LIQUID STRUCTURE OF HYPOEUTECTIC ALUMINIUM-SILICON ALLOYS

CHARACTERIZATION AND APPLICATION OF ATOMIC STRUCTURE INFORMATION OF LIQUID HYPOEUTECTIC ALUMINIUM-SILICON MELTS

By

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Abstract

The liquid structure of Al-Si hypoeutectic binary alloys with and without the addition of 0.04wt% Sr was characterized from diffraction experiments using a high energy X-Ray (Synchrotron) beam source. The high temperature liquid diffraction experiments were carried out for pure aluminum and Al alloys with 3, 7, 10 and 12.5 (eutectic) weight percent Si concentration, respectively. Further, two levels of Sr addition to these alloys at 0 and 0.04 weight percent were carried out. The diffraction data for all the alloys were obtained at various melt temperatures. The salient structure information such as structure factor (SF), pair distribution function (PDF), radial distribution function (RDF), coordination number (CN) and atomic packing densities (PD) have been quantified as a function of Si concentration and melt temperatures. Reverse Monte Carlo (RMC) analysis was carried out using the diffraction experimental data to quantify the partial pair correlation functions such as partial structure factor, partial pair distribution function (PPDF) and partial radial distribution function. Further, the partial pair distribution function and the liquid atomic structure information were used in a semi empirical model to evaluate the viscosity of these liquid alloys at various temperatures. The results show that Sr has a profound effect in changing the atomic structure of the liquid Al-Si hypoeutectic alloys at various Si concentrations and melt temperatures. Further, the effect of Sr is more pronounced at lower melt temperatures closer to the liquidus temperature. The study has shown conclusive evidence that the addition of trace levels of Sr changes the atomic arrangement of the liquid Al-Si alloys which could be validated by the significant change in melt viscosity values. The mechanism of modification of the morphology of the eutectic phases (both eutectic Al and Si) due to Sr addition in these alloys during solidification, from a coarse plate-like eutectic Si phase to a fine fibrous phase, and a significant refinement of the eutectic Al grains can be attributed to the changes in the nucleation mechanism of these alloys effected by the addition of trace levels of Sr. Sr causes more disorder in the atomic structure and delays the nucleation event causing significant undercooling before the evolution of the eutectic phases which in turn refines the morphology of these phases. The Al-Si hypoeutectic alloys in this study have a significant commercial value, especially in shape casting application for automotive, aerospace, domestic and defense sectors. The addition of Sr has been carried out for nearly eight decades but the mechanism for the morphological changes effected by this addition has been eluding researchers globally during all these years. This study presents conclusive evidence to propose a valid mechanism for the effect of Sr addition on the solidified microstructure of these alloys. Another significant contribution of this study would be the development of a valid methodology to evaluate partial pair distribution functions of liquid alloy structures and the evaluation of the melt viscosity using a semi-empirical model along with the atomic structure information. This methodology could be extended to evaluate other fundamental physical properties of binary metallic alloys.

The following presents a brief summary of the results from this study.

- Addition of Si to the Al results in decrease in the value of the first shell CN and PD of atoms. For each alloy, the same decreasing trend in CN and PD was observed for increasing alloy melt temperature.

- Addition of Sr decreases CN and PD for every alloy compositions at any particular melt temperature.

- The $CN_{Al\text{-}Al}$, $CN_{Al\text{-}Si}$ decreases with increasing melt temperatures for every composition of Si and Sr in the alloy. However, no specific trend was observed with respect to change in $CN_{Si\text{-}Si}$ as a function of melt temperature. The same trend was observed for the three partial PD as well.

- The partial CN for the Al-Al pair of atoms in the melt, $CN_{Al\text{-}Al}$ decreases with increasing Si content in the alloy for any given melt temperature. The same trend was observed for the partial $PD_{Al\text{-}Al}$ as well. The partial CN for both the Al-Si and Si-Si pairs of atoms in the melt, $CN_{Al\text{-}Si}$ and $CN_{Si\text{-}Si}$ increases with increasing Si content in the alloy for any given melt temperature. The same trend was observed for the partial $PD_{Al\text{-}Si}$ and partial $PD_{Si\text{-}Si}$ as well.

- Sr addition to the alloy melt decreases the three partial CN and PD values for the respective Al-Al, Al-Si and Si-Si pair of atoms for any given alloy melt temperature.

- The melt viscosity evaluated from a semi-empirical model decreases with increasing Si content in the alloy melt and increasing melt temperatures, respectively.

- Addition of Sr to the alloy melt decreases the melt viscosity at any given Si content and alloy melt temperature.

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CHAPTER 1 INTRODUCTION AND BACKGROUND

This chapter presents a brief introduction to the topic of this research and further presents elaborate background information from prior-art on the various notable topics in the present scope of research.

1.1 INTRODUCTION

Al-Si alloys are widely used in the casting of domestic, military, automotive and aerospace components [1]. The high strength to weight ratio coupled with good castability have brought Al-Si alloys to the forefront of commercial shaped casting applications. These alloys typically have irregular (or divorced) eutectic phases. Moreover, addition of trace elements such as Na and Sr [2,3,4,5,6] result in a modification (refinement) of the morphology of the eutectic phases in these alloys thus improving their mechanical and performance properties. A thorough understanding of the underlying mechanism during the evolution of the eutectic phases and the modification of the eutectic phases in these alloys is critical to improve predictability of the porosity levels and properties of the cast components. The study of these alloys has been of interest to academic researchers ever since Pacz [2] discovered the modification of Al-Si alloys with addition of trace levels of Na. Following this, several hypotheses [4,5] have been proposed to understand the mechanism of the evolution of the eutectic phases in the solidified cast part and their modification by Sr or Na additions. However, there is no conclusive evidence supporting any one of the hypotheses and the mechanism is still unclear and is the subject of much academic debate [7,8,9,10,11,12].

In the case of modified alloys, recent experimental evidence [13, 14] shows that small Sr additions (in the order of 0.01 to 0.04 weight percent) to the Al-Si eutectic melt changes the viscosity of the melt and alters the nucleation environment and sequence of the solidifying phases resulting in a morphological refinement of both the Al and Si eutectic phases. Further experiments on the liquid phases and rheological properties were deemed imperative to understand the nucleation mechanism in Sr-modified Al-Si hypoeutectic alloys. Understanding the structure and properties of the liquid phase of Al-Si alloys is essential to understand the nucleation environment during solidification.

The theory that trace levels of Sr and Na additions alter the physical properties of the inter-dendritic liquid during the final stages of solidification of Al-Si hypoeutectic alloys can be justified only by demonstrating that the atomic structure of the inter-

dendritic liquid is sufficiently altered to effect a change in the physical properties. There are very few experimental techniques to demonstrate this change in physical properties. Recently, Bian et al [15] presented qualitative evidence to show that the atomic structure of Al-Si eutectic melts change with Sr addition and Malik [14] showed that Sr additions change rheological properties, specifically the melt viscosity of these alloys.

This work aims to carry out extensive High energy X-ray (synchrotron beam) diffraction experiments to quantify the atomic structure of liquid Al-Si hypoeutectic alloys in both the unmodified and Sr modified Al-Si hypoeutectic alloys. The liquid structure parameters such as Structure Factor (SF), Pair Distribution Function (PDF), Radial Distribution Function (RDF), Coordination Number (CN) and Packing Density (PD) were quantified. The data obtained from the X-ray diffraction experiments were used in Reverse Monte Carlo (RMC) analysis to evaluate partial pair correlation functions of the Al-Al, Al-Si, and Si-Si pairs of atoms in the liquid alloys. Further, the results of partial pair correlations were used to quantify the melt viscosity by using a semi empirical model.

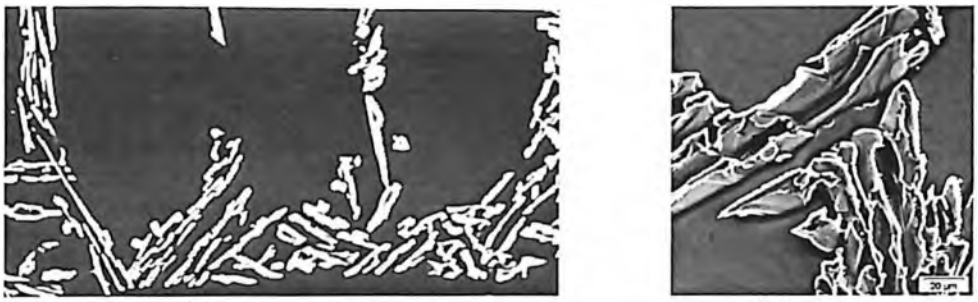
The subsequent sections of this chapter would present comprehensive background information on the following relevant and critical topics within the scope of this research:

- Modification of Eutectic Phases in Al-Si alloys
- Diffraction of Liquid Binary Alloys
- Partial Pair Correlation Functions
- Viscosity of Binary Liquid Alloys

1.2 MODIFICATION OF EUTECTIC PHASES IN AL-SI ALLOYS

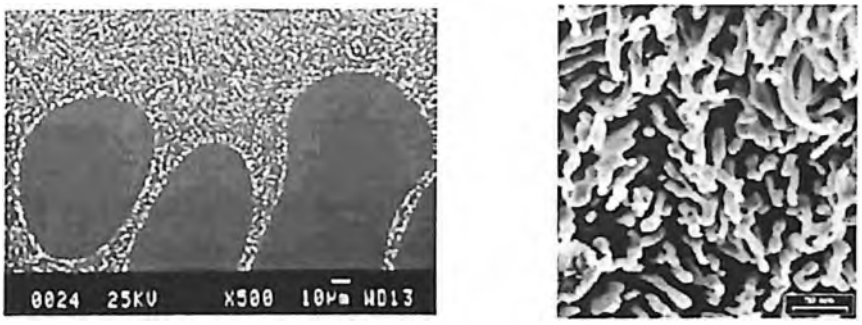
Al-Si system is a simple eutectic system in which the eutectic reaction occurs at 577.6°C and 12.6%Si [16]. In the Al-Si eutectic alloy, the Si phase solidifies in a faceted manner (atomically smooth interface) and the Al phase as non–faceted (atomically rough interface) [4]. It is well established [13] that the Al–Si eutectic can exhibit either of two morphologies; an unmodified and a modified morphology. In the unmodified morphology, the eutectic Si phase is typically coarse plate-like and eutectic Al grains are large and few in number. The microstructure of an unmodified Al–Si eutectic is shown in Figure 1-1. The modified morphology has a fibrous and refined eutectic Si with the grains of eutectic Al being highly refined as shown in Figure 1-2. This morphological transformation significantly enhances the mechanical properties and overall performance of components that are cast from these alloys [4]. Elements such as sodium, strontium, calcium, antimony and several rare earth elements are also known to result in varying degrees of modification [4,12]. Even though sodium has a strong effect

on modification, strontium has gained more importance than sodium as a modifier due to its low oxidation sensitivity which eliminates the fume generation and mitigates the fading effect [17]. In addition, a much wider range of strontium concentrations could be used for effective modification as against very low concentrations (~0.001%) of sodium.



(a) (b)

Figure 1-1 **Typical SEM secondary electron images showing microstructure of unmodified Al-Si hypoeutectic alloy. (a) low magnification showing white eutectic Si and dark Al, and (b) high magnification deep etched microstructure showing plate like morphology of eutectic Si.**



(a) (b)

Figure 1-2: **Typical SEM secondary electron images showing microstructure of Sr modified Al-Si hypoeutectic alloy. (a) low magnification showing white eutectic Si and dark Al phases, and (b) high magnification deep etched microstructure showing fibrous morphology of eutectic Si.**

The mechanism of the modification of the eutectic Si phase by Sr addition has eluded several researchers for over six decades [6,7,18,19,20,21,22,23,24,25,26]. Makhlouf et al [5] has presented a comprehensive literature review of the modification mechanisms by Na or Sr addition to the alloy published until the turn of this century. Some of the mechanisms in chronological order are described in the following paragraphs.

In 1922, Guillet [27] and later Search [28] proposed that the change in eutectic Si morphology from plate like to fibrous was due to the removal of oxides and impurities with the addition of sodium fluoride or potassium fluoride. However, Curran [29] contradicted with this fluxing theory proving that the modification occurs even with metallic sodium. Later, Curran [29] proposed a theory that the modification was due to the formation of ternary Al-Si-Na alloy. Edward and Archer [22] in 1924 ruled out the modification mechanism by Al-Si-Na ternary alloy because in this ternary system, the freezing and melting point should coincide and they found in their cooling curve experiments that the melting point remained constant, while freezing point changed upon cooling.

Edward and Archer (1924) [22], later Gweyer and Philips (1926) [30] proposed a theory called dispersed colloidal theory to explain the mechanism of modification in Al-Si alloys. According to this theory, during solidification small colloidal silicon particles coagulate into silicon crystals. When sodium is present, sodium atoms deposit on these colloidal particles and prevent the growth of silicon crystals causing the modification. In 1921, Hume Rothery [31] disagreed with colloidal theory and explained that the term colloids implies the existence of electric charge on the dispersed phase, which would seem less likely in case of the Al-Si alloys because of high electrical conductivity of aluminium. Further, Hume Rothery [31] proposed that during solidification, as liquid metal approaches solidification temperature, atoms group together to form complexes; when these complexes reach a critical size, and nuclei forms. Addition of modifying agents such as Na destroys these complexes, thereby delaying the formation of nuclei and leading to the observed morphological changes.

In 1949, Thall and Chalmers [18] proposed a theory based on the surface energy of Al and Si solid interface. According to them, the addition of a chemical modifier decreases the surface energy of the Al-Si interface by increasing the interface angle, θ as shown in Figure 1-3. This in turn, suppresses the growth of silicon crystal and causes the modification. They also proposed a theory for modification in case of high cooling rates of the alloy. Since pure Al has a high thermal conductivity compared to the pure Si, as well as the difference in latent heat of fusion between Al and Si is large, the Al phase leads the growth during solidification and encases the silicon phase (restricting its growth) as shown in Figure 1-4, thereby by causing the modification. Later it was confirmed that the Al was the leading growth phase at the Al-Si interface in Sr modified Al-Si alloys and the Si was the leading phase in the unmodified Al-Si alloys. [5, 32].

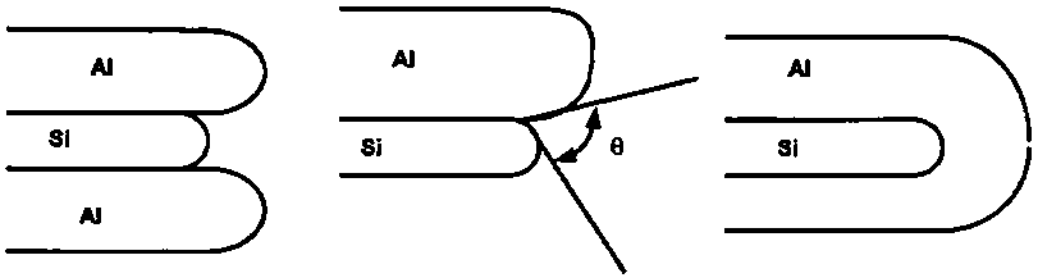


Figure 1-3: Eutectic solidification in sodium modified Al-Si alloys [18].

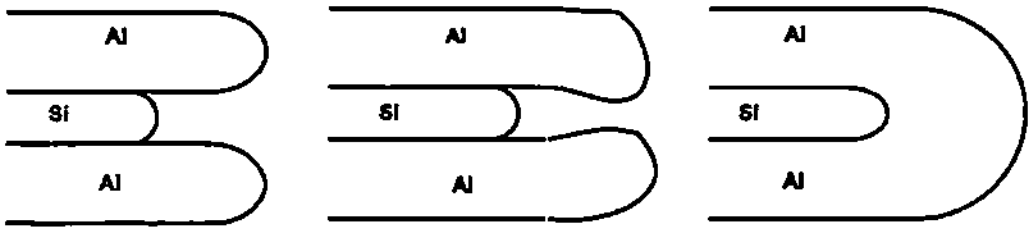


Figure 1-4: Eutectic solidification in unmodified chill cast Al-Si alloys [18].

Tzumara (1957) [21] found that in Al-Si alloys modified with Na, Na has low solubility in solid Al and in solid Si, hence segregates ahead of growing interface and restricts the diffusion of silicon in the melt. He proposed that this reduced diffusion of silicon is responsible for the observed morphological changes in the alloy. Later Davies and West (1964) [33] carried out diffusion experiments and proved that the reduced diffusion rate of silicon in molten Al-Si alloys was not responsible for chemical modification of the eutectic phases in the Al-Si alloys.

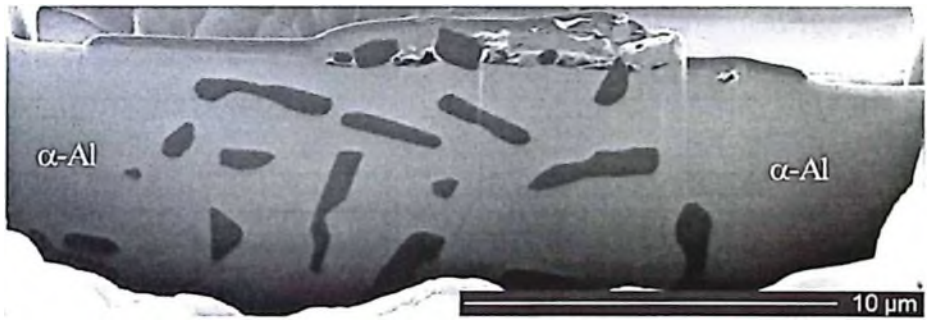
In 1960's, Mondolfo [34, 35] carried out experiments to understand the formation of eutectic structure in various alloys and proposed that the poisoning of nucleation sites due to the addition of modifying elements was the reason for morphological changes in the eutectic structure of Al-Si alloys. He explained that the presence of AlP particles in the Al-Si melt act as nucleating agents for the formation of primary aluminium and eutectic silicon. He also mentioned that during solidification of hypoeutectic Al-Si alloys, the undercooling required for nucleation of eutectic silicon by primary Al is more than the undercooling required for eutectic silicon to nucleate on AlP. He proposed that the addition of sodium to the melt poisons the nucleation sites by reacting with AlP particles there by forming sodium phosphide.

A popular mechanism during the third quarter of last century, proposed for modification was the impurity induced twinning wherein the observation of multiple twins on a few {111} planes of eutectic Si in Sr-modified alloys was attributed to

promoting the growth of fibrous eutectic silicon. Replica techniques by Jekinson and Hogan [23] as well as thin foil studies by Lu and Hellawell [24] propose that impurity elements such as sodium and strontium promote twinning and cause smaller fibers of silicon instead of long flakes and the impurity elements produces higher twin density in the eutectic silicon fibers. They have also mentioned that the efficiency of the modifier depends primarily on the size factor i.e specific radius ratio ($r_{modifier}/r_{silicon}$ = 1.646) and this size factor could be the principal requirement for promoting the impurity induced twinning and subsequent modification of the eutectic phases. However, Na was outside the prescribed ratio and Sr was at one of the extremities of this ratio, and a few elements that were well within this ratio did not show any modification.

Recently, Hegde et al [26] has presented an additional literature review of the various newly proposed mechanisms for the effect of Sr addition to the eutectic structure. The proposal in the last century that Sr addition alters the growth of Si phase during solidification is now widely contested and it has been proposed that the altering of the nucleation events of the eutectic phases during solidification directly results in the refinement of the eutectic phase morphology [8,9,10,13,25]. These new mechanisms state that there are three possible nucleation sites for the eutectic Si to nucleate in an alloy without any Sr addition. These include, an iron containing intermetallic phase [6,13], AlP phase [25,26] and oxide bi-films inherently present ahead of the solidifying Al dendrites [9]. It has been proposed in these mechanisms that the addition of Sr to the alloy renders these potent nucleating sites ineffective and results in a significant undercooling of the inter-dendritic liquid at the eutectic temperature and resulting in a refined morphology of the solidified eutectic phase. Shankar et al [13,11] has proposed that the addition of Sr alters the structure of the inter-dendritic liquid, specifically, the interfacial energies and rheological properties such as melt viscosity, so that the nucleation event of the eutectic Si phase is postponed until a significant undercooling in temperature is achieved. This undercooling results in the super-saturation of the inter-dendritic liquid with Si caused by the continual growth of the primary Al dendrite phases. This results in a refined solidified morphology of the Al and Si eutectic phases. Further, the theory [13] also states that contrary to popular belief that addition of Sr or Na not only refines the morphology of the eutectic Si phase but also refines the grain size of the eutectic Al grains. This is evident from Figure 1-5(a) showing a Ga ion beam Scanning Electron Microscope (SEM) image for Al-7%Si alloy modified with 0.024%Sr showing the fine Al eutectic grains while Figure 1-5 (b) represents an Al-7%Si unmodified alloy with no Al eutectic grains in it. Further, there is emphatic experimental evidence to show that Sr addition to the Al-Si hypo-eutectic alloy significantly changes the viscosity of the alloy at various liquid temperatures [6,13,14], but, there is no fundamental explanation for such a significant change in physical properties with only about 200 parts per million level addition of Sr to the alloy.

(a)



(b)

Figure 1-5: Ga ion beam SEM images comparing the microstructure and the morphology of the eutectic phases in Sr-modified and unmodified hypoeutectic Al-Si alloys , (a) An Al-7% Si-0.024.%Sr alloy with the fine equiaxed Al eutectic grains. (b) An Al-7%Si alloy showing no discernible Al eutectic grains [13].

One common feature in all the mechanistic research on the modification of eutectic phases in Al-Si hypoeutectic alloy by Sr or Na, is that the studies have been carried out only on the solidified cast structure of the alloy and no attention has been paid towards understanding the effect of Sr on the liquid structure of these alloys prior to solidification (nucleation) event. The present research project was carried out with the premise that if Sr alters the nucleation event or environment of the eutectic phases during solidification (nucleation), then the effect of Sr addition should show discernable changes in the liquid structure of these alloys as well. The only work available in the literature on the liquid structure of Al-Si alloys with Sr addition was by Bian et al [15] which showed that there is qualitative evidence that Sr alters the liquid structure of

these alloys. However, these experiments were performed in reflection mode diffraction where the data is collected from the surface of the liquid alloy using Mo source X-rays, wherein the experiment data may be tainted by surface artifacts such as inherent oxide layers. The use of high energy X-rays (synchrotron beam source) enables us to perform the diffraction experiments in transmission mode through the bulk of the sample.

1.3 DIFFRACTION OF LIQUID BINARY ALLOYS

The knowledge of liquid atomic structure is essential for the advancement of condensed matter theory, in developing predictive models, in establishing structure-property relationships in metallurgy & materials sciences and to understand the phase transitions and the fundamental properties of an alloy melt [36,37,38,39,40,41].

The liquid structure was commonly determined by x-ray, neutron diffraction and X-Ray Absorption Fine Spectroscopy (XAFS) methods [40,41,42,43,44,45,46]. The diffraction of x-rays by liquids and non crystalline materials was first reported by Fedrich in 1913 [after 47]. Later, in 1916, Debey and Scherer obtained the diffraction data for several liquids [47]. In 1922, Keesom and de Smedt [after 47] reported the diffraction data for liquid elements and later Gingrich [47] presented a literature review on the contributions of various investigators on the diffraction of x-rays by liquid elements [47]. Further, Thomas and Gingrich [48,49] studied the effect of temperature on the atomic distribution in liquid K and the atomic distribution in the allotropic form of P by x-ray diffraction (Molybdenum source) experiments. Following this, several studies have been carried out on the atomic structure of various liquid metals, non-metals and binary alloy systems by x-ray and neutron diffraction studies as a function of melt temperature and alloy composition [50,51,52,53,54,55,56,57,58,59,60].

The diffraction pattern obtained from a liquid differs from the solid and gaseous states [40,41]. In solids, the diffraction pattern shows sharp peaks at regular intervals because atoms in a solid are arranged in a regular periodic arrangement. However, for gases, the x-ray diffraction shows a continuous scattering intensity with no maxima. This is because of the lack of any atomic arrangement (periodicity). In case of liquids, the diffraction pattern shows a few defined peaks (broad) peaks. The atoms in a liquid have a certain short range order due to the appreciable packing density, but show no long range order owing to their thermal excitation and motion [41].

The important parameter used in the study of liquids and amorphous materials is the pair distribution function, PDF represented by g(r). The PDF corresponds to the probability of finding another atom at a distance *r* from an atom at the origin position (at the point r = 0) [40,41]. The structure and properties of liquids are best described in terms of PDF. The PDF, as shown in Figure 1-6(a), corresponds to the probability of finding an atom at a distance r from an arbitrary origin atom at location 'O' (at the point r = 0). In a binary alloy, the origin atom and the atom at distance r can be either of the two atom types in the melt. The PDF is a time-averaged structure over all atoms in the

melt [61,62]. PDF provides only the magnitude and distribution probability of any pair-wise correlation as a function of distance but not their orientation dependence [41]. Figure 1-6(b) shows a typical plot of the PDF as a function of radial distance r. In Figure 1-6(b), if we have an atom of a species at origin 0, then the maximum probability of finding the next nearest neighbouring atom of any species is at r_m. This maximum probability is represented by the function $g_m(r)$. Also, in Figure 1-6(b) it can be seen that the value of g(r) attenuates at unity for large radial distances, showing that the probability of finding an atom of any species at these distances from the origin atom is unity, representing the short range order in the liquid system.

Since the PDF is obtained from diffraction data, this experimental information plays a significant role in understanding and determining the structure and properties of liquid materials. The PDF, is obtained from the SF information, S(Q) of the liquid.

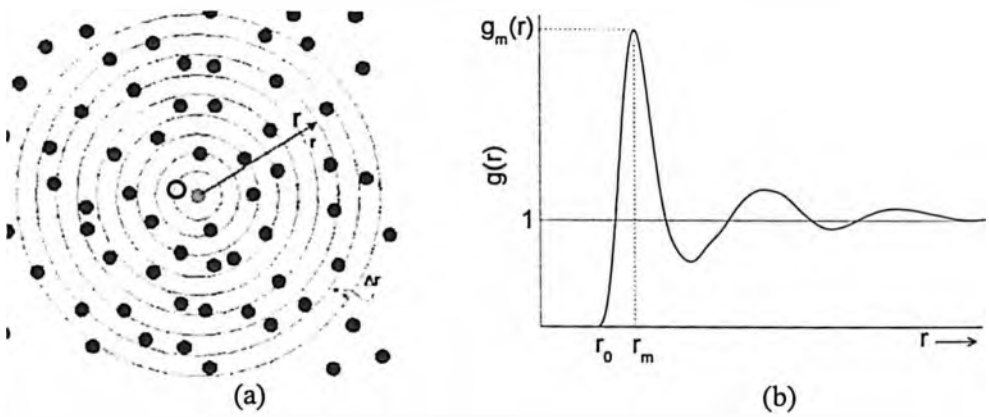


Figure 1-6: Pair Distribution Function, g(r). (a) Schematic showing the definition of g(r) as the probability of finding any atom from a distance r from any origin atom at location O (r = 0). (b) Typical curve of g(r) versus r showing the maximum probability, $g_m(r)$ of finding the nearest neighbor atom at r_m from an atom at the origin, 0 [63].

The raw data from a diffraction experiments collects information of total intensity, *I*, as a function of the scattering angle, θ. After applying corrections for multiple scattering, Compton scattering and geometric corrections, the x-ray intensity scattered coherently, I_{coh}, (electron units (eu)) is derived as a function of the wave vector, *Q* as shown in Equation (1.1).

$$I_{eu}^{coh} = \langle f^2 \rangle + \langle f \rangle^2 \cdot \int_0^{\infty} 4\pi r^2 \left[\rho(r) - \rho_o\right] \frac{\sin Qr}{Qr} dr \qquad (1.1)$$

In Equation (1),

$$Q = \frac{4\pi \sin\theta}{\lambda} \tag{1.2}$$

$$\langle f^2 \rangle = \left(c_i f_i^2 + c_j f_j^2 \right), \text{ and } \langle f \rangle^2 = \left(c_i f_i + c_j f_j \right)^2 \tag{1.3}$$

and

$$\rho(r) = \sum_i \sum_j c_i f_i f_j \rho_{ij}(r) \Big/ \langle f \rangle^2 \tag{1.4}$$

In Equations (1.2) to (1.4), λ is the wavelength of the incident beam, c_i is atomic fraction of i-type atoms, f_i is the atomic scattering factor of species i, $\rho(r)$ is the average number density function, $\rho_{ij}(r)$ is the number of i-type atoms found at a radial distance r from j-type atom at the origin.

From Equation (1.1), the SF, S(Q) is evaluated [40] by the expression shown in Equation (1.5). S(Q) defines the structure of the liquid and is directly measured from diffraction experiments.

$$S(Q) = \left(\left[I_{eu}^{coh}(Q) - \langle f^2 \rangle + \langle f \rangle^2 \right] \Big/ \langle f \rangle^2 \right) \tag{1.5}$$

The Fourier transformation of S(Q) provides the atomic PDF, g(r), as represented in Equation (1.6).

$$g(r) = 1 + \frac{1}{2\pi^2 r \rho_o} \int_0^\infty Q[S(Q) - 1] \sin(Qr) dQ \tag{1.6}$$

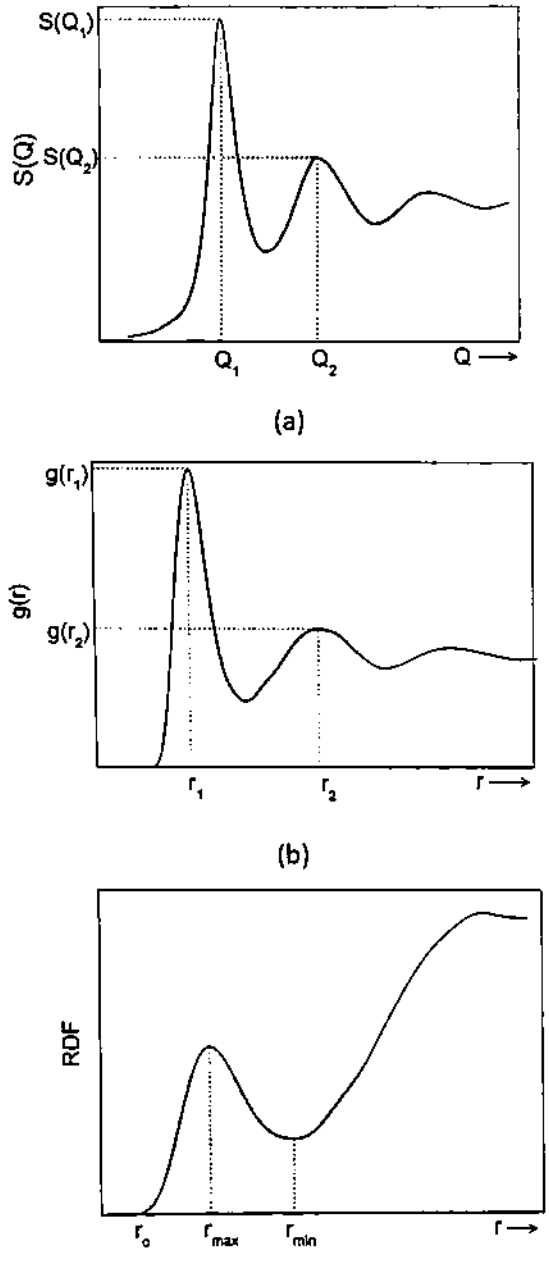


Figure 1-7: **Schematic of the (a) SF, S(Q), (b) PDF, g(r) and (c) RDF for a typical liquid metal.**

The PDF represents the time-averaged probability of atom distribution in the structure of the liquid alloy and when the PDF is multiplied by the linear atom density in two dimensional spaces, the radial distribution function, RDF could be obtained as shown in Equation (1.7).

$$RDF = 4\pi r^2 \rho_0 g(r) \tag{1.7}$$

Figure 1-7 shows a schematic of the SF, PDF and RDF, respectively of a typical metallic liquid system. Figure 1-7(a) shows the notations Q_1, Q_2, $S(Q_1)$ and $S(Q_2)$ in the SF, representing the first peak position, second peak position, first peak height and second peak height, respectively. Figure 1-7(b) shows the notations r_1, r_2, $g(r_1)$ and $g(r_2)$ in the PDF, representing the first peak position, second peak position, first peak height and second peak height, respectively. Figure 1-7(c) shows the notions r_0, r_{max} and r_{min} in the RDF, representing the cut-off position, maximum probability position and outer position of finding an atom in the first coordination shell from an atom placed at the origin, respectively. The notations in Figure 1-7 would be used for analysis of the experimental data in the subsequent sections of this dissertation.

There are four methods to estimate the CN for the RDF [40]. Figure 1-8 shows schematics of the four methods. In all four methods, the area under the first peak of the RDF graph represents the first shell CN. The more popular methods are shown in Figure 1-8(b) and Figure 1-8(d) and the corresponding mathematical expression to evaluate the first shell CN are presented in Equation (1.8)(a) and Equation (1.8)(b), respectively. Between them, the expression in Equation (1.8)(b) is more popular.

$$CN = 2 \cdot \int_{r_0}^{r_{max}} \left(4\pi r^2\right) \cdot \rho_0 \cdot g(r) dr \qquad \rightarrow \text{Figure 1-8(b)} \tag{1.8)(a}$$

$$CN = \int_{r_0}^{r_{min}} \left(4\pi r^2\right) \cdot \rho_0 \cdot g(r) dr \qquad \rightarrow \text{Figure 1-8(d)} \tag{1.8)(b}$$

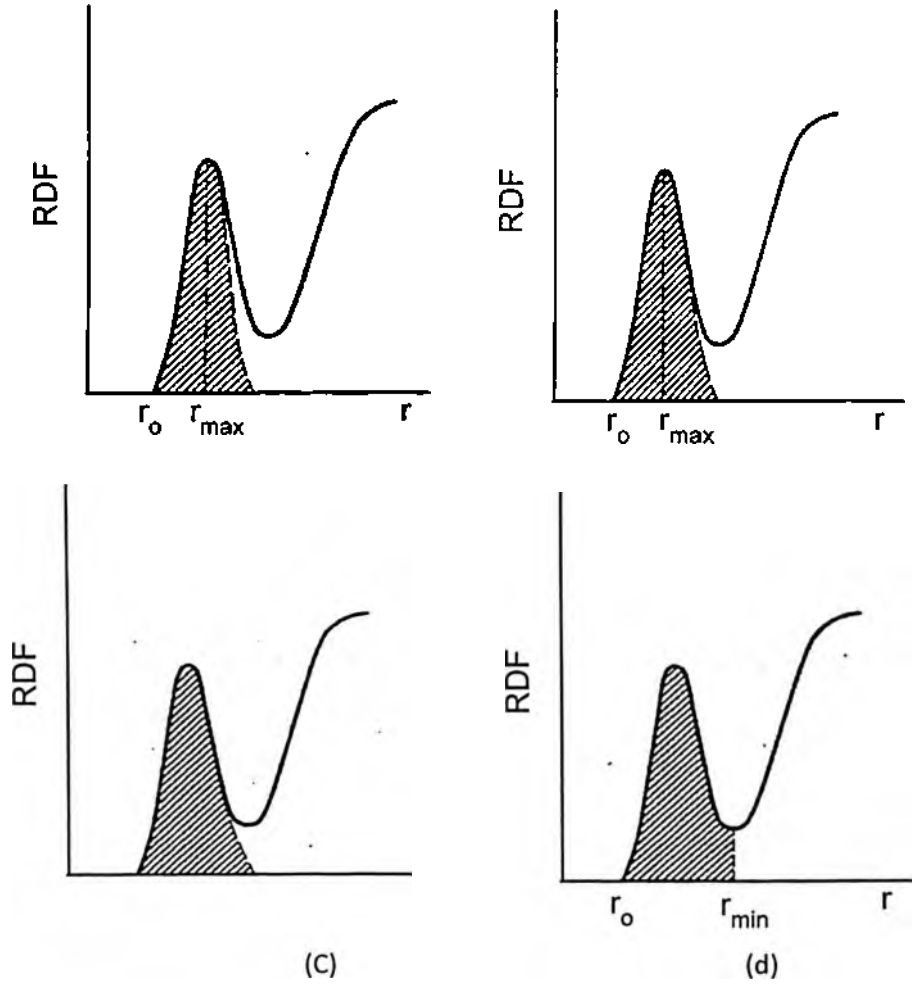


Figure 1-8: Schematic showing four techniques used to evaluate coordination number from the plot between RDF and r [40].

The Packing Density (PD) of atoms in the first coordination shell of the liquid structure is the ratio of the total volume of the liquid to the volume occupied by the atoms in that liquid assuming that the atoms are hard spheres [40]. Equation 1.9 presents the expression to evaluate PD.

$$\mathbf{PD} = \frac{\pi}{6}\rho_o\sigma^3 \tag{1.9}$$

In Equation (9), ρ_o is the number density and σ is the hard sphere diameter [40]. For most metal systems, the hard sphere diameter could be evaluated from r_1 in the PDF as given in Equation (1.10).

$$\sigma = \frac{r_1}{1.145} \tag{1.10}$$

1.4 PARTIAL PAIR CORRELATION FUNCTIONS

In a binary alloy with two components *i* and *j*, there are three atom pair interactions, namely, *i-i*, *i-j* and *j-j*. The PDF obtained from the diffraction experiments provides the total structure information of liquid metals and is composed of three Partial Pair Distribution Functions (PPDF); one for each type of atom pair interaction. The PPDF presents a more detailed understanding of the liquid structure of binary alloys [41,42,64,65]. In case of a binary alloy with components *i* and *j*, three PPDF i.e. $g_{ii}(r)$, $g_{ij}(r)$ & $g_{jj}(r)$ are required for a complete description of liquid structure. The PPDF can be written as:

$$4\pi r^2 \rho_0 [g_{ij}(r) - 1] = rG_{ij}(r) = \frac{2}{\pi}\int_0^\infty Q[S_{ij}(Q) - 1]\sin(Qr)dQ \tag{1.11}$$

In Equation (1.11) $S_{ij}(Q)$, $G_{ij}(r)$, $g_{ij}(r)$ represents the Partial Structure Factor (PSF), reduced partial pair distribution function and PPDF, respectively.

The total structure factor S (Q) obtained from diffraction experiment can be expressed in terms of three PSF, as shown in Equation (1.12).

$$S(Q) = W_{ii}S_{ii}(Q) + W_{jj}S_{jj}(Q) + 2W_{ij}S_{ij}(Q) \tag{1.12}$$

where,

$$W_{ij} = {c_i c_j f_i f_j} \Big/ \left\langle c_i f_i + c_j f_j \right\rangle^2 \tag{1.13}$$

The separation of these individual structures is one of the most important subjects in the structural study of liquids. As shown in Equation (1.12), the structure of a binary alloys with components *i* and *j* is expressed by two like atom pairs (*i-i* and *j-j*) and

one unlike atom pair (*i-j*). The equation to determine PSF can be re- written in a matrix form as shown in Equations (1.14 and (1.15)

$$|\mathbf{A}| = |\mathbf{W}|^{-1} |\mathbf{S}_T| \tag{1.14}$$

Where

$$|A| = \begin{pmatrix} S_{ii}(Q) \\ S_{jj}(Q) \\ S_{ij}(Q) \end{pmatrix};\ |W| = \begin{pmatrix} w_{11} w_{12} w_{13} \\ w_{21} w_{22} w_{23} \\ w_{31} w_{32} w_{33} \end{pmatrix};\ \text{and}\ |S_T| = \begin{pmatrix} S_1(Q) \\ S_2(Q) \\ S_3(Q) \end{pmatrix} \tag{1.15}$$

The CN each of the three atom pairs, particle CN, is evaluated by Equations (1.16a) and (1.16b), wherein the definitions of r_0, r_{max} and r_{min} are shown schematically in Figure 1-6.

$$(CN)_{ij} = 2 \cdot 4\pi \int_{r_o}^{r_{max}} \rho_{ij} \cdot r^2 \cdot g_{ij}(r) \cdot dr \tag{1.16a}$$

$$(CN)_{ij} = 4\pi \int_{r_o}^{r_{min}} \rho_{ij} \cdot r^2 \cdot g_{ij}(r) \cdot dr \tag{1.16b}$$

In Equations (1.16a) and (1.16b), ρ_{ij} is the partial number density of the atom pair *ij*, which is evaluated by Equation (1.17).

$$\rho_{ij} = \rho_o \sqrt{c_i \cdot c_j} \tag{1.17}$$

In Equation (1.17), ρ_o is the total number density of the alloy at any given temperature.

Since, we would need three different total SF, namely, $S_1(Q)$, $S_2(Q)$ and $S_3(Q)$ as shown in Equation (1.15), we would need one of the following four techniques [40] to be adopted to evaluate the three PSF, $S_{ii}(Q)$, $S_{jj}(Q)$ and $S_{ij}(Q)$.

1. Three different incident radiations to obtain three SF,
2. Isotope enrichment of one of the components to obtain three variations in the binary alloy,
3. Anomalous scattering technique to vary the incident beam wavelength to obtain three unique SF, and
4. Concentration independence rule, wherein three different binary alloy compositions at identical melt superheat above their respective liquidus temperatures were assumed to have identical three PSF.

Enderby et al [66] derived three PSF on Cu-Sn alloys using the isotope enrichment technique and neutron beam diffraction experiments by changing the scattering powers of the constituents using different isotopes of elemental Cu. Though this method is considered to be the best method of deriving partial pair correlations of individual atom pairs, it has two limitations. One being that the isotopes are very expensive and second that it is not easy to obtain stable isotopes for all elements.

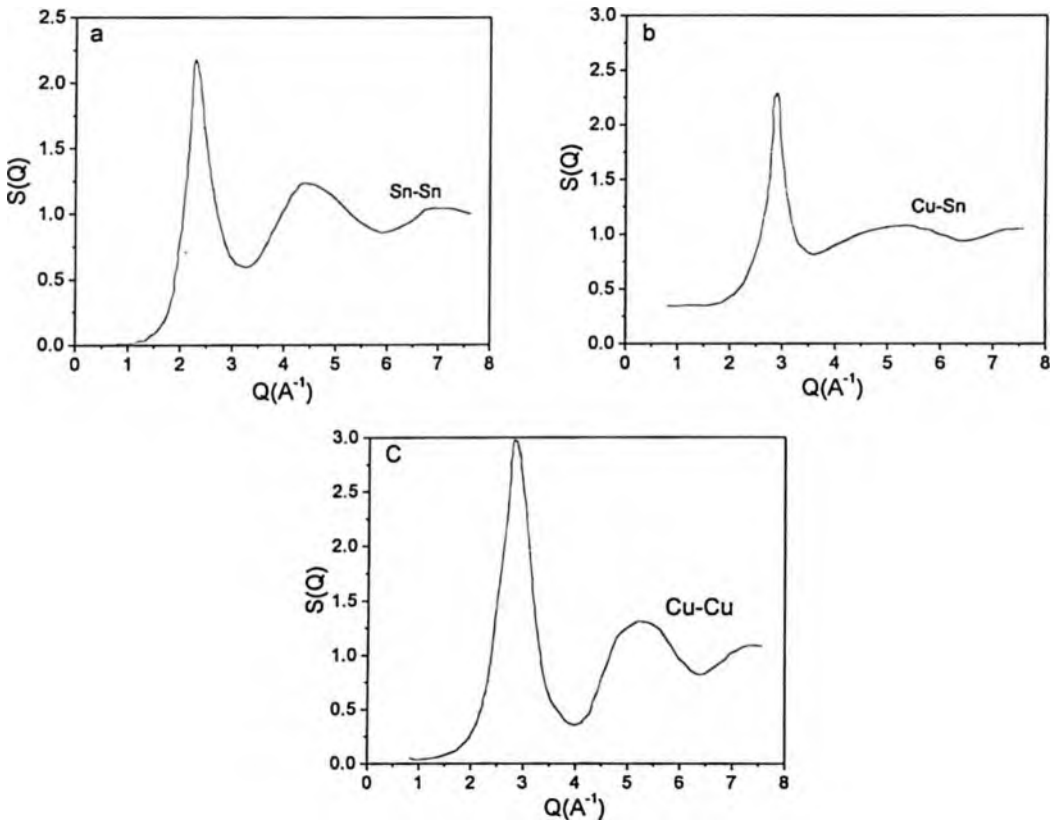


Figure 1-9: Partial structure factors of Cu-Sn alloy derived by Isotope enrichment method [66].

Ramesh and Ramaseshan [67] suggested the anomalous scattering technique to derive three PSFs in liquids and amorphous materials. Later, Waseda et al [68] derived three PSF for liquid Ni-Si alloys by anomalous scattering technique. They had chosen Ni-Si alloy because the absorption edge of nickel atom (1.488 Å) is located near the readily available wave lengths of X-ray targets (Cu-1.542Å; Co-1.1063Å; Ni-1.659 Å). Figure 1-10

shows the partial structure factors for Ni-Si liquid alloy melt derived by using the anomalous scattering technique.

Halder et al [69] used the concentration independence rule for the first time on Ag-Sn alloys, wherein it was validated that the partial structure factors are independent of alloy composition. The three independent partial structure factors were derived based on this assumption and by changing the concentration in weighting factor equation given by Equation (1.13). Following the work of Halder et al, this method has been applied by several authors on a number of liquid binary alloys [40].

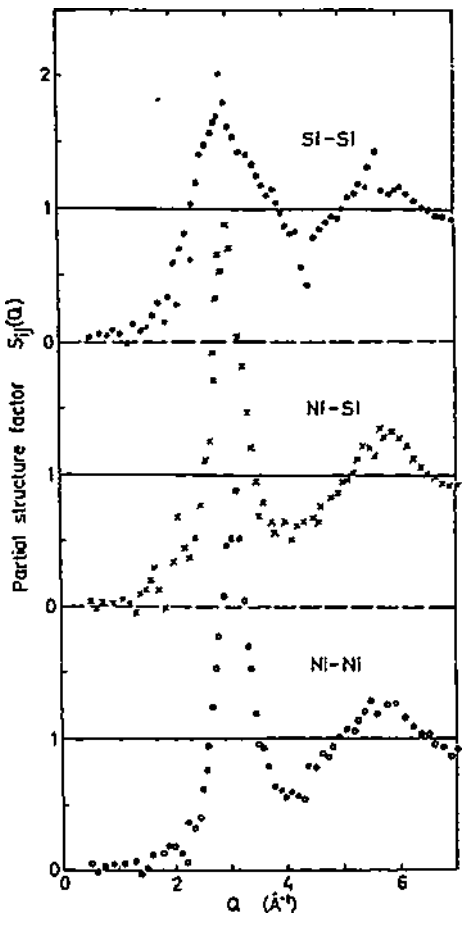


Figure 1-10: Partial structure factors of liquid Ni-Si alloy melt derived by anomalous scattering technique [68].

In principle, partial interference functions vary with the change in concentration and the assumption of concentration independence was not satisfied with binary alloys such as liquid Cu-Te [40] and liquid Ce-Ni alloys [70]. Following this, Bellissent-Funel et al [71] studied the structure of liquid eutectic Ag-Ge alloy by neutron diffraction to assess the validity of the concentration independence of the SF and PSF. They had carried out structural studies using isotopic substitution as well as concentration method and found that the partial structure factors derived from concentration method are not in good agreement with those derived from the more accurate isotopic substitution method.

Considering the difficulties associated with deriving the partial pair correlations due to non availability of Isotopes or three beam radiation sources (as described in section 1.3), researches developed an alternative approach to derive partial correlation functions by using x-ray and neutron diffraction experimental data along with Reverse Monte Carlo (RMC) analysis. RMC analysis is a method of structural modelling based on the experimental data [72,73,74,75]. RMC method was adopted by Keen and McGreevy [76] for vitreous silica to generate structural models from X-ray diffraction experimnent data using the reflective method. Subsequently, Kohara et al [77] further developed and refined the RMC analysis method to derive the partial radial distribution functions for same vitreous silica using experiment data in the high Q-range obtained from the transmission diffraction experiments using neutrons and hard x-ray sources. De Jong et al [78] used RMC method to analyze neutron diffraction data on liquid Li-Si alloy to derive the partial pair correlation functions. Petkov et al [79] studied the atomic structures of liquid Sn, Ge and Si by generating three dimensional structure models using RMC analysis method fitted with XRD experiments data. They observed that the RMC results are in excellent agreement with the results of abinitio molecular dynamics simulations. The results of Petkov et al [79] demonstrate that the RMC method which does not require the use of the interatomic pair potential functions produces results comparable to those obtained from abinitio molecular dynamic simulations which require the use of the interatomic potential functions.

Recently, Gruner et al [80] studied the atomic clusters in Cu-Sn alloy using x-ray and neutron diffraction data coupled with RMC analysis and observed that the derived partial structure factors are comparable to those obtained by neutron diffraction experiments with isotope substitution by Enderby et al [66]. Following this, Takeda et al [81] studied the atomic structure of liquid Au-Si alloys by transmission method using high energy X-ray source. They derived the partial pair correlation functions using RMC analysis and fitted the experimental data as shown in Figure 1-11. This approach of using X-ray and neutron data with RMC modelling eliminates the difficulties associated with the non availability of isotopes and three radiation sources to derive partial pair correlation functions.

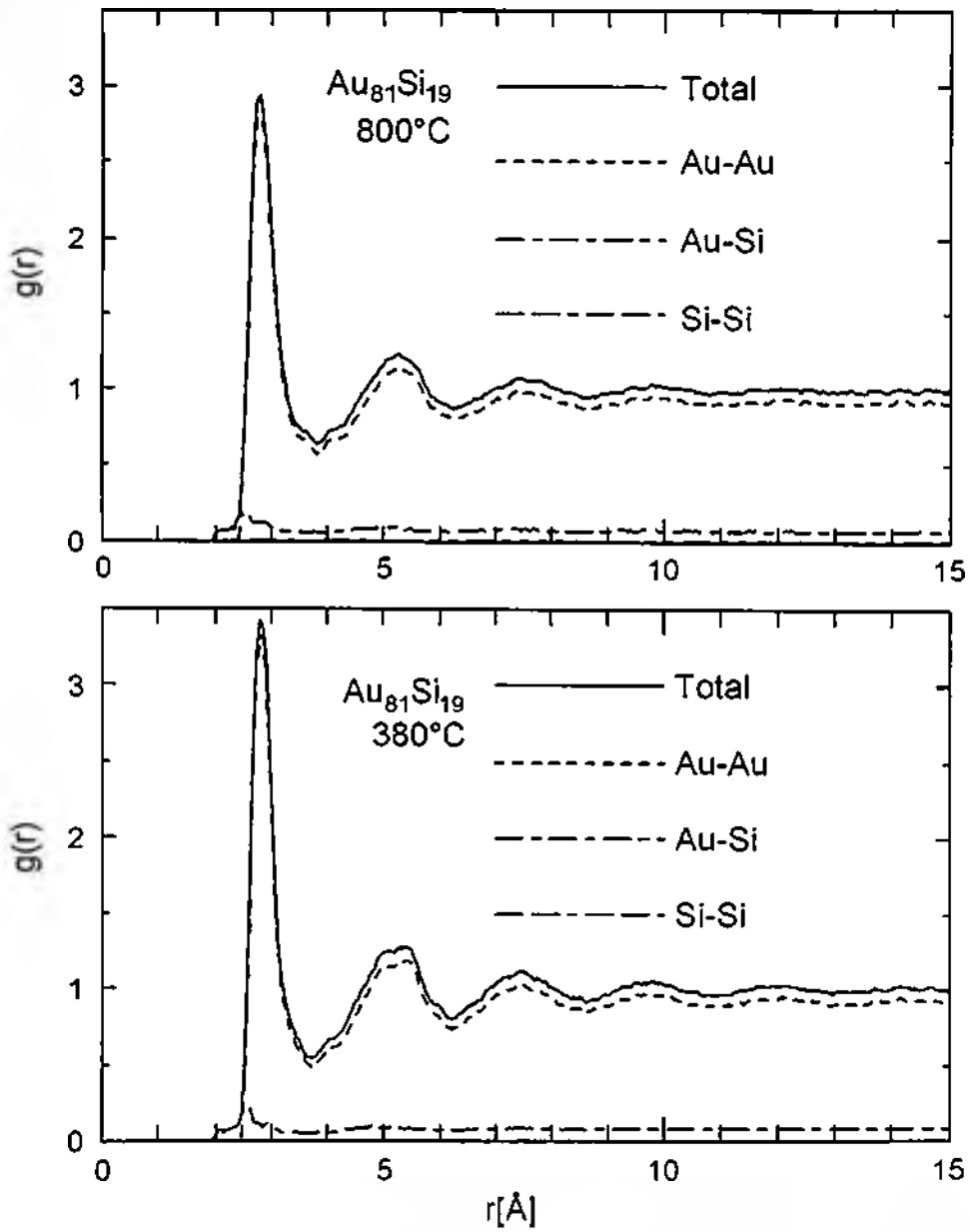


Figure 1-11: **Partial pair distribution functions weighted by concentration obtained for liquid Au-19 at% Si alloy melt at 380K and 800K using RMC analysis method [81].**

1.5 VISCOSITY OF BINARY LIQUID ALLOYS

The following is the nomenclature used in this sub-section.

σ effective hard sphere diameter

c concentration

g (r) pair distribution function

$g_{ii}(r)$ Partial pair distribution function of atoms type i

$g_{jj}(r)$ Partial pair distribution function of atoms j

m atomic mass

M molecular weight

n number density

T_b boiling point

T_m melting point

T Temperature

P(T) Probability that the atom will stay in a state of oscillation around a fixed coordinate position.

R universal gas constant

x_i Concentration of component i

x_j Concentration of component j

v_o frequency of oscillations

V_m molar volume

K_B Boltzmann constant

a (au) softness parameter

ø pair potentials

ζ friction coefficients

D diffusion coefficient

H Hard Part

S Soft part

K Thermal conductivity

ρ density

η Viscosity

Viscosity of liquid metals and alloys has been studied extensively by various experiments [14,41,82,83,84] and theoretical models [40,41,85,86,87,88,89,90]. Quantified viscosity is extensively used in studies of solidification, solidification simulations, metallic glass formation and various other metallurgical applications [41,91]. The physical properties of liquid metals can be evaluated from the atomic structure of liquids by coupling experiment diffraction data with appropriate theories [41,91]. Rice and Allnat (RA) [86] used the concept of pair potential and pair distribution functions to evaluate the viscosity of liquid metals and binary alloy. Kitajima et al [87] extended the concept of pair potential and pair distribution function method to evaluate the viscosity of Na-K binary alloy. Later, Bhuyan et al [88] have calculated the viscosity of Ag-In alloys using the RA theory. The following sections elaborate the popular theories of evaluating viscosity from fundamental atom arrangement information.

1.5.1. Rice and Allnat theory

The expression for the coefficient of viscosity is shown Equation (1.18) as proposed by Kitajima et al [87] and Bhuyan et al [88].

$$\eta_v = \eta_v(\sigma) + \eta_k + \eta_v(r > \sigma) \tag{1.18}$$

Where, η_k is the kinetic contribution to the viscosity, $\eta_v(\sigma)$ is the contribution of the hard part of the potential, and $\eta_v(r>\sigma)$ the soft potential contribution. The different parts of Equation (1.18) can be expressed as follows:

$$\eta_k = \sum_{i=1}^{2}\sum_{j=1}^{2}\left[\frac{5k_BT}{8g_{ij}\sigma_{ij}}\times\frac{1+4\pi n_j g_{ij}(\sigma_{ij})\sigma_{ij}^3/15}{(4\pi K_BT/m_i)^{1/2}\sigma^2_{ij}+\left[5\zeta_i^{(S)}\Big/4m_in_ig_{ij}(\sigma_{ij})\right]}\right] \tag{1.19}$$

$$\eta_v(\sigma) = \sum_{i=1}^{2}\sum_{j=1}^{2}\left[\frac{5k_BT}{36}\frac{m_{ij}n_j}{m_in_i}\times\frac{12\pi\ \sigma_{ij}^3/5g_{ij}(\sigma_{ij})+(4\pi\ \sigma_{ij}^3n_\alpha/5)^2}{(4\pi K_BT/m_i)^{1/2}\sigma_{ij}^2+[5\zeta_i^s/4m_in_ig_{ij}(\sigma_{ij})} + \frac{8\pi k_jT}{15}\frac{n_{ij}n_j\sigma_{ij}^6g_{ij}(\sigma_{ij})}{(4\pi K_BT/m_i)^{1/2}\sigma_{ij}^2}\right] \tag{1.20}$$

$$\eta_v(\sigma) = \eta_{11}^H+\eta_{12}^H+\eta_{22}^H+\eta_{21}^H \tag{1.21}$$

$$\eta_v(r>\sigma) = 4\pi\sum_{i=1}^{2}\sum_{j=1}^{2}\frac{m_{ij}}{30}\left(\frac{1}{\zeta_i^{(s)}}+\frac{1}{\zeta_j^{(s)}}\right)X_{ij}(r) \tag{1.22}$$

Where,

$$X_{ij}(r) = n_in_j\int_{r>i}^{\infty}(\phi_{ij}''(r)+\frac{4}{r}\phi_{ij}'(r))(g_{ij}(r))(r)^4\,dr \tag{1.23}$$

In Equations (1.21) and (1.22), H and S stand for hard and soft parts, respectively.
In Equations (1.17) to (1.21), the friction coefficient, ζ, is given by:

$$\zeta_i^{(s)} = \eta_i\zeta_{ii}^{(s)}+\eta_j\zeta_{ij}^{(s)} \tag{1.24}$$

where

$$\zeta_{ij}^{(s)} = \left(\frac{1}{\zeta_i} + \frac{1}{\zeta_j}\right) c_{ij}, \tag{1.25}$$

and,

$$c_{ij} = \frac{m_{ij}}{3} \int \left(\phi'' + \frac{2}{r}\phi'\right) r^2 g_{ij}(r) dr \tag{1.26}$$

In the Equations (1.25) to (1.26), the single and double primes denote the first and second derivatives with respect to r, respectively,

It can be observed from Equations (1.18) to (1.23) that the RA theory has four important parameters such as the pair potential function, pair distribution function, effective hard sphere diameter and friction coefficient to enable evaluating the viscosity for binary alloys.

The main difficulty associated with this approach is to ascertain the partial pair potential functions by molecular dynamics simulations, which is very expensive, and the number of atoms used in simulations are about 100 at most [92,93]. Further, obtaining valid and reliable pair potential functions for binary metallic alloy at various melt temperatures is still an ongoing research study.

1.5.2. Born-Green Theory

Born and Green [85] derived an expression for evaluating the viscosity of liquid metals based on the PDF and pair interatomic potential function as given in Equation (1.27)

$$\mu = \frac{2\pi}{15}\left(\frac{m}{kT}\right)^{1/2} n^2 \int_0^\infty g(r) \frac{\partial \phi(r)}{\partial r} r^4 dr \tag{1.27}$$

Using Equation (1.27), the viscosity for various liquid metals have been evaluated and it was found that the viscosity values match with the experimental data for most metals at their melting point [41]. However, the temperature dependence of viscosity could not be satisfactorily validated using the Born-Green Theory due to the lack of confidence in determining the pair potential functions by simulation techniques [41].

1.5.3. Moment Method

The moment method has been developed only for pure liquid metals and not for binary alloys; and further, work carried out by Kitajima et al [87] and Bansal [94] have shown that the melt viscosity evaluated by the moment method for liquid sodium and potassium was underestimated by a factor of 0.5 to 0.6. This method utilizes the transverse momentum correlation functions and relates these functions to the transverse angular frequency which in turn relates to the shear viscosity of the melt [40, 41].

1.5.4. Hard Sphere Theory

The packing density (PD) of a liquid metal can be calculated from the hard sphere diameter (Equation (1.9)) and the viscosity of dense fluids is expressed interms of packing density as shown in Equation (1.28)[95].

$$\mu = 3.8*10^{-8}\frac{(MT)^{\frac{1}{2}}}{V^{\frac{2}{3}}}\frac{(PD)^{\frac{4}{3}}\left(1-\frac{PD}{2}\right)}{(1-PD)^{3}} \quad \text{(in PaS)} \qquad (1.28)$$

Where, M is the molecular weight and V is the molar volume

This method has shown to under-predict the shear viscosity of the alloy melt by a factor of 0.3. We have used this method as well to evaluate the shear viscosity of the alloys in this study by assuming the alloy as one integral fluid with a specific PD.

1.5.5. Semi Empirical Model

A semi empirical method to evaluate viscosity of liquid metals was proposed by Iida et al [41] by expanding the model proposed by Andrade [96] to obtain an expression for melt viscosity using fundamental properties such as pair distribution function and average inter-atomic frequency. Viscosity is a structure sensitive property and microscopically viscosity was related to the transfer of momentum between the nearest neighboring atoms in the liquids [41]. The information about the nearest neighboring atoms could be readily obtained from the pair distribution function, g(r) [40]. Iida et al [41] proposed an equation to evaluate the viscosity of Newtonian liquids using the concept of pair distribution function g(r) as represented by Equation (1.29).

$$\mu = \frac{8\pi}{9} \nu_0 P(T) m n^2 \int_0^{\infty} g(r)\ r^4 dr \tag{1.29}$$

In Equation (1.29), the upper limit of the integral could be changed to the distance over which the nearest neighbor interactions occur in the liquid metals by assuming that the momentum transfer occurs mostly between nearest neighboring atoms which is represented by the r_{min} in the g(r) curve as shown in Figure 1-7(b). Equation (1.26) could be rewritten as Equation (1.30).

$$\mu = \frac{8\pi}{9} \nu_0 P(T) m n^2 \int_0^{r_{min}} g(r)\ r^4 dr \tag{1.30}$$

In Equation (1.30), ν_0 is a constant and calculated from the Lindemann's melting point atomic frequency formula modified for metals by Iida et al and given in Equation (1.31).

$$\nu_0 P(T) = \beta \nu_L = \beta c \left(\frac{RT_m}{MV_m^{\frac{2}{3}}} \right)^{1/2} \tag{1.31}$$

Where β is a correction factor which is related to the surface tension (γ_m) and molar volume (V_m) of the liquid at the melting point

$$\beta = 2.2X10^3 \left(V_m^{1/3} \right) \left(\frac{\gamma_m}{RT_m} \right)^{1/2} \tag{1.32}$$

In Equation (1.30), P(T) is the probability function that the atom will stay in a state of oscillation around a fixed coordinate position. In Equation (1.31), c is a constant (9.0×10^8), and P(T) is dependent on temperature and decreases with increasing temperature. P(T) could be evaluated by Equation (1.32).

$$P(T) = 1 - \int_{\varphi}^{\infty} (2\pi)^{1/2} \exp\left(-\frac{\varphi^2}{2} \right)\ d\varphi \tag{1.33}$$

Where,

$$\varphi = \frac{\sqrt{3}}{2}\left(\frac{T_b - T}{T}\right) \quad (1.34)$$

Based on Equation (1.29), Djemili et al [97] proposed an equation for evaluating the viscosity of binary alloys as shown in Equation (1.35). Using Equation (1.35), the viscosity of Cd-In binary alloy was evaluated and validated by viscosity experiments [97].

$$\mu = \frac{8\pi}{9} v_0 n^2 \left[x_i^2 P(A) m_\alpha \int_0^a g_{ii}(r) r^4 dr + x_j^2 P(B) m_j \int_0^b g_{jj}(r) r^4 dr + x_i x_j \left\{ m_i P(A) + m_j P(B) \right\} \int_0^c g_{ij}(r) r^4 \, dr \right] \quad (1.35)$$

In Equation (1.35), the upper limits of the integrals, as represented by a, b and c, correspond to the r_{min} values of $g_{ii}(r)$, $g_{ij}(r)$, $g_{jj}(r)$ respectively.

A critical analysis of the above-mentioned five methodologies (theories) to evaluate melt viscosity using the atomic structure information of liquid alloys showed that the Semi-Empirical approach was the most feasible to carry out within the scope of this project.

CHAPTER 2 OBJECTIVES AND PROJECT PLAN

This section of the thesis presents the research objectives of this project and the plan adopted to obtain the deliverables fulfilling these objectives.

2.1 OBJECTIVES

The aim of this project is to create an in-depth understanding of liquid properties of Al-Si alloy melts via diffraction experiments using a High energy X-ray (synchrotron) beam source.

- Evaluate the atomic structure of liquid Al-Si hypoeutectic alloys as function of melt temperature above the liquidus temperature and silicon content.
- Evaluate the effect of trace additions of Sr (0.04 weight percent) on the atomic structure of liquid Al-Si hypoeutectic alloys.
- Determine the partial pair correlation functions of Al-Al, Al-Si and Si-Si pairs of atoms in the liquid Al-Si hypoeutectic alloys by Reverse Monte Carlo (RMC) analysis.
- Evaluate fundamental physical properties of liquid metals such as viscosity by using the atomic structure information of Al-Si alloys obtained from diffraction experiments and RMC analysis.

Project Plan

The project was carried out in three phases as explained below:

Phase I

- Design of experiments and preparation of alloy cast samples for liquid diffraction experiments. Communication/visit to various Synchrotron and Neutron laboratories to see the feasibility of liquid Al-Si alloy diffraction experiments. Writing project proposals to obtain the beam time to perform diffraction experiments.
- High energy X-ray diffraction experiments on Liquid Al-Si hypoeutectic alloys. High energy X-ray diffraction experiments on Sr modified Liquid Al-Si hypoeutectic alloys.

Phase II

- Analysis of diffraction experiment data.

- Determine the effect of Si and melt temperature on total liquid structure of the alloys
- Determine the effect of Sr on total liquid structure of the alloys.

Phase III

- Reverse Monte Carlo analysis of experiment data to evaluate the partial pair correlation functions of the alloys.
- Viscosity of Liquid Al and Al-Si hypoeutectic alloys with and without the addition of Sr.

Figure 2-1 presents an overview of the project plan showing the three phases adopted to fulfill the objectives of this project.

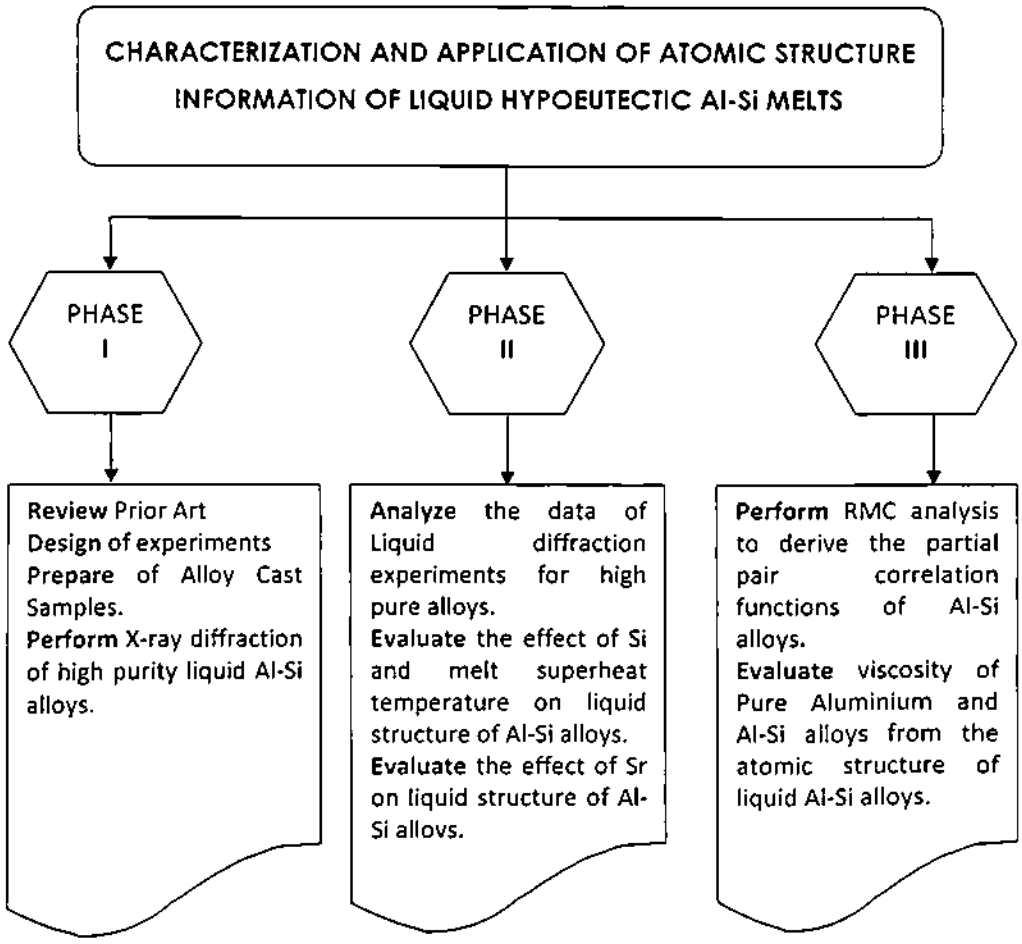


Figure 2-1: Overview of the project plan adopted in this project.

CHAPTER 3 EXPERIMENTS

This chapter elaborates the relevant topics dealing with the material and procedures involved in the various experiments of this study.

3.1 MATERIALS AND ALLOYS

Alloy samples were prepared from 99.999 % purity Al ingots, electronic grade (99.9999% purity) elemental Si and 99.9% purity elemental Sr. Each alloy sample was placed in a clean alumina crucible, melted in an electric furnace and poured into a cylindrical copper mold of 15 mm diameter and 70 mm height to form a cast specimen. Al-10%Sr master alloy was prepared with the Al and Sr elements and this was added to the Al-Si alloy to attain the required Sr level of 0.04 weight percent.

The alloy chemistry was measured with Inductively Coupled Plasma (ICP) and confirmed with Glow Discharge Optical Emission Spectroscopy (GDOES). Thermal data during solidification was collected from each alloy composition at a solidification rate of 48 °C/min to evaluate the liquidus temperature. Figure 3-1 shows the thermal data obtained for Al-12.5%Si eutectic alloy during solidification of the alloy. Similar plots were obtained for all the alloy compositions to determine the liquidus temperature of the alloys. The alloy compositions and corresponding liquidus temperatures are presented in Table 3-1. All alloy compositions presented in this dissertation are in weight percent.

Table 3-1: Alloy Chemistries and the respective liquidus temperature measured in this study.

Alloy	Al	Al-3Si	Al-7Si	Al-10Si	Al-12.5Si
Liquidus Temperature (K)	933	909	879	870	849

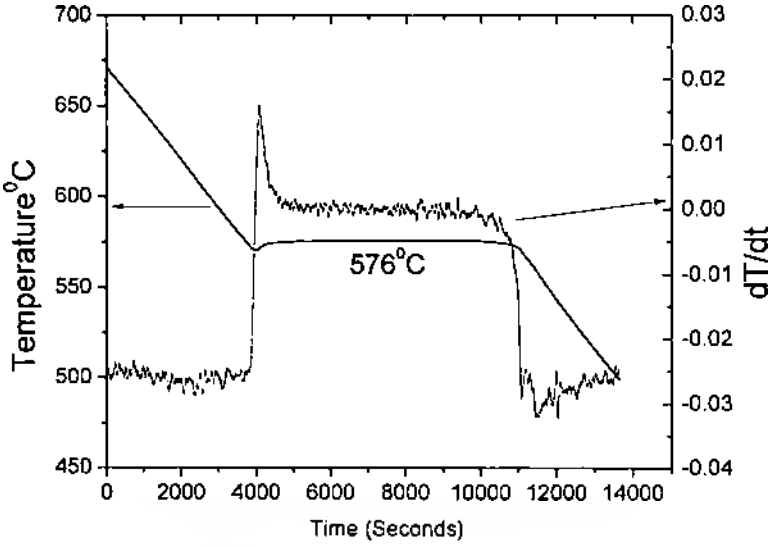


Figure 3-1: Thermal data during the solidification of Al-12.5%Si alloy.

3.2 HIGH ENERGY X- RAY DIFFRACTION

A cylindrical sample of 1.5 mm diameter and 10 mm length was machined out of the cast sample (Section 3.1) and placed in a transparent quartz tube of 2 mm in diameter and 10 mm in length. The tube was subsequently evacuated and sealed with Ar gas to minimize oxidation of the alloy melt. Figure 3-2 represents the phase diagram for a typical Al-Si hypoeutectic alloy binary system [98]. The data markers superimposed in Figure 3-2 are presented and these are the Si content and melt temperature of the alloys used for diffraction experiments. Figure 3-3 shows a photograph of a typical sample inside a quartz tube for liquid x-ray diffraction experiments.

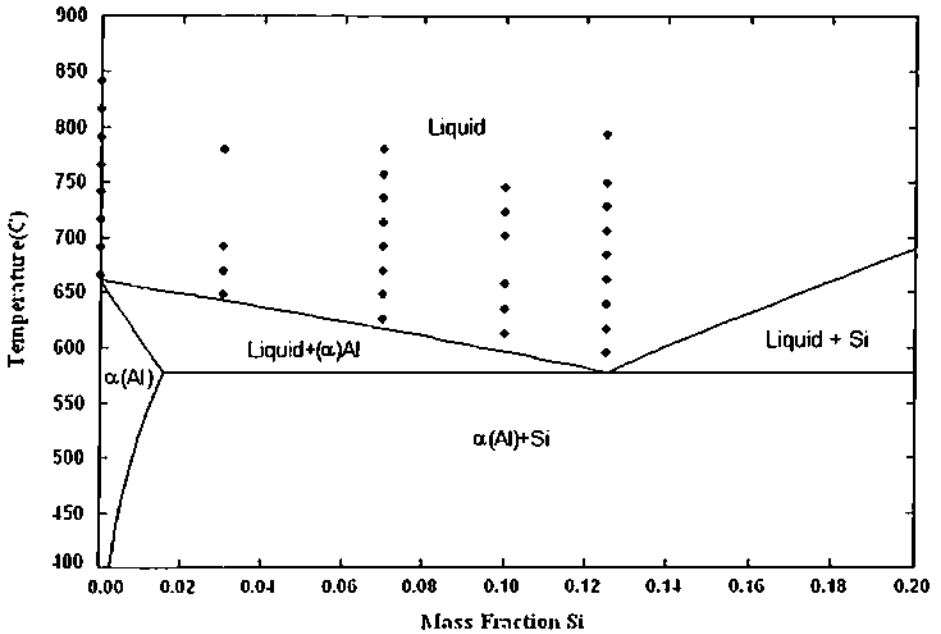


Figure 3-2: **Al-Si binary alloy phase diagram [98] showing the eutectic composition at about 12.5 wt% Si. The spots in the figure represent the Si level and melt temperatures at which the liquid diffraction experiments were carried out as shown in Table 3-2.**

Table 3-2: Alloy temperatures at which diffraction experiments were carried out.

Alloy	Temp (K)	Alloy	Temp (K)
Al	938	Al-3Si	920
	963		942
	988		964
	1013		1052
	1038	Al-7Si	898
	1063		920
	1088		942
	1113		964
Al-12.5Si	867		986
	889		1008
	911		1030
	933		1052
	956	Al-10Si	885
	978		907
	1000		929
	1022		973
	1065		995
			1017
			1039

X-ray diffraction experiments were carried out using high energy synchrotron X-Ray source at Sector 6ID-D, MUCAT (μ-CAT) beam line, Advanced Photon Source (APS), in Argonne National Laboratory (ANL), Argonne, IL, USA. A monochromatic (98.099 KeV) beam (0.1264Å wavelength) was chosen to provide high penetration through the bulk and minimize multiple scattering. Silicon double crystal monochromators were employed to attain the required wavelength. The distance from the sample to the detector was calibrated using Si 920C[•] standard providing an effective range of wave vector, Q from 0 to about 15 $Å^{-1}$. The Debye rings obtained as diffraction data were integrated into a single one dimensional plot of intensity and scattering angle using the FIT2D [99] software program, which also provided a geometric correction for the flat plate detector geometry.

The quartz tube with the sample alloy was placed vertically inside a furnace capable of heating samples to 1500 K. Figure 3-4 shows the schematic of the furnace used for liquid diffraction experiment [100]. The sample was heated to 750K to ensure

[•] National Institute of Standards and Technology, Gaithersburg, Madison, USA.

complete melting. The diffraction data was collected at various liquid superheat temperatures, ranging between 5K and 250K for the Al-Si alloys.

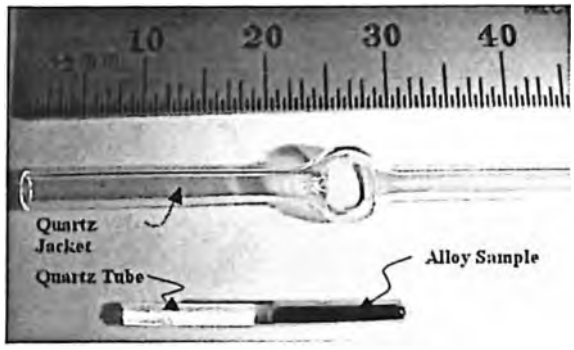


Figure 3-3: Sample inside a quartz tube for Liquid X-ray diffraction experiments.

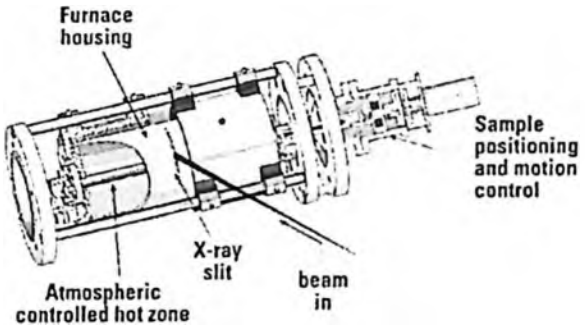


Figure 3-4: Schematic of portable furnace for high temperature liquid X-ray diffraction experiments [100].

Ten scans of 60 s each were obtained at each melt temperature using a MARCCD detector[†]. The diffraction data was also obtained for the empty container (Quartz tube) and the empty furnace for purposes of background subtraction. The sample data along with background and empty container data were analyzed using PDFgetX2[*] software [101] to obtain the SF, S(Q). The analysis included corrections for multiple scattering, compton and geometric corrections to the raw intensity data to obtain $I^{corr}(Q)$, S(Q) and g(r), respectively. The parameters on the SF, PDF and RDF graphical plots (Figure 1-7) were evaluated using a standard academic graphing software program.

[†] 41 cm x 41 cm CsI coated solid state detector manufactured by General Electric, USA.

CHAPTER 4 REVERSE MONTE CARLO ANALYSIS

This chapter elaborates on the procedure used for the Reverse Monte Carlo (RMC) analysis. Figure 4-1 represents the flow chart of the RMC analysis procedure developed in this study. The RMC procedure was divided into five steps and a total of 10,000 Al-Si alloy atoms were used in the analysis. The Al-12.5%Si alloy will be used to describe the various steps in the RMC analysis procedure.

1200 Si atoms for the Al-12.5wt%Si alloy were randomly placed in a box and the dimensions of the box were determined by the total number density of the Al-Si alloy. Si configuration file was created using the RANDOM[‡] program. The remaining 8800 Al atoms were randomly placed in the box containing the initial Si configuration file using the ADDRAND[‡] program. This would give the Al-Si configuration file containing all the 10000 Al and Si atoms together in a square box of 57.02 Å length per side for the Al-12.5 Si alloy temperature of 867K as dictated by the number density of the alloy (0.05393 atoms/Å^3) (refer to Table 6-1).

A program file was created as shown in Figure 4-2 to carry out RMC program[§] on the Al-Si atom configuration obtained from Step 2. The aim of this procedure is to move out all the atoms in the initial box such that any two atoms are at the farthest possible distance without changing the number density of the alloy and the size of the box containing the atoms. The coordination constraints presented in Figure 4-2 dictates that any Al-Al atom pair would be at a minimum distance of 2.35 Å from each other, any Al-Si atom pair would be at a minimum distance of 2.4 Å from each other and any Si-Si atom pair would be at a minimum distance of 2.4 Å from each other. This value of minimum distances is typically about 7 to 9 % of the cut off distance in the PDF (r_o in Figure 1-7) as obtained from the diffraction experiment data. This ensures that the initial condition of the atom arrangement in the box used to fit the experiment data in the next step was such that no clustering or trapping of any atom types was feasible. It is to be noted that if this step was not carried out, many atoms were found trapped and unable to move when the RMC program was performed on the initial box of atoms coupled with the experiment data. Such atom trappings were reflected by abnormal peaks before the first peak in the respective partial pair distribution functions (PPDF). Further, moving in the Al and Si atoms from an initially larger value of r, rather than the cut-off value of r_o to fit an experimental data with RMC proved to be more effective (with respect to time and final peak definitions in PPDF).

[‡] http://www.isis.rl.ac.uk/RMC/downloads/useful.htm

[§] RMCA 3.14 program

The output from Step 3 yielded a box of atoms with the favorable initial configuration which was coupled with the experiment data for the reduced structure factor, (S(Q) -1) and the RMC modeling was carried out with an input program file as shown in Figure 4-3. It must be noted that PDF could also be used for input as experiment data; however, the reduced structure factor was used to avoid errors that could arise from the Fourier transformation used to obtain the PDF. Further, our experience showed that the use of reduced structure factor yielded more repeatable and accurate results for the PPDF. Additionally, the weighting function W_{ij} (Equation (1.13)) varied with Q, whereas this function would have to be assumed constant when PDF was used instead of reduced structure factor as the input data file in the RMC program. Traditionally, PDF was used in the RMC procedure because most of the work in metallic alloys was carried out in the reflection mode with the Mo X-Ray source and this would not yield a highly refined S(Q) data for use in the RMC program. In the RMC program shown in Figure 4-3, two parameters need to be critically controlled for a successful simulation. These are the values of moveout and standard deviation, respectively. Initially, the moveout and standard deviation values were set at 0.05 and 0.05, respectively. The RMC program is allowed to run at these values until the chi-squared (χ^2) stabilized to a nearly constant value. The moveout value was maintained at 0.05 and the standard deviation was lowered to 0.03, 0.01 and 0.001 in subsequent iterations of the program. Each iteration was stopped when the χ^2 reached a nearly constant value. Each iteration mentioned in this step took about two hours to complete.

At the standard deviation value of 0.001, the moveout was reduced to 0.01 and the RMC program was again carried out until the χ^2 reached a nearly constant value at which point the simulation was deemed complete. The last iteration of the program with the moveout value at 0.01 and the standard deviation value of 0.001 would typically take more than 10 hours to completion. The moveout values are in Angstrom units and represent the maximum mobility of the atoms in the simulation box. The standard deviation is the level of accuracy required for fitting the experiment data.

The RMC simulations quantified the partial structure factor values, $S_{ij}(Q)$ for the three types of atom pairs in the binary alloy. Each of these partial structure factor values was used as input into a program to evaluate the respective PPDF by Fourier transformation (Equation (1.11)). The values of PPDF along with the respective values of ρ_{ij} were used to evaluate the partial RDF for the three Al-Al, Al-Si and Si-Si atom pairs and subsequently, the partial CN and partial PD were also quantified.

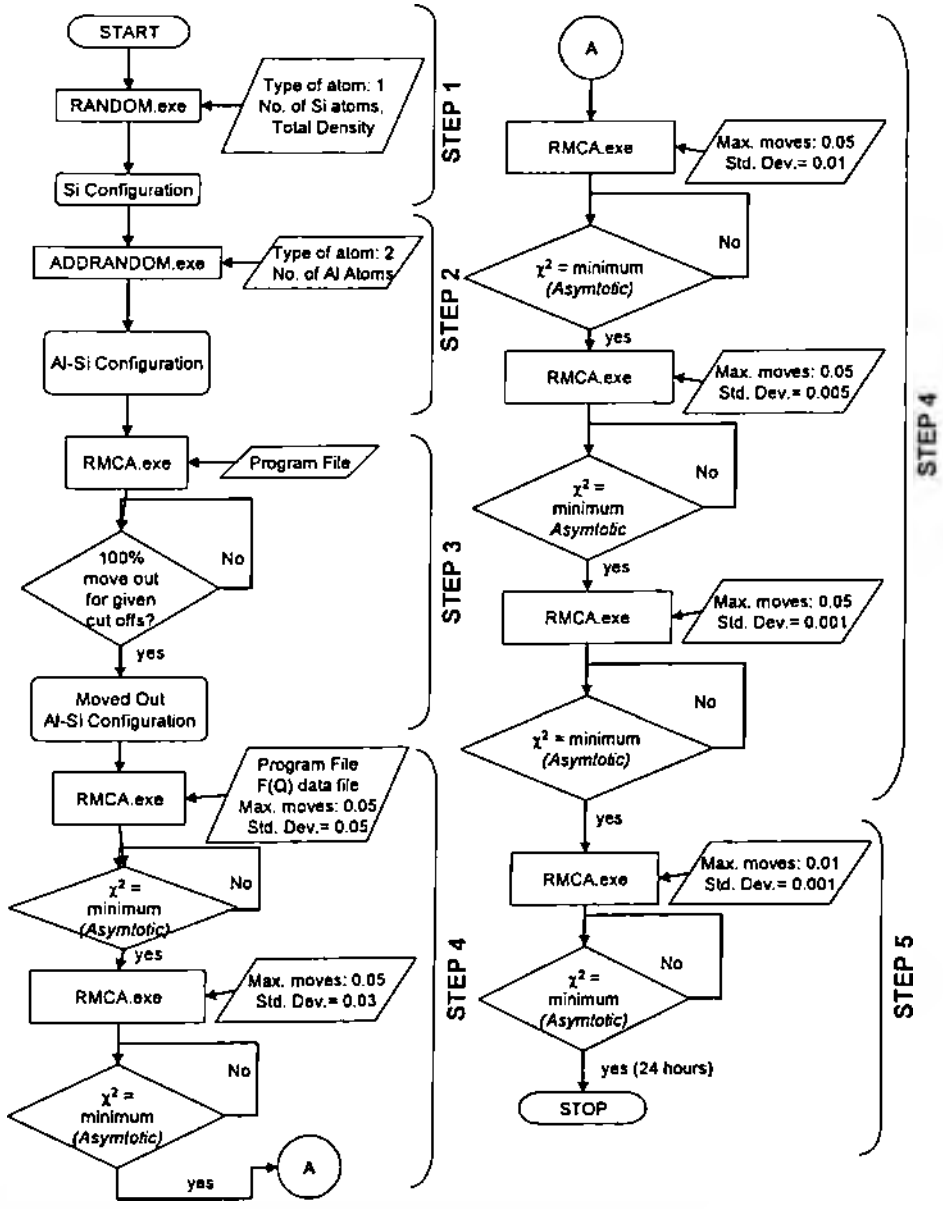


Figure 4-1: Flow-Chart representing RMCA procedure

```
0.053928835                                  ! number density
2.4 2.4 2.35                                 ! cut offs
0.5 0.5 0.5                                  ! maximum moves
0 0                                          ! nswap, swapfrac
0.01                                         ! r spacing
.true.                                       ! moveout option
0                                            ! number of configurations to collect
9000 1                                       ! step for printing
300 3                                        ! Time limit, step for saving
0 0 0 0                                      ! No. of g(r), S(Q), F(Q), EXAFS expts
4                                            ! no. of coordination constraints
2 2 0.0 2.35 0 1.0 0.00001
1 1 0.0 2.4 0 1.0 0.00001
1 2 0.0 2.4 0 1.0 0.00001
2 1 0.0 2.4 0 1.0 0.00001
0                                            ! no. of average coordination constraints
0                                            ! no. of bvs constraints
0                                            ! no. of triplet constraints
.false.                                      ! whether to use a potential
```

Figure 4-2: Initial Al-Si configuration for move out (Al-12.5%Si)

```
0.053928835                                  ! number density
2 2 2                                        ! cut offs
0.01 0.01 0.01                               ! maximum moves
0 0                                          ! nswap, swapfrac
0.1                                          ! r spacing
.false.                                      ! moveout option
0                                            ! number of configurations
to collect
1000 1                                       ! step for printing
6000 10                                      ! Time limit, step for saving
0 0 1 0                                      ! No. of g(r), S(Q), F(Q),
EXAFS expts
x594fq.fq
1 1325                                       ! Range of points used
3 0.001                                      ! Standard deviation
.false.                                      ! whether to convolute
.true.                                       ! whether to renormalise
1                                            ! beta
.false.                                      ! whether to offset
1                                            ! nback
0.                                           ! bcoeff
.false.                                      !
0                                            ! no. of coordination
constraints
0                                            ! no. of average coordination
constraints
0                                            ! no. of bvs constraints
0                                            ! no. of triplet constraints
.false.                                      ! whether to use a potential
```

Figure 4-3: RMC program file to model the alloy with the experiment data Al-12.5%Si)

CHAPTER 5 UNCERTAINITY ANALYSIS

This section presents the uncertainty in the data collected from the high energy x-ray diffraction experiments and the subsequent analysis of the data.

Figure 5-1 shows a schematic of the typical process used in evaluating the 95% confidence interval in the data during each stage of the analysis. Nine to ten scans were collected for each temperature for a particular alloy in the diffraction experiment. Typically, the uncertainties in the diffraction data and the subsequent structure information data for all the alloys at a given temperature were similar in magnitude and hence, a typical uncertainty analysis is presented for nine scans of raw diffraction data obtained and analyzed for pure Al at 938 K as well as for Al-12.5%Si alloy at 889K. The 95% confidence interval of the average data was evaluated by Equation (5.1).

$$\left(M - t\frac{\sigma}{\sqrt{n}}\right) \leq \mu \leq \left(M + t\frac{\sigma}{\sqrt{n}}\right) \qquad (5.1)$$

In Equation (5.1), μ is the mean data within the interval, M is the average of the data, t is the t-value for the 95% confidence (probability of 0.05) with (n-1) degree of freedom in data, σ is the standard deviation of the data set and $(\sigma/(\sqrt{n}))$ is the estimated standard deviation of the average data. The t-value for 10 diffraction data measurement is 2.26.

Figure 5-2 to Figure 5-7 show the typical plots of I(Q), S(Q), first peak features in S(Q) curve, g(r), first shell atoms features in g(r) and RDF, respectively for pure Al at 938 K. Figure 5-8 shows the typical values for CN and PD as a function of alloy temperature for pure aluminium along with the respective 95% confidence interval. The 95% confidence interval for both CN and PD are small showing the reliability in the diffraction data and the subsequent analysis.

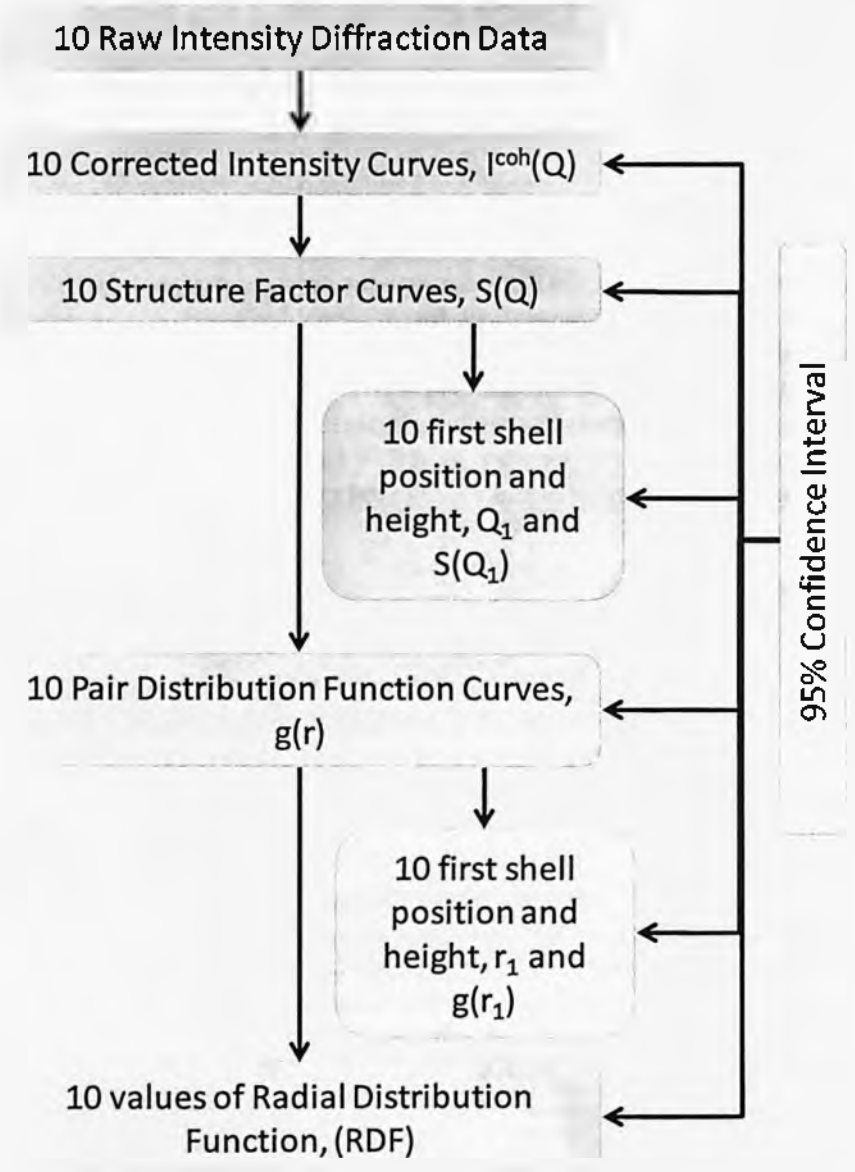


Figure 5-1: Schematic showing the typical uncertainty analysis carried out on the diffraction data at various stages of the analysis.

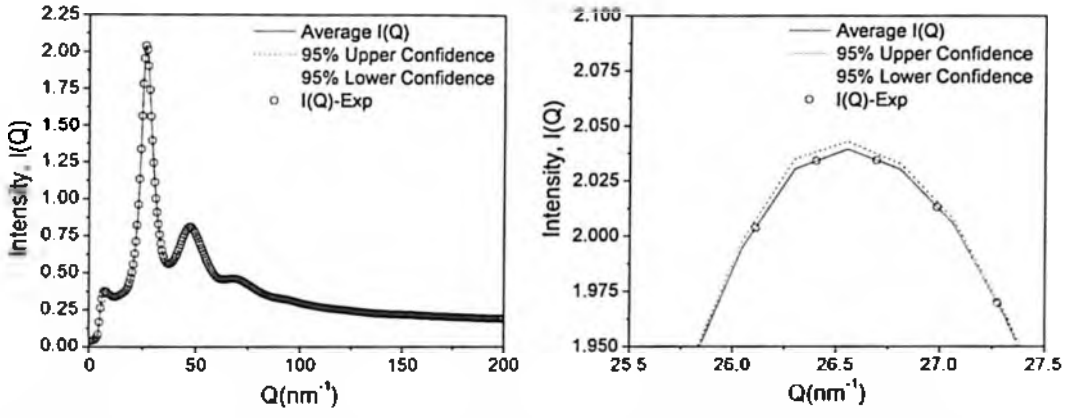


Figure 5-2: **Typical corrected Intensity plot from diffraction data for (a) Pure Aluminium at 938K along with the 95% confidence interval, (b) Magnified image showing the first peak features.**

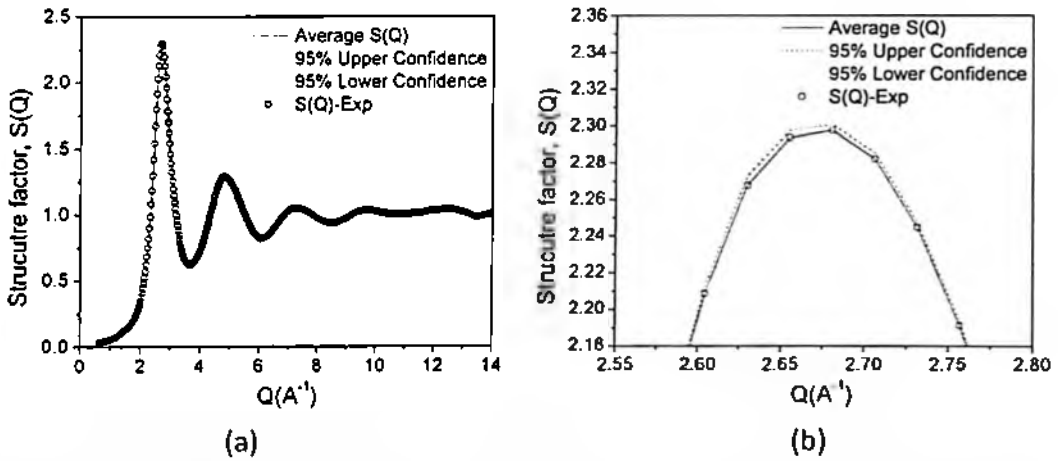
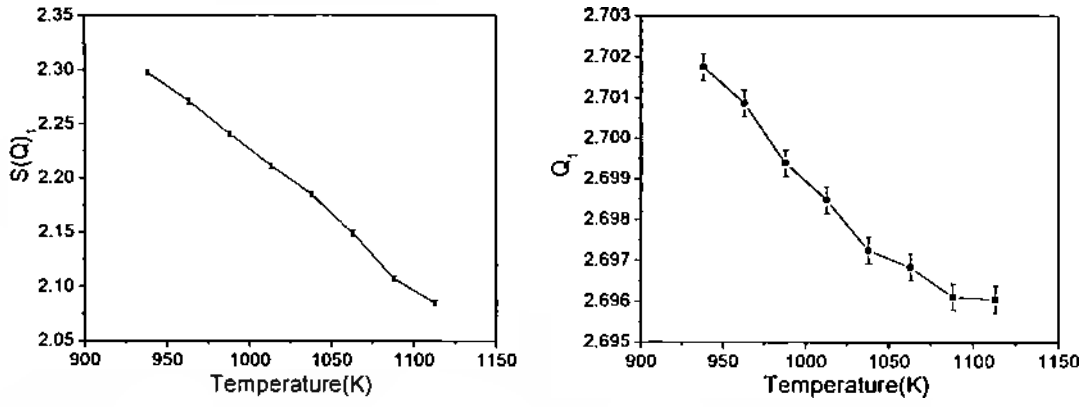
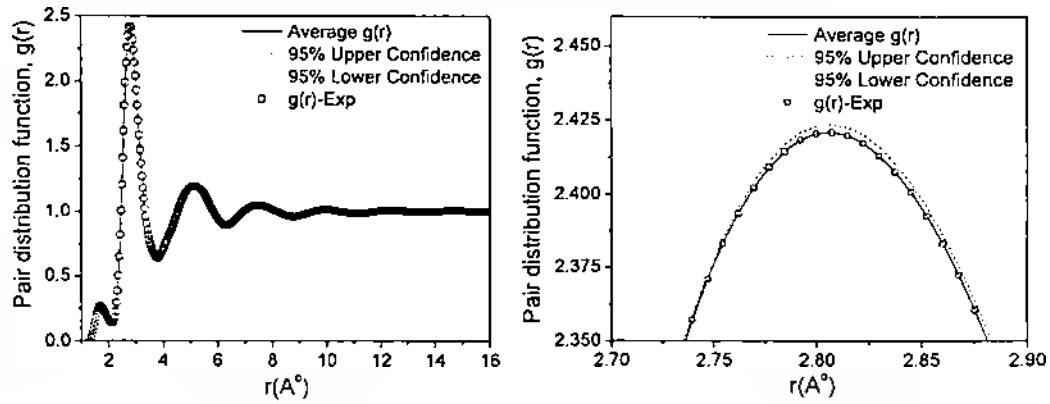


Figure 5-3: **Typical plot of the S(Q) for (a) Pure Aluminium at 938K with the 95 confidence interval, (b) Magnified image of the first atom shell (first peak features).**



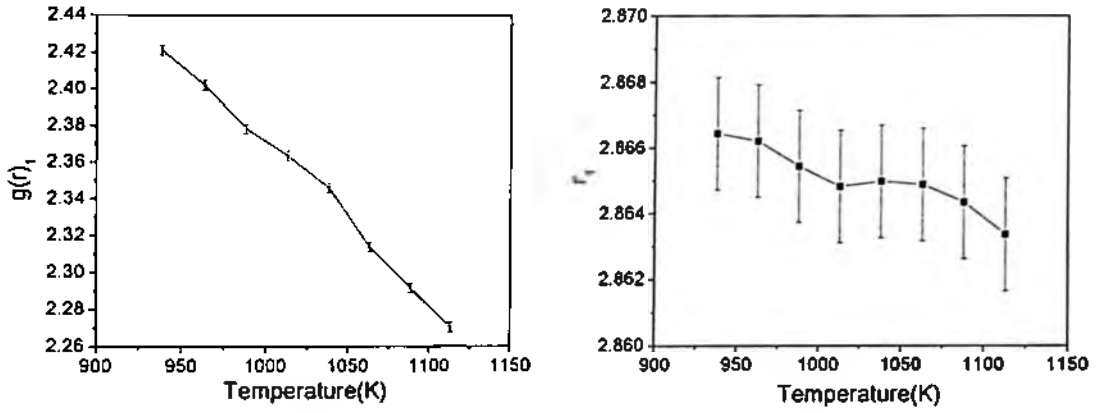
(a) (b)

Figure 5-4: Plot of the first atom shell in S(Q) for Pure Al showing (a) $S(Q_1)$ and (b) Q_1 with the respective 95% confidence interval.



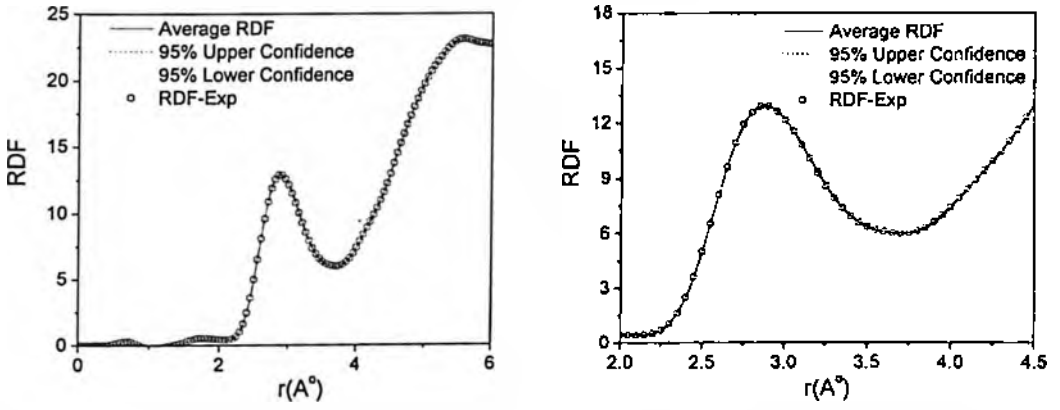
(a) (b)

Figure 5-5: Typical plot of the g(r) for (a) Pure Aluminium at 938K with the 95 confidence interval, (b) Magnified image of the first atom shell (first peak features).



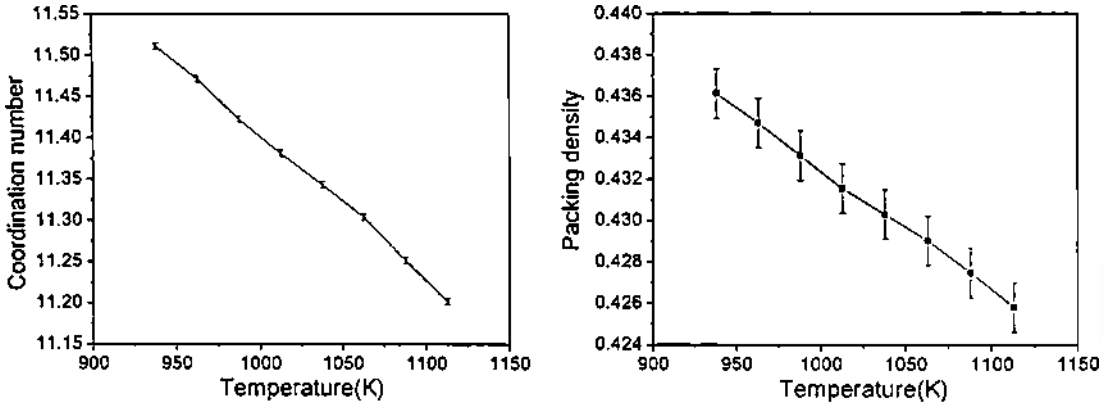
(a) (b)

Figure 5-6: Plot of the first atom shell in g(r) for Pure Al showing (a) $g(r_1)$ and (b) r_1 with the respective 95% confidence interval.



(a) (b)

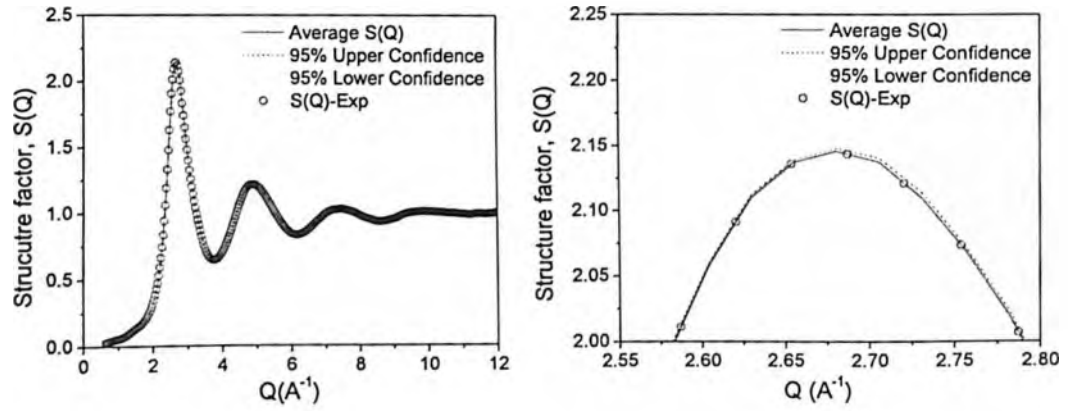
Figure 5-7: Typical plot of the RDF for Pure Aluminium at 938K with the 95 confidence interval, (b) Magnified image of the first atom shell (first peak features).



(a) (b)

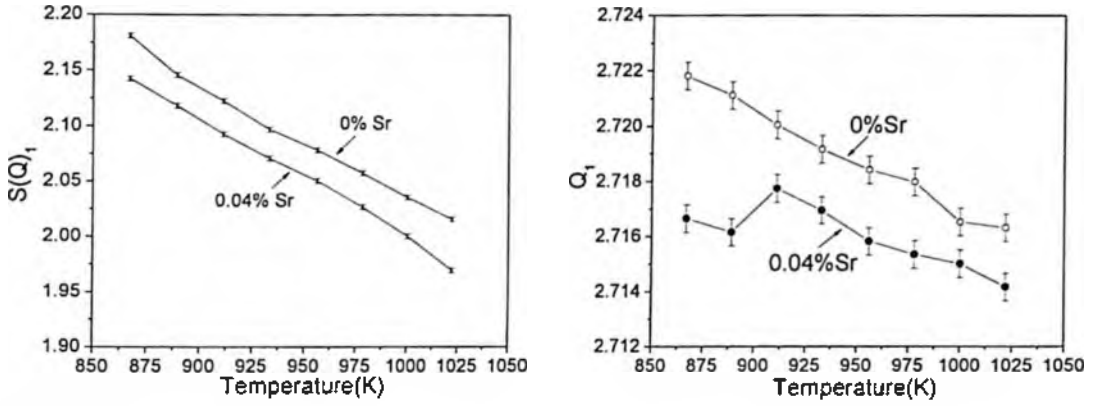
Figure 5-8: Typical plots for Pure Al (a) coordination number, CN and (b) packing density, PD at various temperatures along with the 95% confidence interval.

Figure 5-9, Figure 5-10, Figure 5-11 and Figure 5-12 show the typical plots for first peak features in S(Q) curve, and first shell atoms features in g(r) respectively for the Al-12.5%Si alloy at 889 K. Figure 5-13 shows the typical values for CN and PD as a function of alloy temperature for Al-12.5%Si and Al-12.5%Si-0.04%Sr along with the respective 95% confidence interval. The 95% confidence interval for both CN and PD are small showing the reliability in the diffraction data and the subsequent analysis. Similar results to the uncertainty analysis were obtained for other alloys at various levels of Si and alloy temperature.



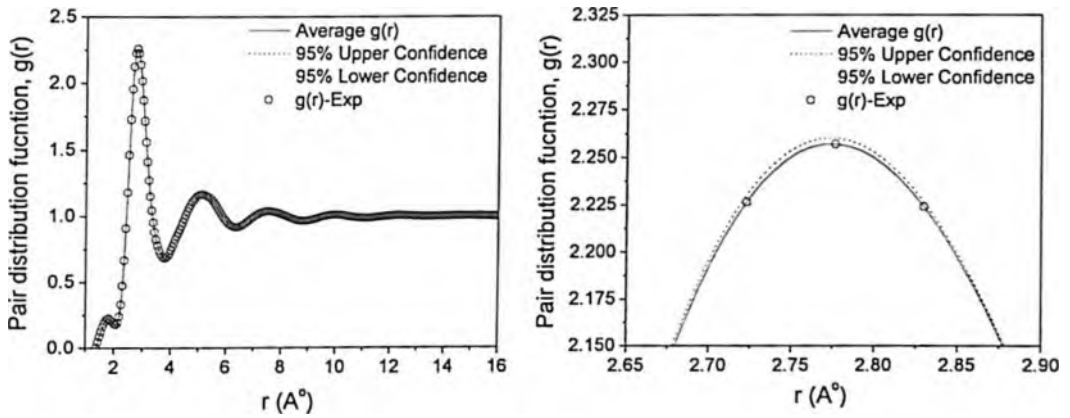
(a) (b)

Figure 5-9: Typical plot of the S(Q) for Al-12.5%Si at 889K with the 95 confidence interval, (b) Magnified image of the first atom shell (first peak features).



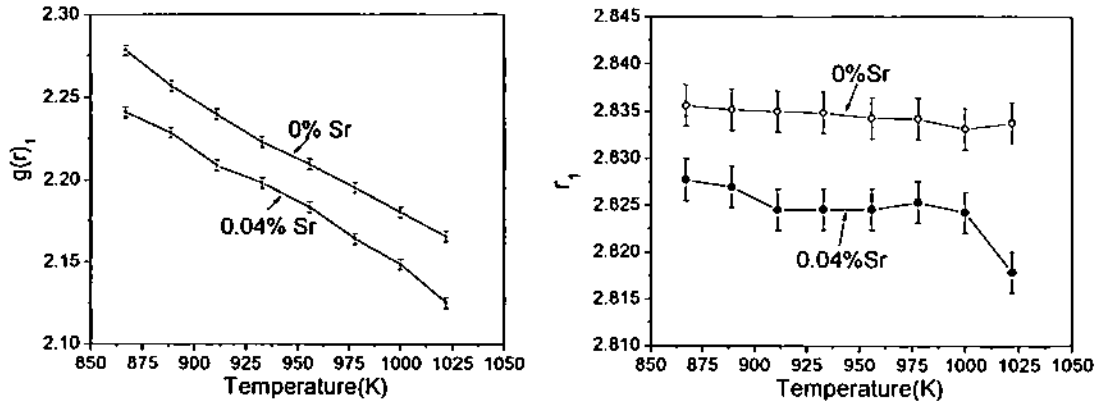
(a) (b)

Figure 5-10: **Plot of the first atom shell in S(Q) for Al-12.5%Si and Al-12.5%Si-0.04%Sr showing (a) $S(Q_1)$ and (b) Q_1 at various temperatures with the respective 95% confidence interval.**



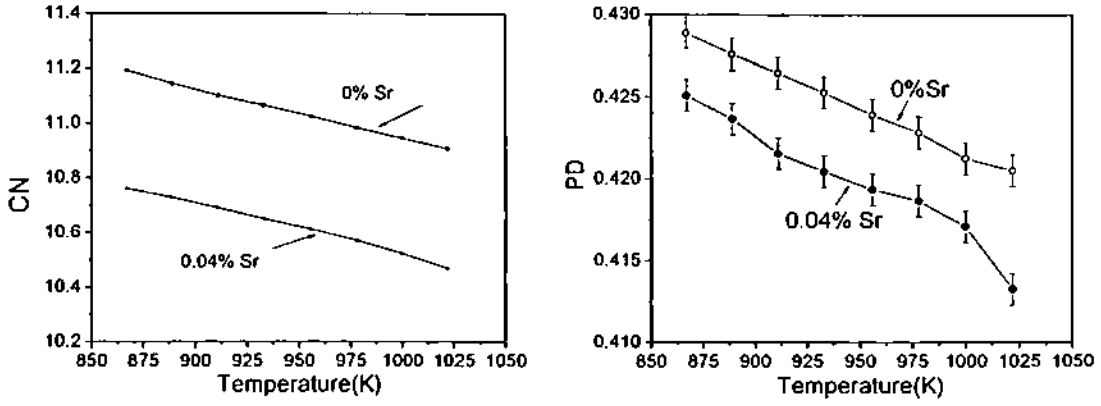
(a) (b)

Figure 5-11: **Typical plot of the g(r) for Al-12.5%Si at 889K with the 95 confidence interval, (b) Magnified image of the first atom shell (first peak features).**



(a) (b)

Figure 5-12: Plot of the first atom shell in g(r) for Al-12.5%Si and Al-12.5%Si-0.04%Sr showing (a) $g(r_1)$ and (b) r_1 at various temperatures with the respective 95% confidence interval.



(a) (b)

Figure 5-13: Typical plots for Al-12.5%Si and Al-12.5%Si-0.04%Sr (a) coordination number, CN and (b) packing density, PD at various temperatures along with the 95% confidence interval.

The uncertainities presented in this chapter were only applicable to the alloy compositions, melt temperatures and the experimental set up used in this study. Any deviations from these parameters may produce different results in uncertainities.

CHAPTER 6 RESULTS AND DISCUSSION

This chapter presents the results and discussion for the following topics:

- Total Liquid Structure of Al-Si Hypoeutectic Alloys.
- Partial Pair Correlation Functions of Al-Si Hypoeutectic Alloys.
- Viscosity of pure Al and Al-Si Hypoeutectic Alloys.

6.1 TOTAL LIQUID STRUCTURE OF Al-Si HYPOEUTECTIC ALLOYS

This section presents the results obtained from the high energy x-ray diffraction experiments of Pure Al and Al-Si hypoeutectic alloys. The effect of Si, melt temperature and 0.04% addition of Sr on liquid structure of Al-Si hypoeutectic alloys are presented and discussed.

6.1.1. Total Structure Information for Unmodified Al-Si alloys

Figure 6-1 shows the structure factor S(Q) for pure Al and is typical for all the alloy compositions. In Figure 6-1 (a), the plot at 938 K temperature is the true evaluated data and the other temperature plots are progressively incremented by a fixed integer for better clarity and visualization. There was no evidence of any pre-peaks in any of the structure factor plots for the alloys investigated in this study. The presence of a prepeak before the first peak of S(Q) in the low Q-region could represents the compound formation tendency in the liquid alloy melt [103]. Figure 6-1(b) represents the magnified image of Figure 6-1 (a) showing the effect of melt temperature on the height and width of the first peak of S(Q). The height of the first peak decreases with increasing temperature from 938 K to 1113 K, as shown in Figure 6-1(b). This is indicative of the loss of order in the atomic structure with increasing temperature of the alloy melt [40].

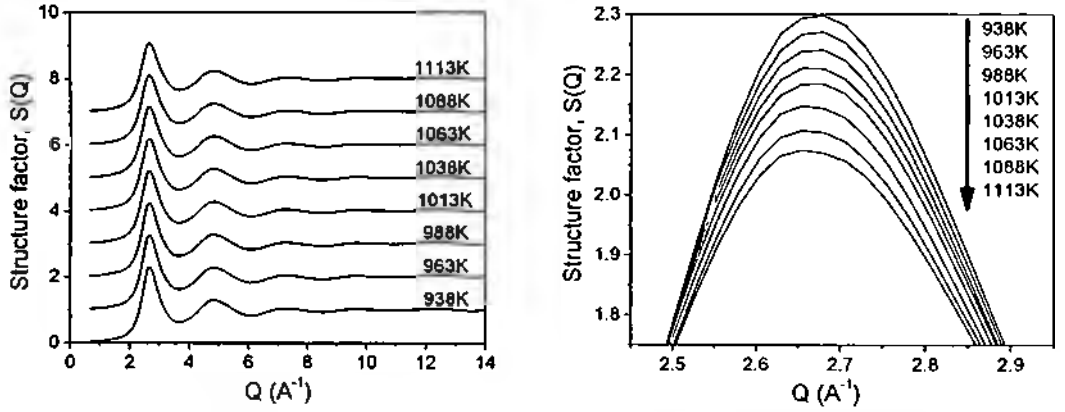


Figure 6-1: Structure factor S(Q) Vs Q for Pure Al (a) at various melt temperatures, (b) magnified region of first peaks shown in (a).

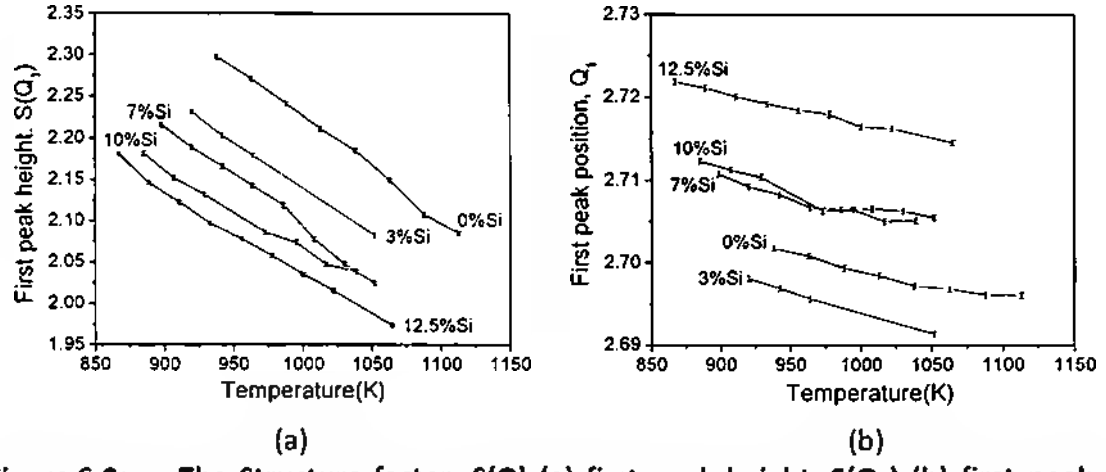


Figure 6-2: The Structure factor, S(Q) (a) first peak height, $S(Q_1)$ (b) first peak position, Q_1 plotted as a function of melt temperature for Al-Si hypoeutectic alloys.

Figure 6-2 shows the features of the first peak, $S(Q_1)$ of the SF plot, plotted as a function of melt temperature for the various alloys. Figure 6-2(a) shows the height and Figure 6-2(b) shows the position of the first peaks. It was observed that the height of $S(Q_1)$ decreases with increasing melt temperature and increasing Si content, independently. The level of atomic order in the liquid decreases with decreasing peak heights; alternately, the atomic order in the liquid decreases with increasing temperature and with increasing Si content in the alloy as well. In Figure 6-2(b), the first peak position of structure factor, Q_1 moves to lower values of Q with increasing melt temperatures for any specific alloy. In Figure 6-2(b), large variations in Si content, for

example from 0 to 12.5 wt% show an observable increase in the position of the first peak. However, smaller changes in Si content of about 3 wt% do not show any appreciable changes in the position of the first peak. Reasonably higher difference in Si levels of about 5wt% or more would be required to observe a change in the position of the first peak of the SF curve in these alloys.

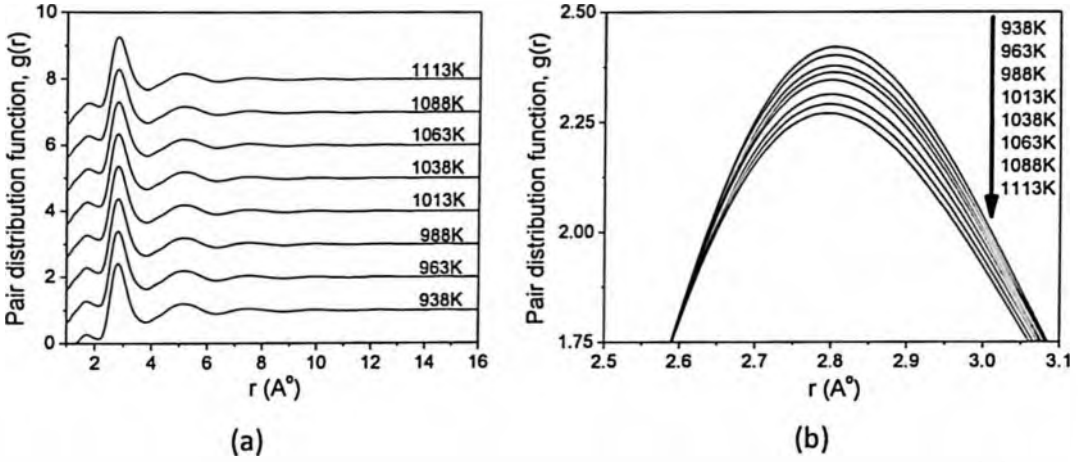


Figure 6-3: The Pair distribution function, g(r) Vs r for Pure Aluminium (a) at various melt superheat temperatures, (b) magnified image of g(r) showing the effect of melt temperature on height of the first peak $g(r_1)$.

The PDF obtained by Fourier transformation of SF for pure aluminium is shown in Figure 6-3. Similar plots were obtained for pair distribution function for all alloy compositions by Fourier transformation of their respective SF functions using the respective alloy number density evaluated and presented in Table 6-1. The number density (ρ_o) at each alloy temperature was evaluated based on the molar weight and molar volume data obtained from the FactSage thermodynamic database software [98, 102]. An empirical equation was formulated to evaluate the number densities of Al-Si hypoeutectic alloys as a function of melt superheat and Si concentration as shown in Equation (6.1).

$$\rho_o = -6 \cdot 10^{-6} \cdot (T - T_L) + 7.495 \cdot 10^{-3} \cdot (C_{Si}) + 0.05315 \qquad (6.1)$$

In Equation (6.1), the units of ρ_o is atoms per cubic angstroms, that for C_{Si} is atom fraction; the terms T and T_L represent the alloy melt temperature and the liquidus temperature of the alloy, respectively. In Equation (6.1), the minimum R-Squared for the equation obtained by regression analysis with T as the variable was 0.999, and that for C_{Si} as the variable was 0.994.

In Figure 6-4, the first peak height of g(r) decreases with increasing melt temperature for all alloy compositions. The peak height is higher in the case of pure Al and decreases with increasing silicon content from 0-12.5%Si as represented in Figure 6-4 (a). The first peak position of g(r) is shown in Figure 6-4 (b). The variation of r_1 with melt temperature is not significant and almost constant with increasing melt temperatures for a given Si level in the alloy. However, the effect of Si content on r_1 shown in Figure 6-4 (b) is similar to the effect of Si content on Q_1 presented in Figure 6-2 (b). Large variations in Si content, for example from 0 to 12.5 wt% show an observable increase in the value of r_1. However, smaller changes in Si content of about 3 wt% do not show any appreciable changes in the position of the first peak. Reasonably higher difference in Si levels of about 5wt% or more would be required to observe a change in the position of the first peak of the g(r) curve in these alloys.

Table 6-1. Evaluated number density values for Al-Si hypoeutectic alloy compositions at various melt temperatures.

Alloy	Temperature (K)	ρ_o (atoms/Å^3)	Alloy	Temperature (K)	ρ_o (atoms/Å^3)
Al	938	0.05309	Al-3Si	920	0.05332
	963	0.05293		942	0.05318
	988	0.05278		964	0.05304
	1013	0.05262		1052	0.0525
	1038	0.05246	Al-7Si	898	0.05359
	1063	0.05231		920	0.05345
	1088	0.05215		942	0.05331
	1113	0.052		964	0.05318
Al-12.5Si	867	0.05393		986	0.05304
	889	0.05379		1008	0.05291
	911	0.05366		1030	0.05277
	933	0.05352		1052	0.05263
	956	0.05366	Al-10Si	885	0.05376
	978	0.05325		907	0.05362
	1000	0.05311		929	0.05349
	1022	0.05298		973	0.05322
	1065	0.05272		995	0.05308
				1017	0.05295
				1039	0.05281

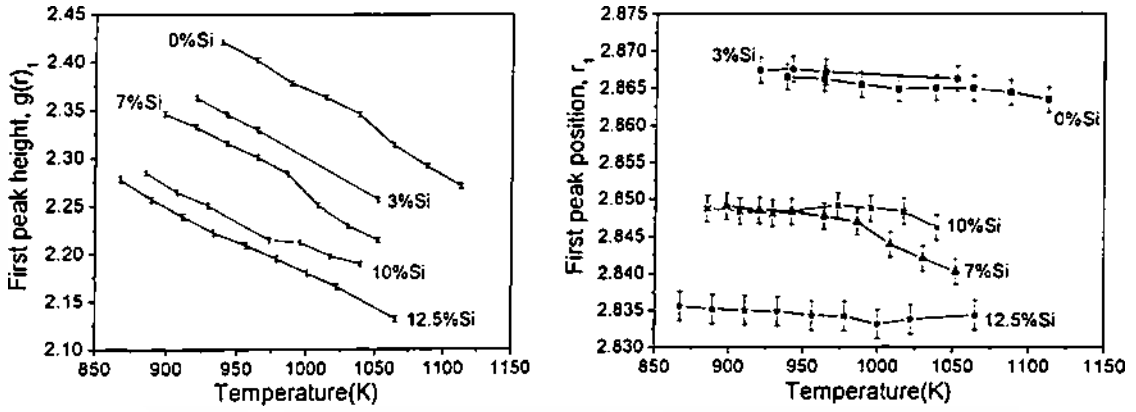
Figure 6-5 shows the variation of coordination number as a function of melt temperature for various Al-Si hypoeutectic alloys. It is evident from Figure 6-5 that the coordination number increases with decreasing melt temperature for the alloys.

Increase in silicon content in the Al results in a decrease of the coordination number at any given temperature. An empirical equation was formulated to enable evaluation of CN as shown in Equation (6.2).

$$CN = -0.0017 \cdot (T - T_L) - 2.4352 \cdot (C_{Si}) + 11.5185 \quad (6.2)$$

In Equation (6.2), the unit of C_{Si} is atom fraction; the terms T and T_L represent the alloy melt temperature and the liquidus temperature of the alloy, respectively. In Equation (6.2), the minimum R-Squared for the equation obtained by regression analysis with T as the variable was 0.999, and that for C_{Si} as the variable was 0.996.

The CN value for pure Al at 938 K was evaluated as 11.51 and this value validates the value of 11.5 evaluated by Waseda [40].



(a) (b)

Figure 6-4: The pair distribution function, g(r), (a) first peak height, $g(r_1)$, (b) first peak position, r_1 as a function of melt temperature for Al-Si hypoeutectic alloys.

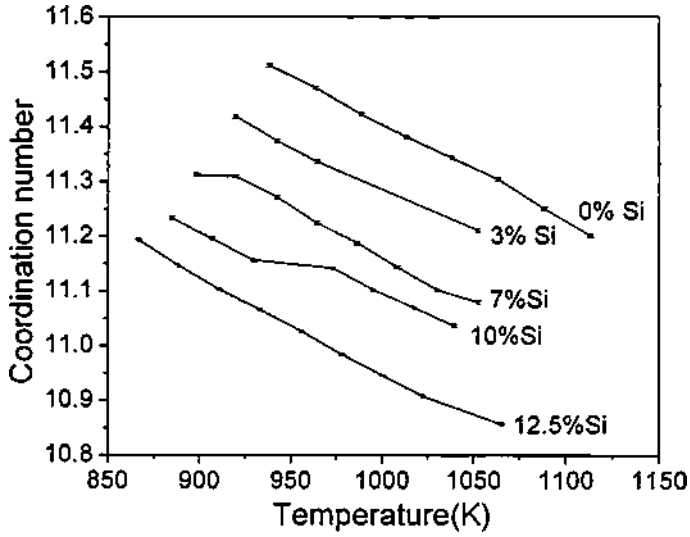


Figure 6-5: Coordination number as a function of melt temperature for various Si concentrations for the Al-Si hypoeutectic alloys.

Figure 6-6 shows the packing density of Al-Si hypoeutectic alloys as function of melt temperature. It is evident from Figure 6-6 that the packing density of any given alloy composition decreases with increase in melt temperature. Further, at any given melt temperature, the packing density of the alloy melt decreases when comparing alloys with 0% Si and 12.5%Si. However, the change is not so significant for increase in Si levels of about 3 wt%.

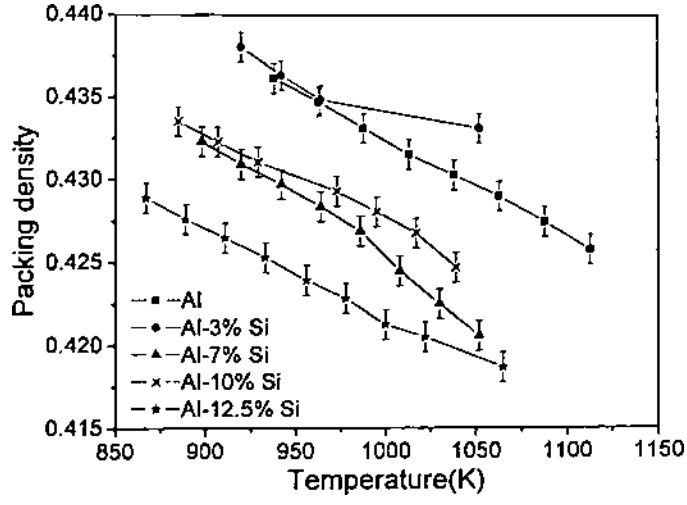


Figure 6-6: Variation of packing density as a function of melt temperature for various Si concentrations for the Al-Si hypoeutectic alloys.

It can be observed from Figure 6-1 to Figure 6-6 that the disorder in the alloy melts increases with increase in melt temperatures for Al and Al-Si alloy melts. This was represented by decrease in peak height of S(Q) and g(r), decrease in CN and PD. In the case of Al-7Si alloy, a sudden change in peak heights, peak positions and PD observed at 986K and this could be resulted from the temperature induced structural changes, where some clusters break to from free atoms or result in new clusters in the melt. However, these changes were not so significant to attribute to anomalous behaviour in the melt as the trend in the plots for structure parameters show a linear behaviour with temperature. Addition of silicon content (0% to 12.5%) to the aluminium melt also causes disorder in the melt. The coordination number of pure Al near the melting point was observed to be 11.5 and the addition of silicon lowers the CN, representing a change in the structure of melt from a closely packed to an open structure. No signs of compound forming tendencies were observed due to the addition of silicon to the Al melt as there were no evidence of prepeaks in the S(Q) plots of all alloy compositions.

6.1.2. Effect of Sr on Total Structure Information of Al-Si Alloys

Figure 6-7 (a) to (d) represent the plots for S(Q) as a function of Q for Al-12.5%Si and Al-12.5%Si-0.04%Sr alloys, respectively at various alloy melt temperatures. The plots shown in Figure 6-7 are typical of those obtained for the other alloys in this study as well. Figure 6-7(c) and (d) show a magnified section of the first peak of S(Q) plots shown in Figure 6-7(a) and (b), respectively. Figure 6-7(c) and (d) show that in eutectic alloy without and with Sr addition, the height of the first S(Q) peak, $S(Q_1)$ decreases and its position (Q_1) shifts to lower Q values with increasing liquid alloy temperature. Also, in Figure 6-7(c) and (d), the addition of Sr to the melt shifts $S(Q_1)$ to a lower value for the same temperature showing that addition of Sr decreases the order in the liquid structure at any given temperature. The absence of any peaks before the first large peak (low Q region) and the absence of any humps in the first peak shown in Figure 6-7 shows the lack of any compound forming tendencies in the liquid alloy [103]. The pre-peaks and humps were absent in the S(Q) data obtained for all the Al-Si alloys with Sr additions, as well. In Figure 6-7 (a) and (b), the plot at 867 K is the true evaluated data and the other temperature plots were progressively incremented by a fixed integer for better visual clarity for the readers.

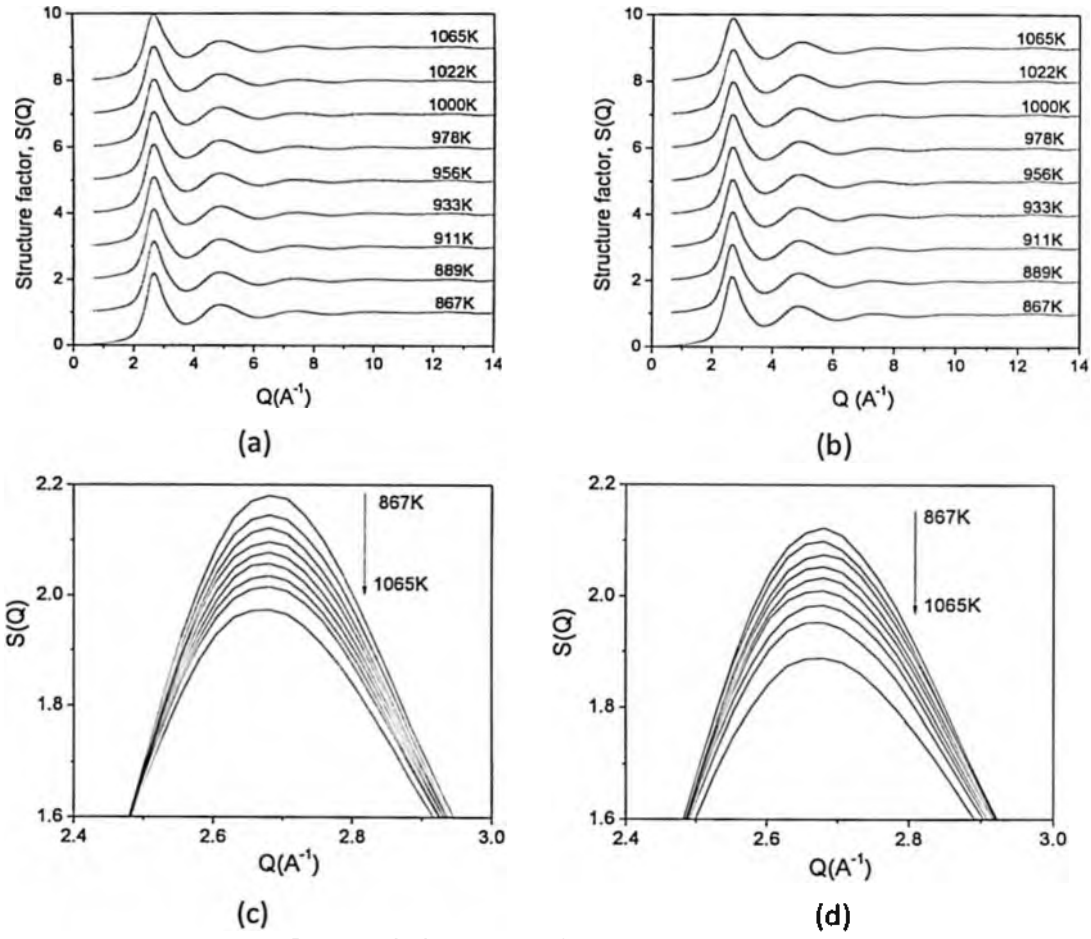


Figure 6-7: **Structure factor S(Q) Vs Q for (a) Al-12.5%Si, (b) Al-12.5%Si-0.04%Sr, (c) magnified region of first peaks shown in (a), and (d) magnified region of first peak shown in (b).**

Figure 6-8 represents the variation of first peak height, $S(Q_1)$ for various alloy compositions in unmodified and Sr-modified conditions. In Figure 6-8(a) to (d), it can be observed that $S(Q_1)$ decreases with increasing melt temperature for all alloy compositions. Further, addition of 0.04 %Sr in each alloy decreases the value of $S(Q_1)$, at any given temperature representing that the melt becomes more disordered.

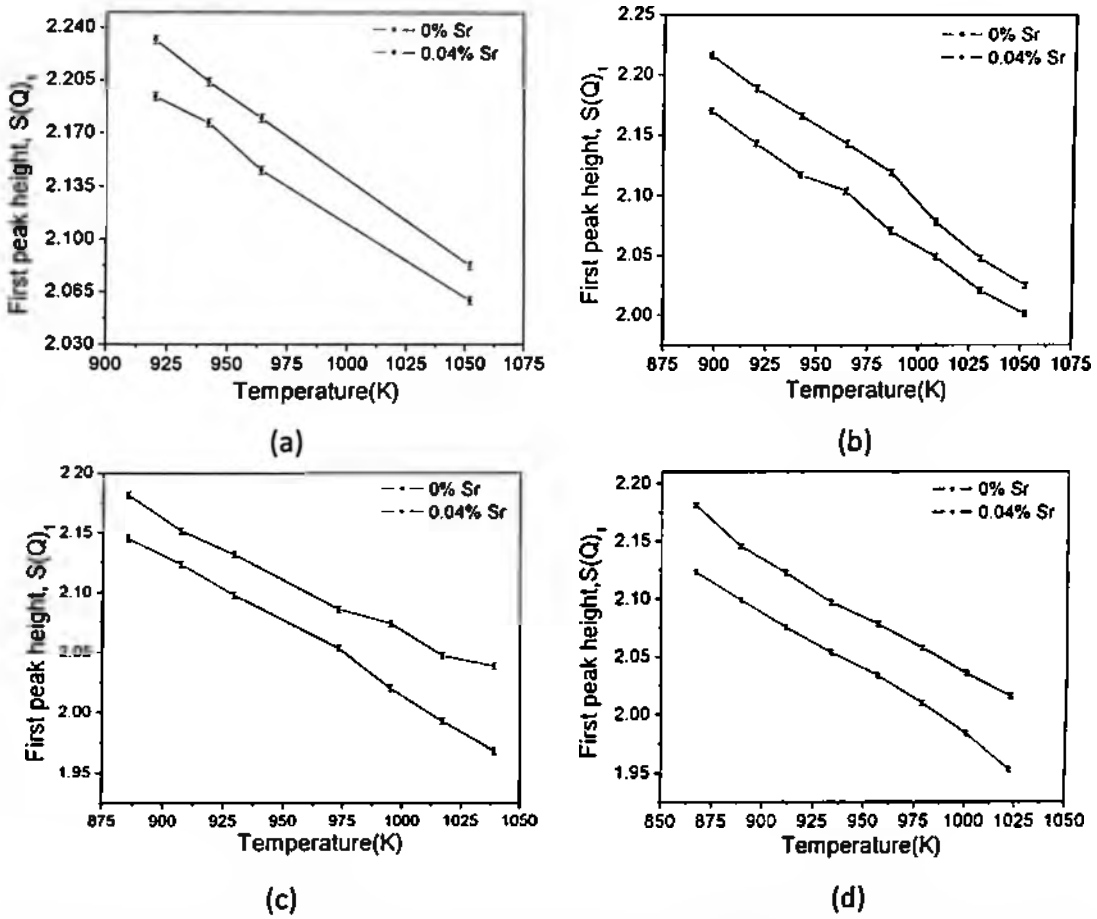


Figure 6-8: Effect of Sr addition on the first peak height, $S(Q_1)$ at various melt temperatures for, (a) Al-3% Si, (b) Al-7% Si, (c) Al-10%Si, (d) Al-12.5%Si.

Figure 6-9(a) and (b) represent the typical pair distribution function, g(r) as a function of the radial distance, r for various liquid alloy temperatures for Al-12.5%Si and Al-12.5%Si-0.04%Sr alloys, respectively. In Figure 6-9 (a) and (b), the g(r) plot at 867 K is a true evaluated data and the other temperature plots were incremented by a fixed integer for clarity. Figure 6-9(c) and (d) show the magnified region of the first peak in the g(r) curves for Al-12.5%Si and Al-12.5%Si-0.04%Sr alloys, respectively at various alloy temperatures. In Figure 6-9(c) and (d), it can be observed that for both the alloys the value of $g(r_1)$ decreases with increasing temperature and the position r_1 remains nearly constant and these observations show that the Fourier transformation of S(Q) carried out by Equation (1.6) were reliable and consistent. The g(r) plots of the other alloys were identical in behavior shown in Figure 6-9. Similar g(r) plots were obtained for all the alloy compositions investigated in this study.

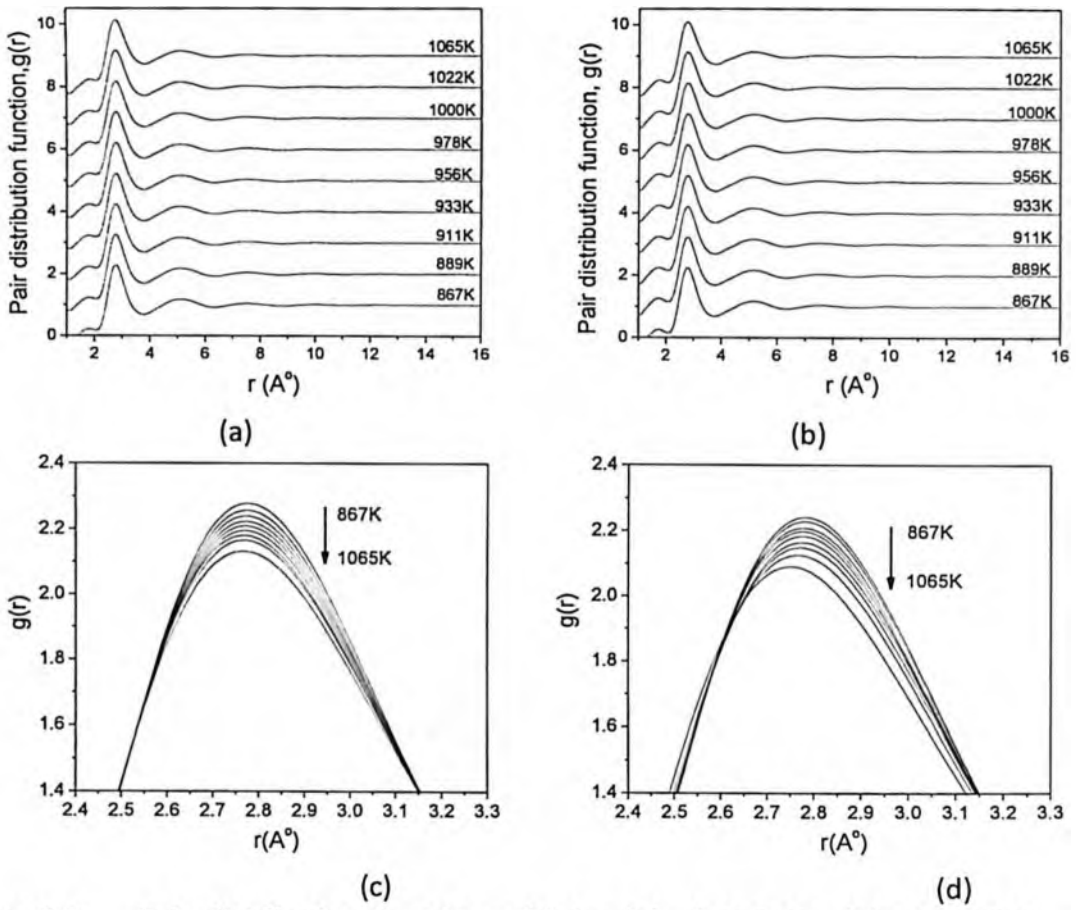


Figure 6-9: Pair distribution function, g(r) for (a) Al-12.5%Si, (b) Al-12.5%Si-0.04%Sr, (c) magnified region of first peaks shown in (a), and (d) magnified region of first peak shown in (b).

The peak height of the PDF represents the atomic ordering in the liquid alloy and the peak position of PDF represents the average nearest neighbor distance between any two atoms. Larger values of $g(r_1)$ represents higher ordering of atoms in the liquid alloy system. Figure 6-10 shows the value of $g(r_1)$ decreases with increasing liquid alloy temperature for each alloy composition (as expected), however, the addition of 0.04Sr to any alloy significantly decreases the value of $g(r_1)$ at any specific liquid alloy temperature. This shows that Sr addition to Al-Si hypoeutectic alloy causes a significant decrease in the ordering of atoms, specifically, the probability of finding the nearest atom at any given distance from an origin atom in the liquid is lower when 0.04 %Sr is added to the alloy melt. Further, Figure 6-11 shows that the addition of 0.04 %Sr to any alloy significantly reduces the value of r_1 (average nearest neighbor distance for any atom in the liquid) at all liquid alloy temperatures, thus establishing that trace level additions of Sr significantly changes the atomic structure of Al-Si hypoeutectic alloys.

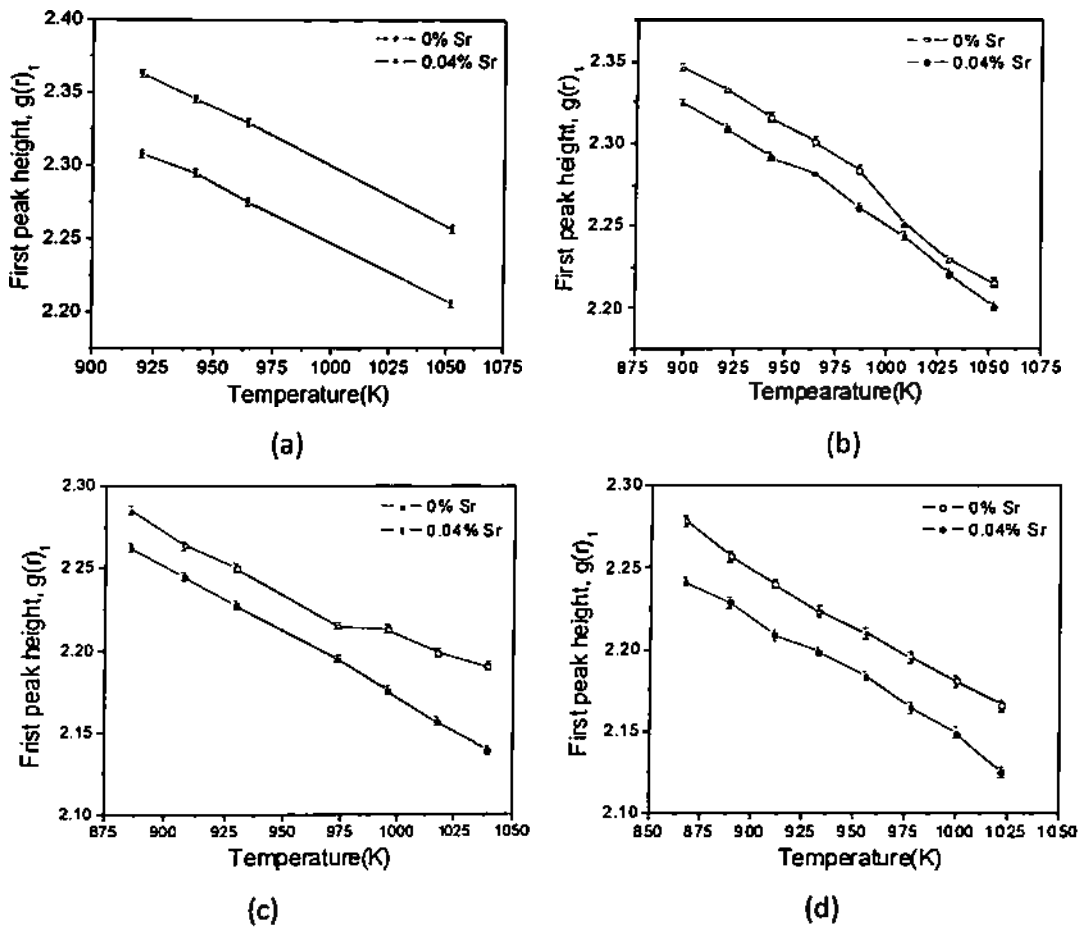


Figure 6-10: **Effect of Sr addition on the first peak height, $g(r_1)$ at various melt temperatures for, (a) Al-3% Si, (b) Al-7% Si, (c) Al-10%Si, (d) Al-12.5%Si.**

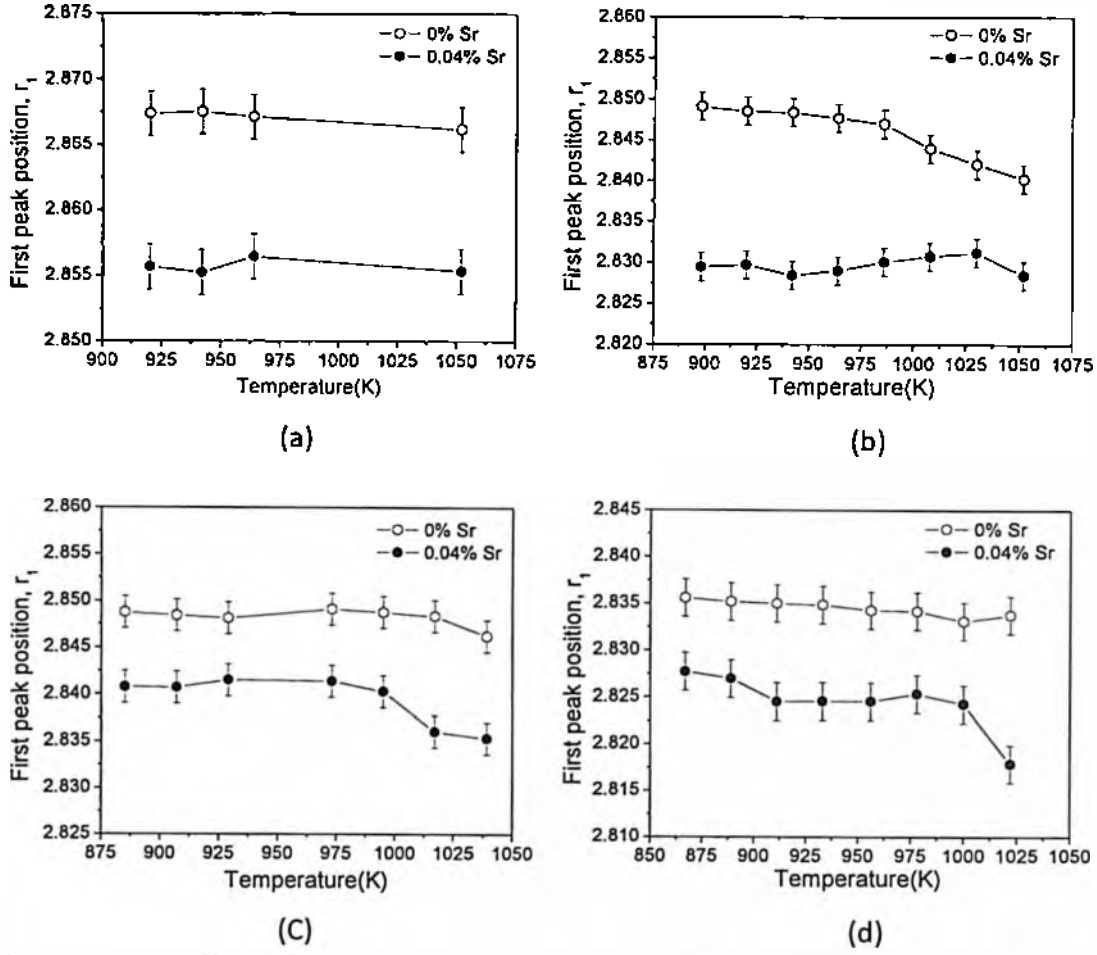


Figure 6-11: Effect of Sr addition on first peak position of PDF, r_1 at various melt temperatures for, (a) Al-3% Si, (b) Al-7% Si, (c) Al-10%Si, (d) Al-12.5%Si.

Figure 6-12 shows the radial distribution function, RDF as a function of r for various melt temperatures. The first peak height decreases with increasing melt temperatures as shown by the magnified image of RDF in Figure 6-12 (b).

Figure 6-13 (a) and (b) represents the total coordination number for Al-Si hypoeutectic alloys in unmodified and Sr modified conditions at various melt temperatures, respectively. The coordination number decreases with the addition of 0.04%Sr to any given alloy composition for any given melt temperature as shown by comparing Figure 6-13(a) and Figure 6-13(b). Figure 6-14 represents the change in coordination number as a function of melt temperature for each Al-Si hypoeutectic unmodified and Sr-modified alloy composition separately. Sr addition to the melt reduces the CN of the liquid alloy at any given temperature and Si level of the alloy as

shown in Figure 6-14. This presents conclusive evidence that the trace level Sr addition significantly changes the atomic structure, specifically the atom arrangement in the first coordination shell.

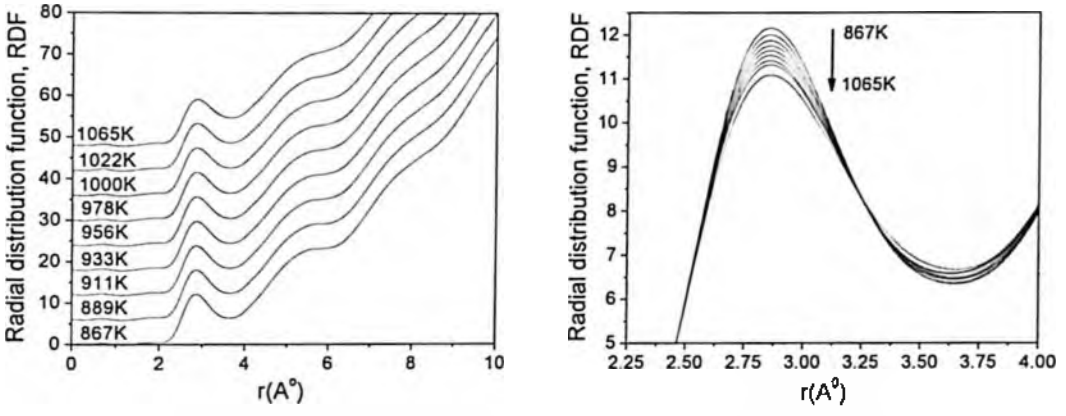


Figure 6-12: **The Radial distribution function, RDF Vs r for Al-12.5wt%Si (a) at various melt temperatures, (b) Magnified image of RDF showing the effect of melt temperature on peak heights of RDF.**

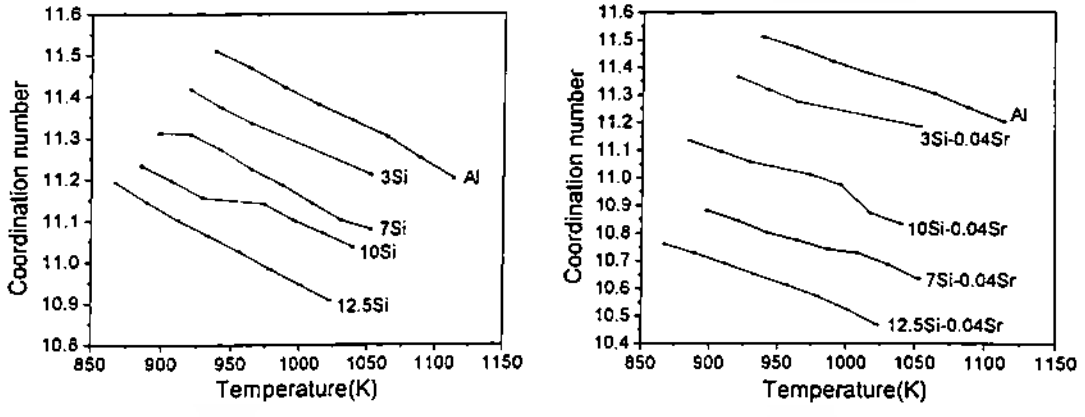


Figure 6-13: **Total coordination numbers of Al-Si hypoeutectic alloys at various melt temperatures for Al-Si hypoeutectic alloys; (a) Unmodified, (b) Sr modified.**

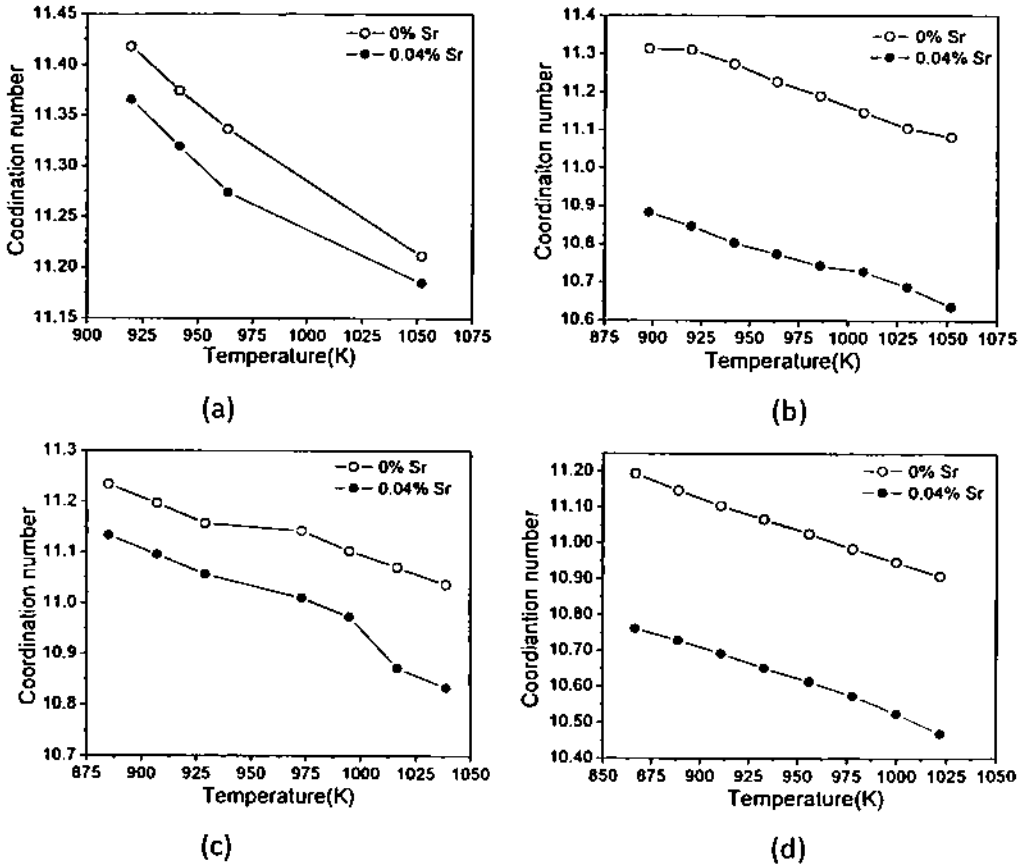


Figure 6-14: Effect of Sr addition on coordination number at various melt temperatures for, (a) Al-3% Si, (b) Al-7% Si, (c) Al-10%Si, (d) Al-12.5%Si.

To elaborate the significant effect of Sr on the second shell of the liquid alloy structure at all Si levels, Figure 6-15 was plotted to show the change in the ratio of the second peak to the first peak in the PDF curve, $\frac{r_2}{r_1}$. Figure 6-15 shows that this ratio increases for most of the alloy compositions at any given melt temperature when 04 %Sr is present in the alloy suggesting that the Sr addition delays the formation of the clusters of atoms as the alloy melt temperature decreases or in other words, at any alloy temperature, the size of atom clusters in the first two atomic coordination shells is significantly smaller when the alloy contains 0.04 %Sr. The trace level addition of Sr inhibits or delays the clustering tendencies of the liquid atoms which at the liquidus temperature lead to the formation of a critical nuclei. Specifically, the eutectic alloy which is mostly in contact with the primary Al dendrite phase at the eutectic temperatures would have significantly lower first and second shell coordination numbers (Figure 6-14(d) and Figure 6-15(d)) and hence, would have lower clustering

tendencies of atoms which in turn might delay the nucleation of the eutectic phases during solidification.

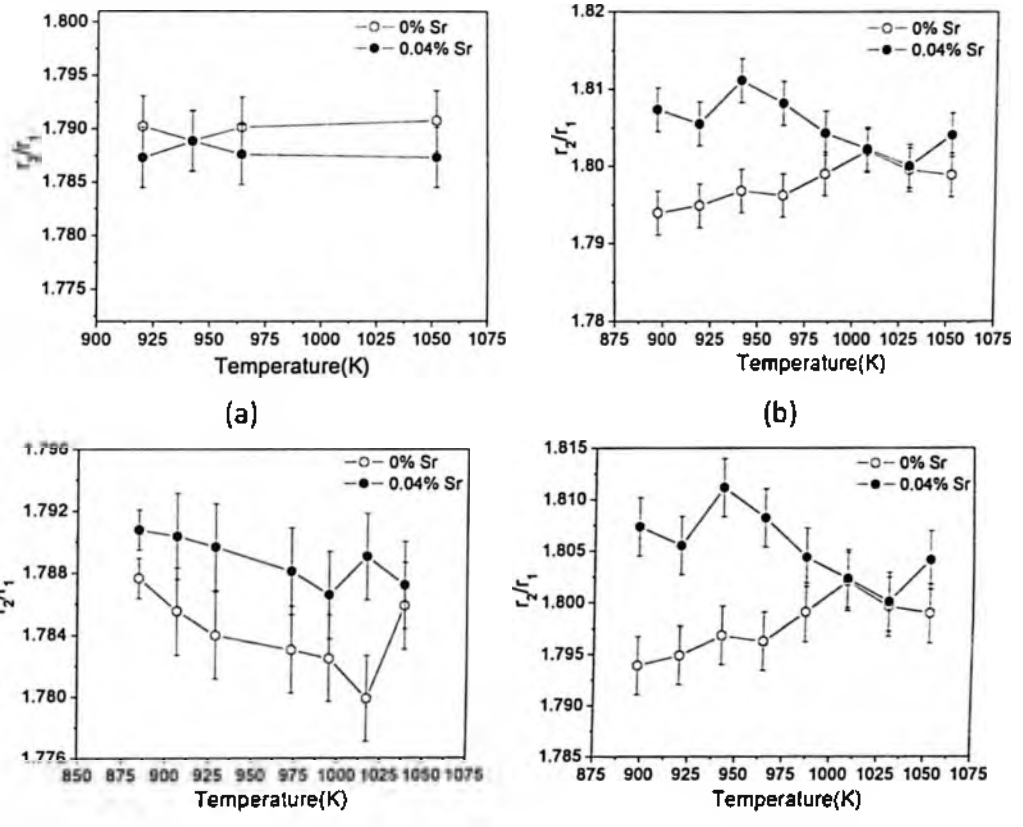


Figure 6-15: Effect of Sr addition on the ratio of r_2/r_1 of g(r) at various melt temperatures for, (a) Al-3% Si, (b) Al-7% Si, (c) Al-10%Si, (d) Al-12.5%Si.

Figure 6-16(a) and Figure 6-16(b) represent the packing density of unmodified and Sr modified Al-Si hypoeutectic alloys at various melt temperatures respectively. Figure 6-17 further emphasizes the significant role of trace levels of Sr addition in these alloys. The packing density is defined as the ratio of the total volume of the liquid to the total volume occupied by the atoms in the liquid [40], or in other words, the packing density in liquids is synonymous with the atomic packing fraction evaluated in the crystal structures of solids. Figure 6-17 shows that 0.04 %Sr addition to various Al-Si hypoeutectic liquid alloys markedly changes the packing density of atoms in the respective liquids at any given alloy temperature. This means that the number of atoms in a unit of volume of any alloy liquid decreases at any specific temperature when 0.04 %Sr was added to the alloy.

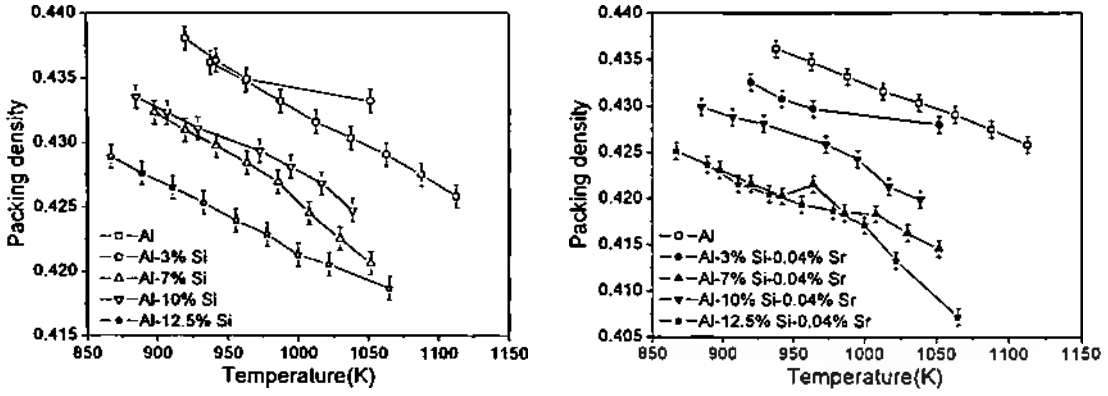


Figure 6-16: Packing density of Al-Si hypoeutectic alloys at a various melt temperature for (a) Unmodified, (b) Sr modified.

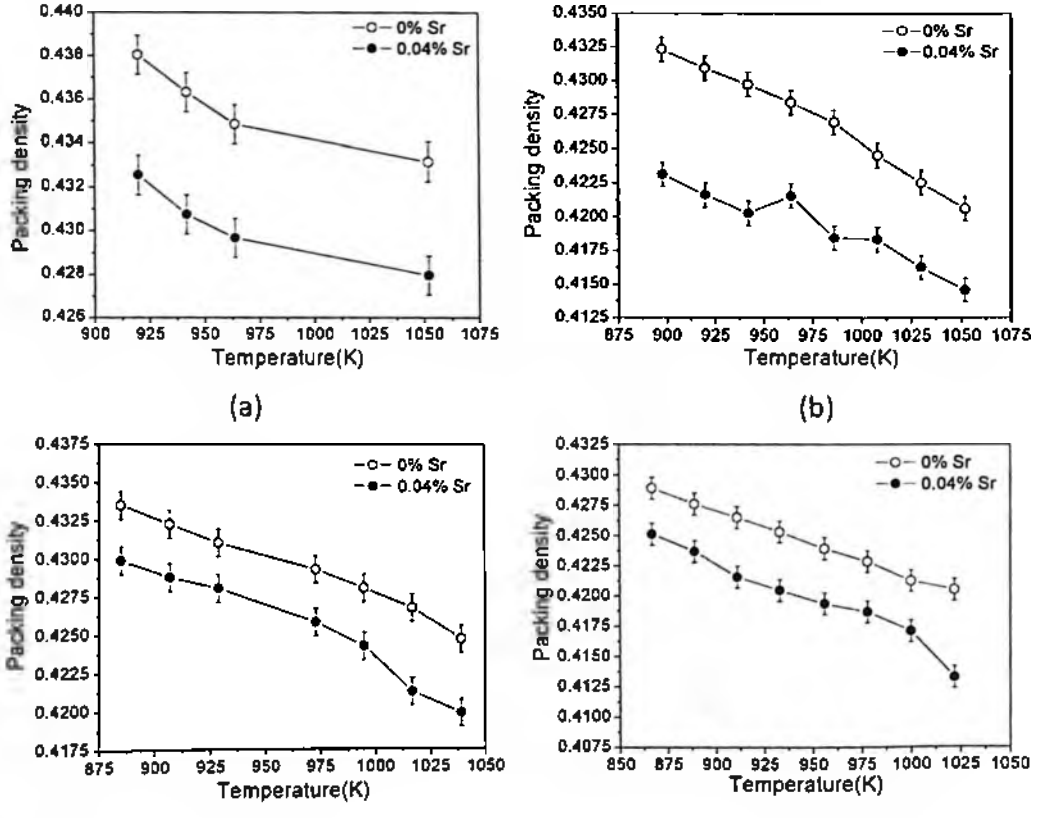


Figure 6-17: Effect of 0.04 % Sr addition on liquid atomic packing density at various alloy temperatures for Al-Si hypoeutectic alloys. (a) Al-3% Si, (b) Al-7% Si, (c) Al-10%Si, (d) Al-12.5%Si.

All the data for the total structure information obtained for the curves of SF, PDF, RDF, CN and PD for all the alloy compositions and temperatures are presented in APPENDIX A.

Figure 6-8 to Figure 6-17 show that Sr addition significantly alters the liquid structure of these alloys at all Si content and alloy melt temperatures. Addition of Sr causes more disorder in the alloy melt for all the alloy compositions. Further, Figure 6-14 to Figure 6-17 show that Sr addition to these alloys delay or inhibit the clustering tendencies of the atoms towards the nucleation event. When Sr is added to the eutectic alloy, atom clustering may not be sufficient at the eutectic temperature to effect a nucleation event and this would lead to undercooling of the inter-dendritic liquid to reach a labile temperature at which spontaneous crystallization of the Si phase would occur on the primary Al phases which acts as heat sinks during solidification. The evidence of spontaneous nucleation and the subsequent evolution of the eutectic phases have been presented earlier with sufficient experimental and analytical validations [13]. The results of this section on total liquid structure of Al-Si hypoeutectic alloys presents emphatic evidences to support the fact that the morphological modification of the eutectic phases in Al-Si hypoeutectic alloys begin with the marked changes to the atomic structure of the alloy liquid which leads to changes ir fundamental physical properties of these alloy liquids.

6.2 PARTIAL PAIR CORRELATION FUNCTIONS OF Al-Si HYPOEUTECTIC ALLOYS

The structure information obtained from the SF, PDF and RDF from high energy x-ray diffraction experiments as presented in the previous sub section provides only the total structural changes due to the addition of Sr to the Al-12.5%Si alloy melt. The limitation of studying the total structure information alone is that it cannot explain what pair of atoms is mostly affected by Sr additions. In order to understand the effect of Sr addition on the liquid structure of Al-Si hypoeutectic alloys, we have carried out RMC (Reverse Monte Carlo) analysis to obtain the partial pair correlations using the experimental data obtained from diffraction experiments. The procedure for the RMC analysis was explained in Chapter 4 of this dissertation. The results of these analyses are presented and discussed in this section.

The RMC analysis was carried out for all the diffraction data obtain in this study as presented in Table 3-2. The results of the RMC analysis showed that the modeling of the atoms was found to be valid for all the diffraction data. The eutectic alloy (Al-12.5Si) at 867 K has been used to demonstrate the validity of the RMC analysis in this section. The results for all the other alloys at various temperatures are presented in APPENDIX B of this dissertation.

Figure 6-18 shows the comparison of experimental S(Q) (Open circle) with the S(Q) obtained from RMC analysis (dark black line) at 867 K. The total structure factor from X-ray diffraction experiments were used as input data into the RMC analysis. The S(Q) from RMC analysis, $S_{RMC}(Q)$ is the summation of weighted partial structure factors (Equation (1.15)) and shown in Figure 6-18. The $S_{RMC}(Q)$ is in excellent agreement with the experimental S(Q) as shown in Figure 6-18. The weighting factors were calculated using Equation (1.13). It could be worth mentioning here that no smoothening of the data was necessary on the results obtained from the RMC analysis.

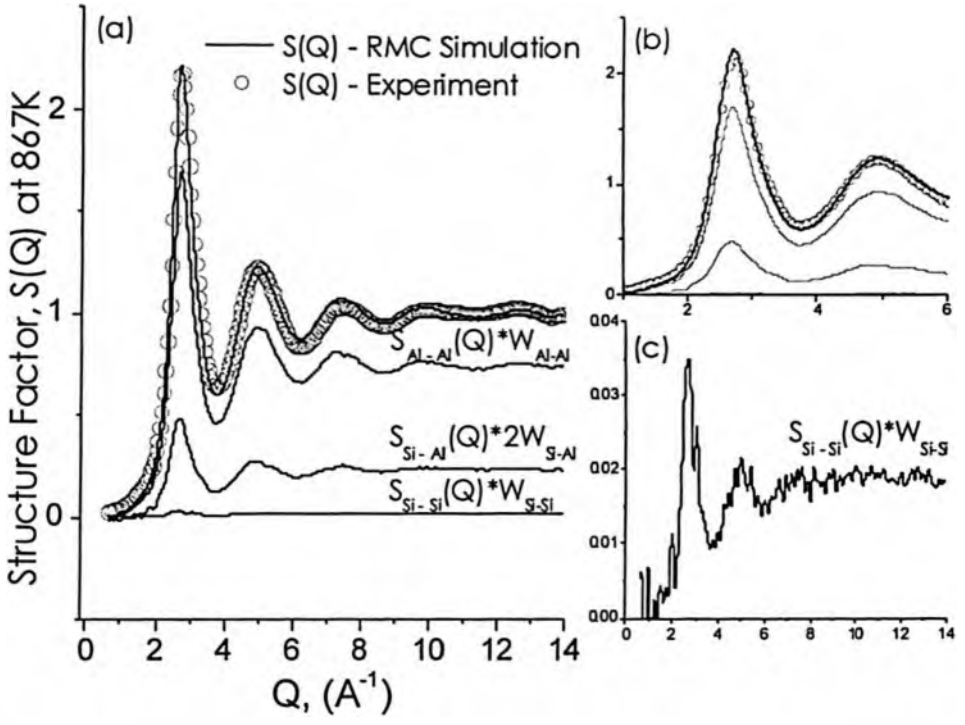


Figure 6-18: The variation of total and partial structure factors for Al-12.5wt%Si alloy at 867K. All three graphs have the same variables in the respective axes. (b) and (c) are magnified sections of (a) to show the first two peaks and the $S_{Si-Si}(Q)$, respectively.

The three PPDF, $g_{Si-Si}(r)$, $g_{Al-Si}(r)$ and $g_{Al-Al}(r)$ were obtained from the Fourier transformation of the three respective PSFs: $S_{Si-Si}(Q)$, $S_{Si-Al}(Q)$, $S_{Al-Al}(Q)$. Figure 6-19 shows the variation of total and partial pair distribution functions with r for Al-12.5%Si alloy at 867 K. All three graphs in Figure 6-19 have the same variables for the respective abscissae and ordinates. Figure 6-19(b) and Figure 6-19 (c) are magnified sections of Figure 6-19 (a) to show the first two peaks and the $g_{Si-Si}(r)$ respectively. The total PDF from RMC analysis is in good agreement with the experimental $g(r)$ as shown in Figure 6-19. No smoothening has been applied to the curves. The $g_{Si-Si}(r)$ is much smoother showing first and second peaks very clearly as compared to those reported by Wang et al [104]. The smoothness of the PPDF curves shown in Figure 6-19 may be attributed to the modified algorithm to carry out the RMC analysis developed in this study and described in Chapter 4.

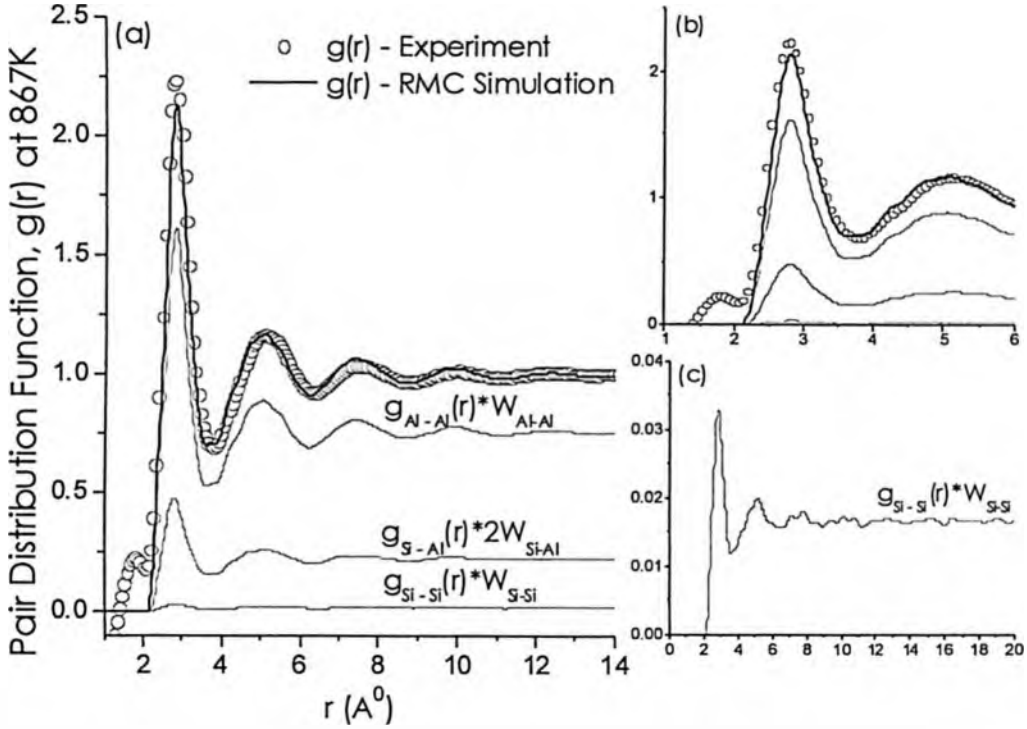


Figure 6-19: The variation of total and partial pair distribution functions with r, for Al-12.5wt%Si alloy at 867K. All three graphs have the same variables in the respective axes. (b) & (c) are magnified sections of (a) to show the first two peaks and the $g_{si-si}(r)$, respectively.

Figure 6-20 (a), Figure 6-20(b) and Figure 6-20(c) represents the typical PPDF of Al-Al, Al-Si and Si-Si pair of atoms obtained from RMC analysis for the Al-12.5%Si alloy at various melt superheat temperatures, respectively, to show that the nature of such data.

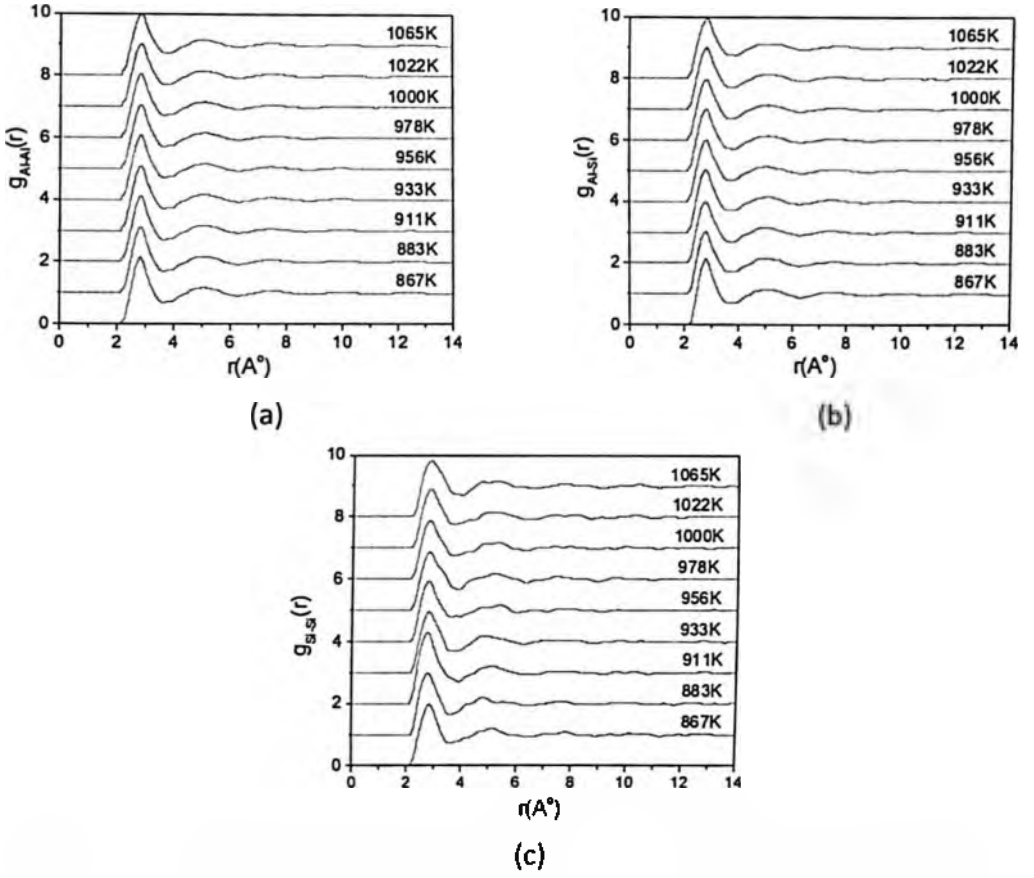


Figure 6-20: Partial pair distribution functions obtained from RMC for Al-12.5%Si at various melt temperatures (a) $g_{Al-Al}(r)$, (b) $g_{Si-Al}(r)$, (C) $g_{Si-Si}(r)$.

The first shell coordination number for Al-Al, Al-Si, and Si-Si pairs of atoms for a Al-12.5% Si alloy decrease with increasing melt temperatures as shown in Figure 6-21. Two methods as presented in Equations (1.16a) and (1.16b) were used to evaluate the CN shown in Figure 6-21. Since, the trend of the CN is identical by both the methods, the Equation (1.16b) was solely used for the other alloy systems to evaluate CN. Figure 6-22 shows the coordination number of Al-Al, Al-Si and Si-Si in unmodified Al-Si hypoeutectic alloys. The coordination number of Al-Al and Al-Si atoms decreases uniformly with increasing melt temperature, where as in case of Si-Si atoms the change is not uniform with temperature due to the small volume fraction of Si atoms (1200 atoms) in the total of 10,000 atoms used in the RMC analysis. Further, the coordination number of Al-Al atoms decreases with increasing silicon content from 0% to 12.5%, whereas, in case of Al-Si and Si-Si, the coordination number increases with increasing silicon content in the alloy at any given melt temperature as one would expect. The partial coordination numbers results in this study were compared with the results of abinitio molecular dynamics by Wang et al as shown in Figure 6-23. The data from Wang

et al [104] was digitized from the original publication and plotted along with the present study results. Wang et al [104] reported that the CN_{Al-Al} and CN_{Al-Si} decreases with increasing melt temperature as observed in the present study. In case of CN_{Si-Si}, they stated that the CN_{Si-Si} increases with increasing melt temperature though the plot shown in the publication presents no such trend, as shown in Figure 6-23(c). Even though, the trends look similar in both the studies, the actual CN values show a difference and this could be due to the method of evaluation in determining the r_{min} positions in RDF curve as well as due to the significant differences in the number density values used in both the studies.

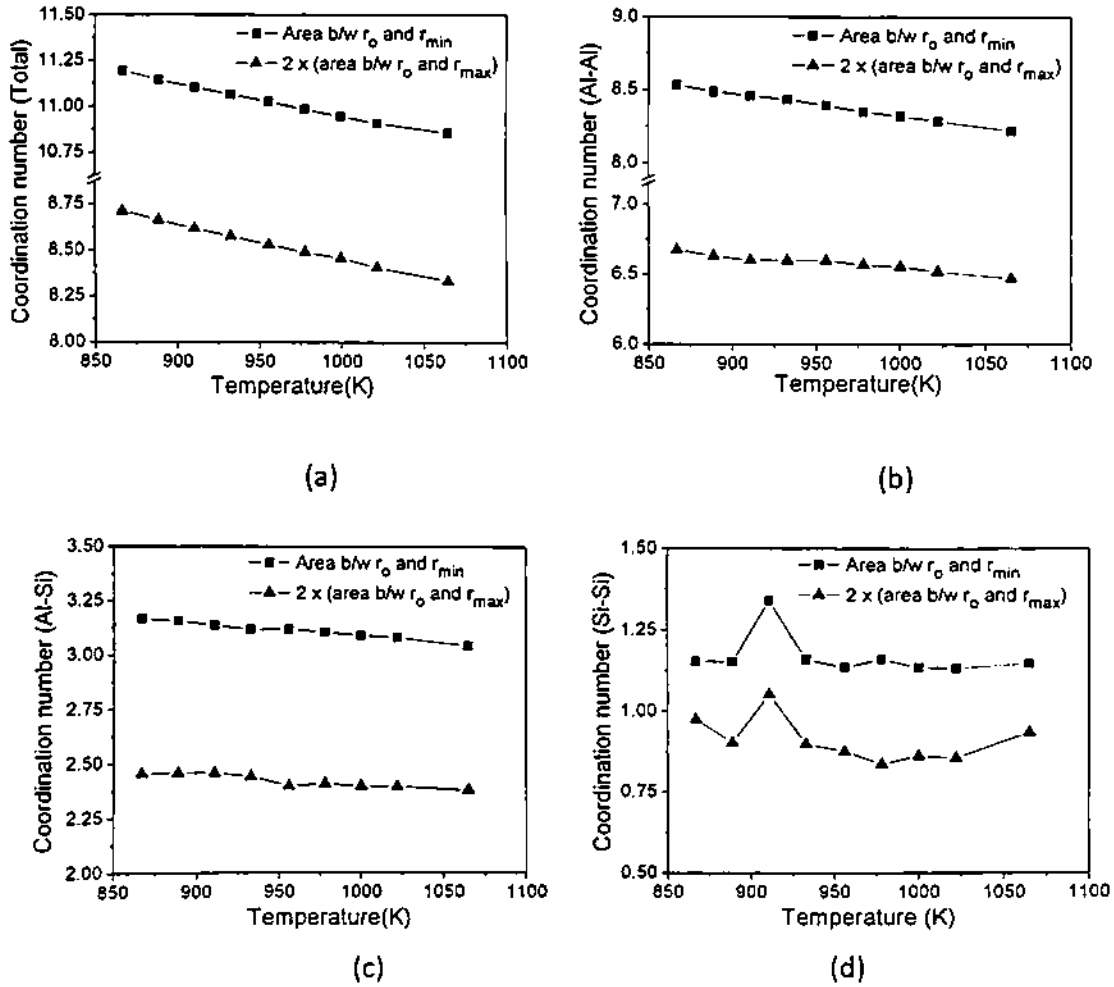
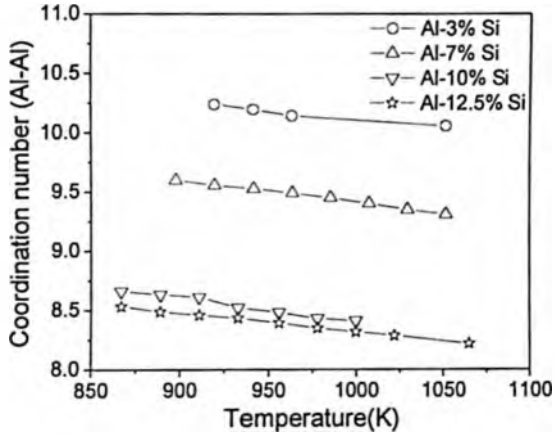
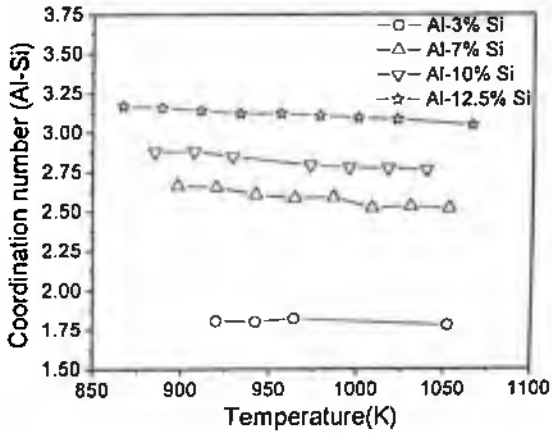


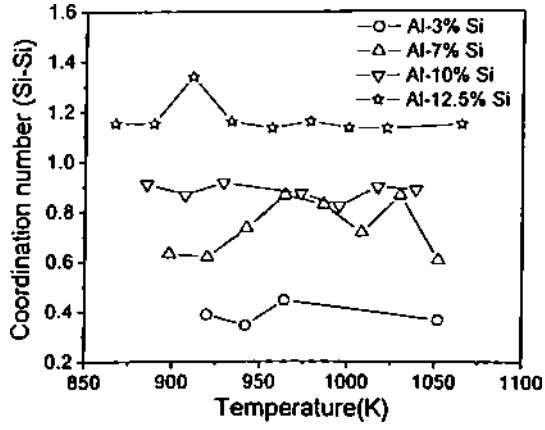
Figure 6-21: Coordination number as function of melt temperature for Al-12.5wt%Si. (a) Total, (b) Al-Al, (c) Al-Si, (d) Si-Si.



(a)



(b)



(c)

Figure 6-22: Coordination number as a function of melt temperature for Al-Si hypoeutectic alloys (a) Al-Al, (b) Al-Si, (c) Si-Si.

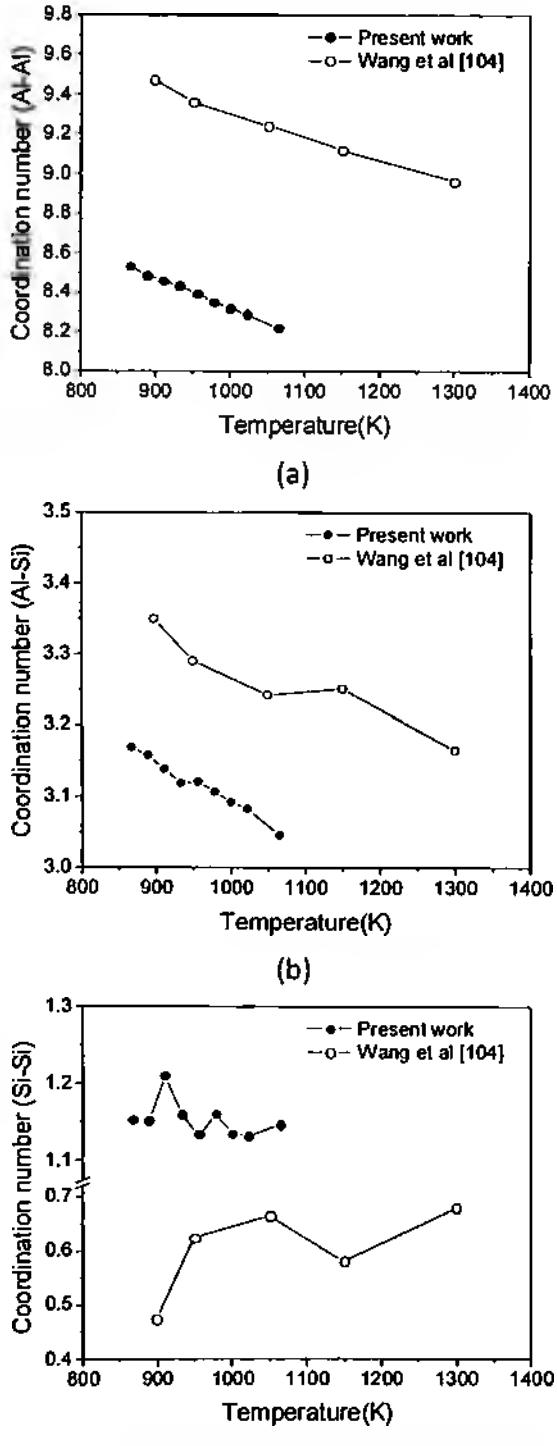


Figure 6-23: Comparison of partial coordination numbers, (a) Al-Al, (b) Al-Si, (c) Si-Si for Al-12.5%Si alloy with abinitio results by Wang et al [104].

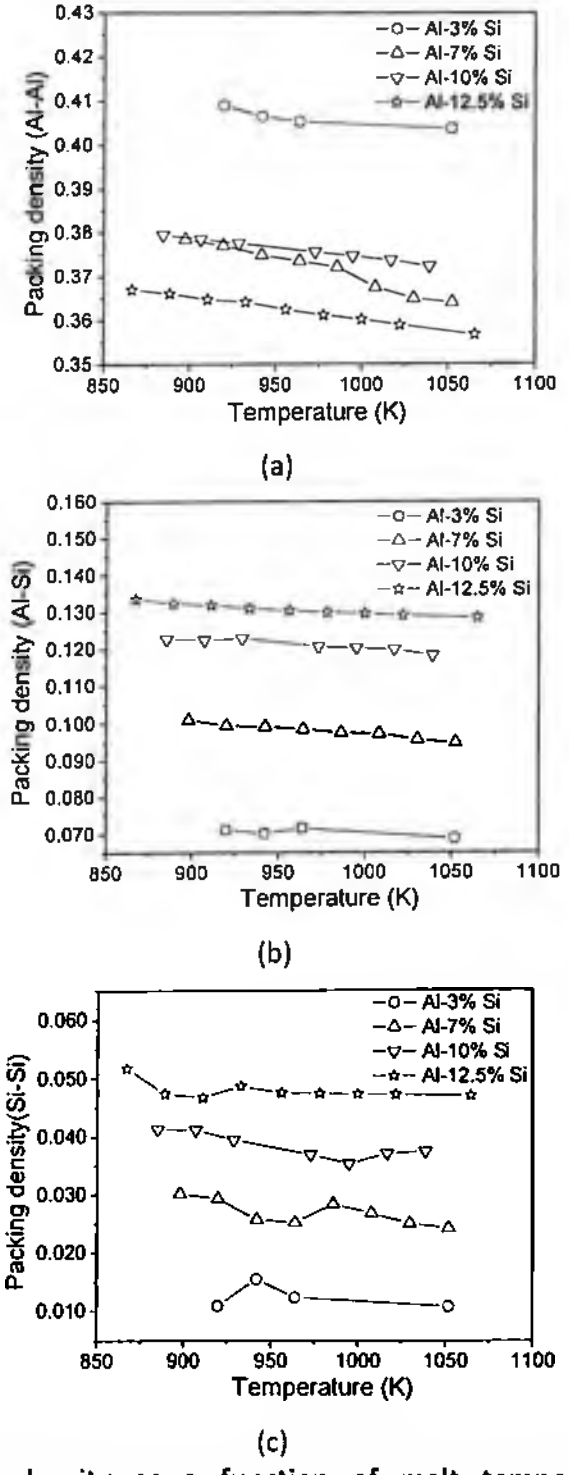


Figure 6-24: Packing density as a function of melt temperature for Al-Si hypoeutectic alloys (a) Al-Al, (b) Al-Si, (c) Si-Si.

Figure 6-24 shows the packing density of Al-Al, Al-Si and Si-Si pair of atoms in unmodified Al-Si hypoeutectic alloys at various melt temperatures. The packing density of Al-Al and Al-Si decreases uniformly with increase in melt temperature for any given alloy composition. However, in the case of Si-Si the variation in packing density with temperature is not smooth due to the small volume fraction of Si atoms (1200 atoms) in the total of 10,000 atoms used in the RMC analysis. Further, the packing density of Al-Al decreases with increasing silicon content at any given melt temperature, whereas, in the case of Al-Si and Si-Si packing density increases with increasing Si content in the alloy as one would expect.

6.2.1. Effect of Sr on the partial pair correlations of Al-Si hypoeutectic alloys

The effect of 0.04% addition of Sr on partial pair correlations of Al-Si hypoeutectic alloys obtained from RMC analysis of experimental diffraction data are presented in this section.

In order to show the effect of Sr, the $g_{Si\text{-}Si}(r)$, $g_{Al\text{-}Si}(r)$, $g_{Al\text{-}Al}(r)$ for Al-12%Si and Al-12.5%Si-0.04%Sr compositions were plotted separately at each melt temperature as shown in Figure 6-25 to Figure 6-27. All the plots were magnified between r values of 2Å to 4 Å to clearly show the effect of Sr on the first shell of atoms (first peak height and first peak position of g(r)). Figure 6-25, Figure 6-26and Figure 6-27 represent the $g_{Si\text{-}Si}(r)$, $g_{Al\text{-}Si}(r)$, $g_{Al\text{-}Al}(r)$ of Al-12.5%Si and Al-12.5%Si-0.04%Sr alloys respectively. It is evident from Figure 6-25 that the addition of strontium decreases the peak height of $g_{Si\text{-}Si}(r)$ at any given temperature. This effect is more pronounced at lower melt temperatures as represented by 867K, 889K and 911K. There is no significant effect of Sr on the peak height of $g_{Al\text{-}Si}(r)$ at any given melt temperature except at 867K where a marginal decrease in the first peak height is observed as shown in Figure 6-26. There is no discernable effect of Sr observed on the first peak height of $g_{Al\text{-}Al}(r)$ as shown in Figure 6-27.

Further, from Figure 6-25 to Figure 6-27, it was observed that the first peak position r_1 of $g_{Si\text{-}Si}(r)$ shifted to lower r values due to the addition of Sr to Al-Si alloy melt. However, this effect was not significant for Al-Si and Al-Al pair of atoms as compared to Si-Si atoms. APPENDIX B shows the numerical values for partial pair distribution function information such as first peak height, first peak position, second peak height and second peak position for Si- Si, Al-Si and Al-Al pair of atoms for all the alloy compositions at various melt temperatures used in this study. Table 6-2, Table 6-3 and Table 6-4 presents the numerical values for the r_2/r_1 ratio of Si-Si, Al-Si and Al-Al pair of atoms obtained from RMC analysis for Al-7%Si, Al-10%Si and Al-12.5%Si alloys in

unmodified and Sr modified conditions. The ratio of r_2/r_1 for Si-Si pair of atoms increased with Sr addition to the alloy melt as compared to Al-Si and Al-Al as shown in Table 6-2, Table 6-3 and Table 6-4 . Further, it can be observed that this effect is more significant at lower melt temperature near the liquidus temperature of the alloy.

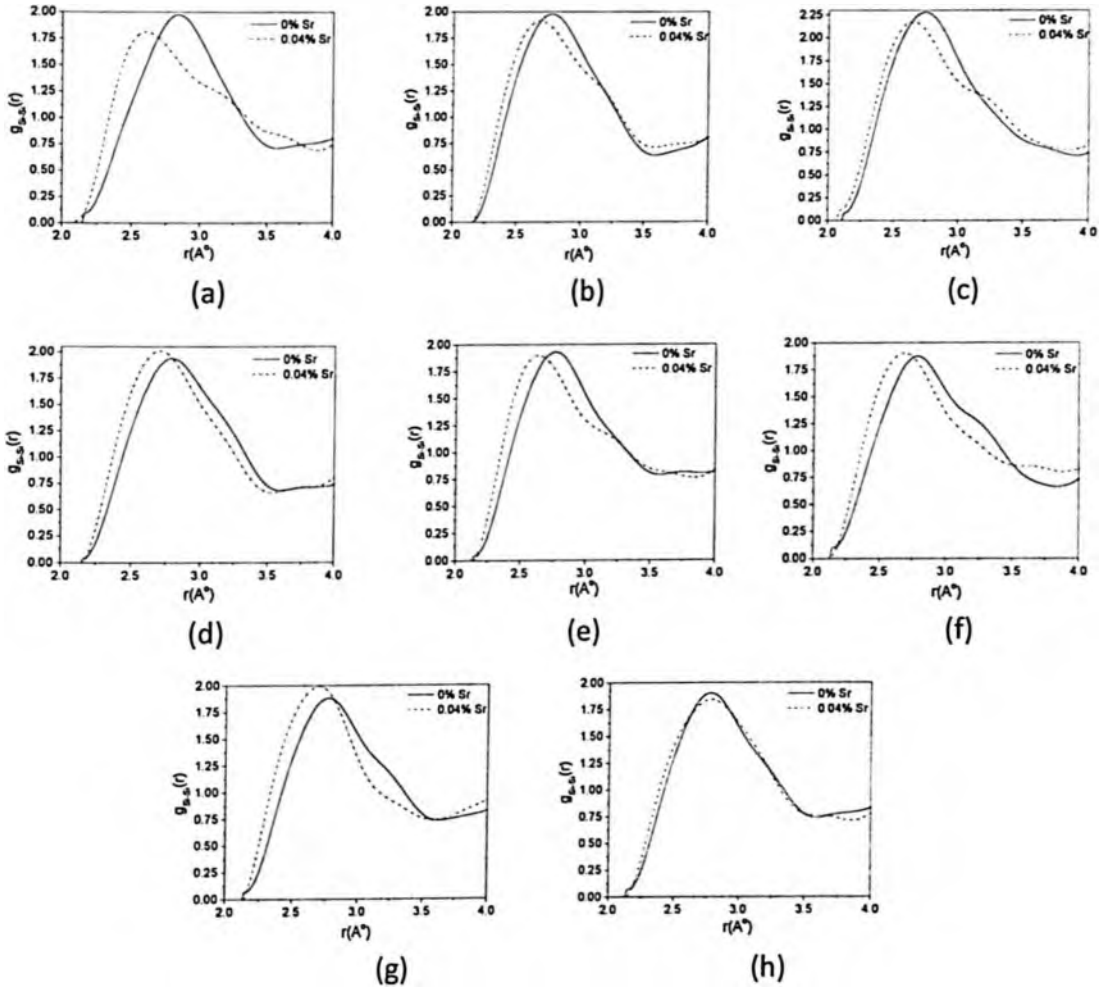


Figure 6-25: **Effect of Sr on the partial pair distribution function $g_{Si\text{-}Si}(r)$ at various melt temperatures for Al-12.5%Si eutectic alloy (a)867K, (b)889K, (c)911K, (d)933K, (e)956K, (f)978K, (g)1000K, (h)1022K.**

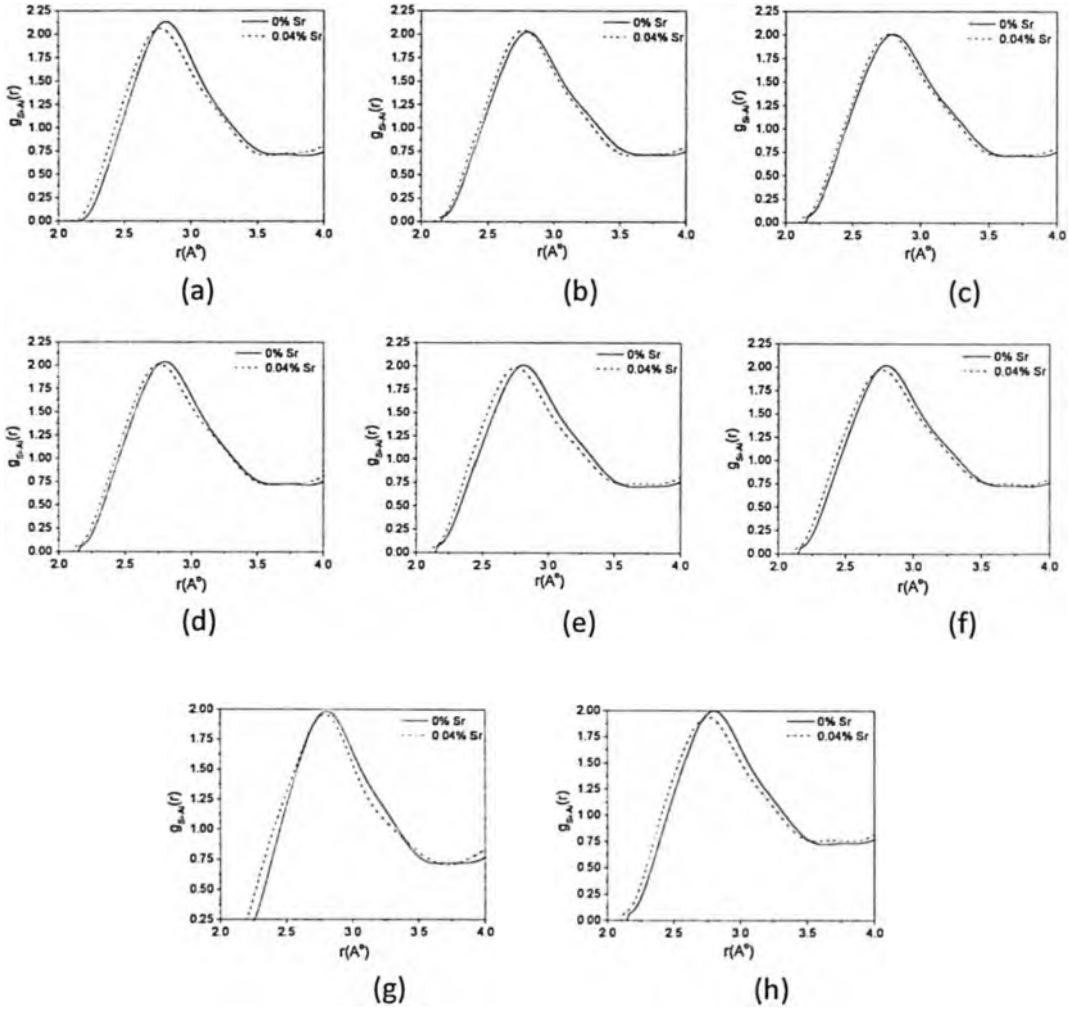


Figure 6-26: **Effect of Sr on the partial pair distribution function $g_{Si\text{-}Al}(r)$ at various melt temperatures for Al-12.5%Si eutectic alloy (a)867K, (b)889K, (c)911K, (d)933K, (e)956K, (f)978K, (g)1000K, (h)1022K.**

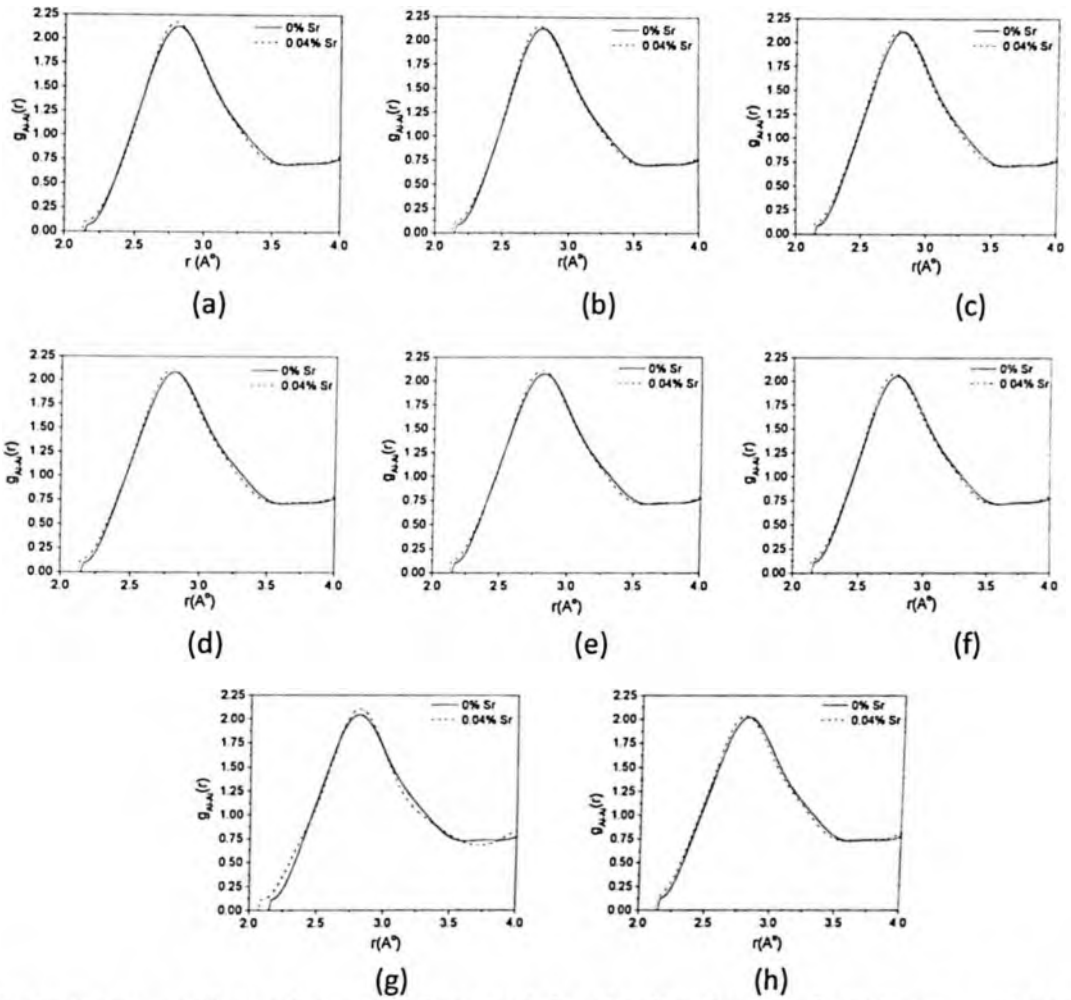


Figure 6-27: Effect of Sr on the partial pair distribution function $g_{Al\text{-}Al}(r)$ at various melt temperatures for Al-12.5%Si eutectic alloy (a)867K, (b)889K, (c)911K, (d)933K, (e)956K, (f)978K, (g)1000K, (h)1022K.

The first shell coordination number of Si-Si, Al-Si and Al-Al pairs of atoms for Al-Si hypoeutectic alloys were evaluated by integrating the area under the respective RDF curves between r_0 and r_{min} as presented in Equation (1.16)(b). The coordination number of Si-Si and Al-Si and Al-Al pair of atoms for Al-Si alloys in unmodified and Sr-modified alloys are shown in Figure 6-28, Figure 6-29 and Figure 6-30 respectively. The coordination number of Al-Al, Al-Si decreases uniformly with increasing melt temperature. However, the effect of temperature on the coordination number of Si-Si was observed to be non uniform with lots of scatter in the data. Further, addition of 0.04%Sr to any given Al-Si alloy composition decreases the coordination number of Al-Al, Al-Si and Si-Si pair of atoms at any given melt temperature as shown in Figure 6-28(b), Figure 6-29(b) and Figure 6-30(b). In order to show the effect of Sr on the coordination

number of partial pair of atoms in a discernable way, separate plots were made for Al-12.5%Si and Al-12.5%Si-0.04%Sr alloy as shown in Figure 6-31. It was observed that the addition of 0.04%Sr decreases the coordination number of Al-Al, Al-Si and Si-Si atoms at any given melt temperature as shown Figure 6-31(a), Figure 6-31(b) and Figure 6-31(c) respectively. Further, it was observed that the there were abnormal behavior of CN_{si-si} shown in Figure 6-31(c) in both the unmodified and modified conditions; wherein the random behavior of the curves were notoriously identical in both the unmodified and Sr-modified alloy and a viable explanation for such a unique behavior could not be presented without further investigation.

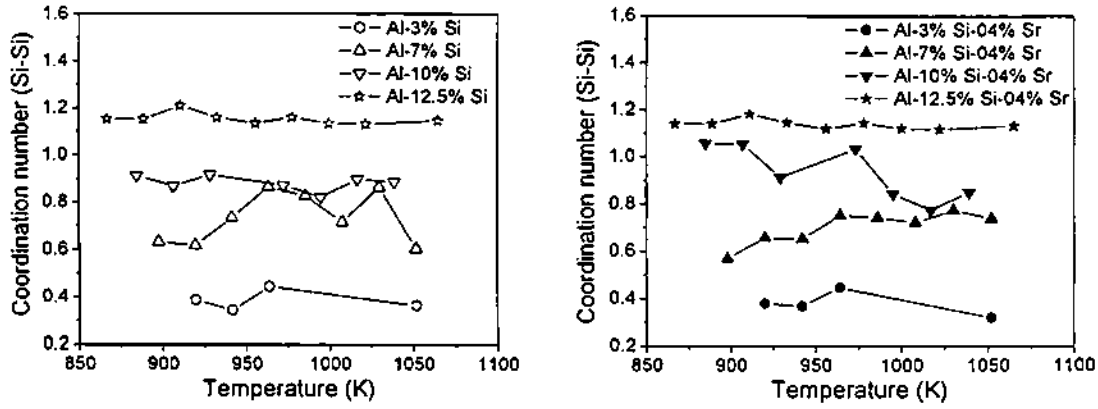


Figure 6-28: Coordination number of Si-Si atoms for Al-Si hypoeutectic alloys, Unmodified alloys, (b) 0.04% Sr modified alloys.

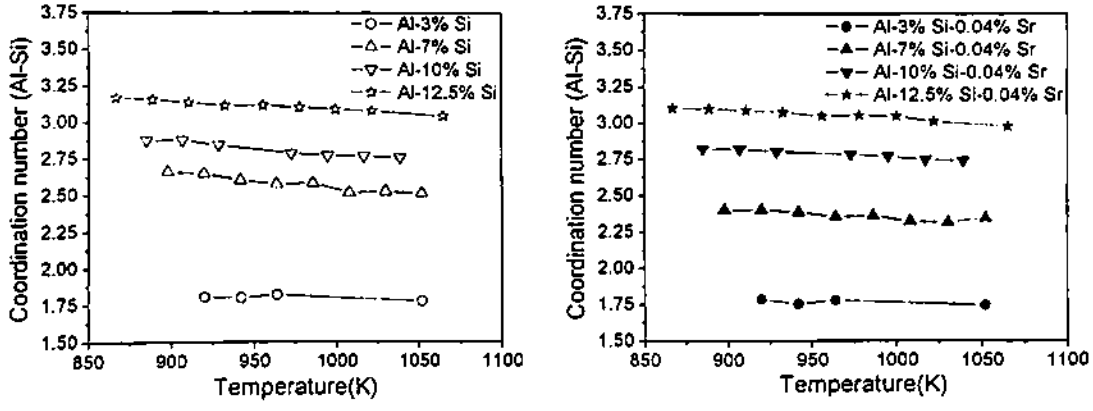
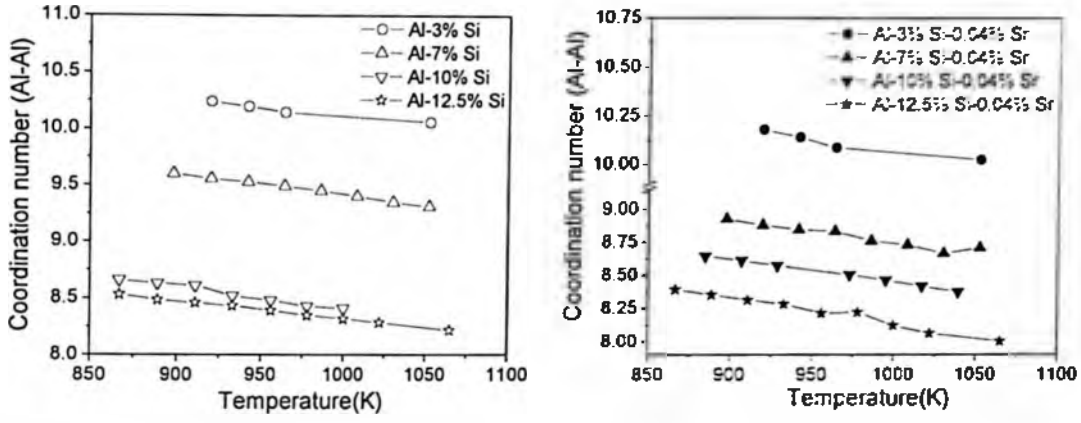


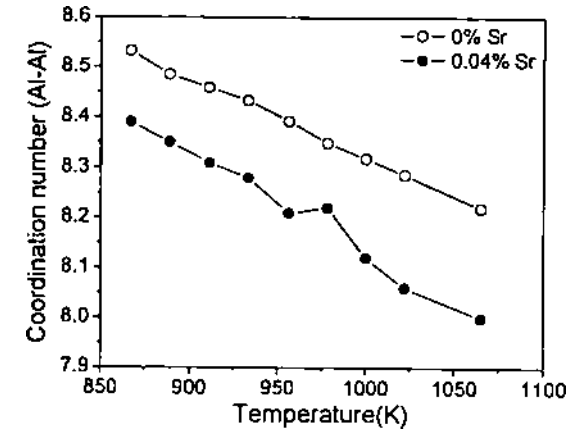
Figure 6-29: Coordination number of Al-Si atoms for Al-Si hypoeutectic alloys, (a) Unmodified alloys, (b) 0.04% Sr modified alloys.



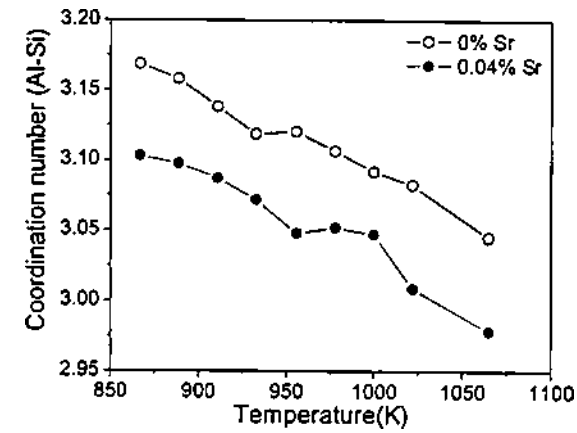
(a) (b)

Figure 6-30: Coordination number of Al-Al atoms for Al-Si hypoeutectic alloys, (a) Unmodified alloys, (b) 0.04% Sr modified alloys.

The effect of Sr on the packing density of Al-Al, Al-Si and Si-Si pair of atoms of Al-12.5%Si has been presented in Figure 6-32 . The packing density for Al-Al, Si-Al decreases uniformly with increase in melt temperature as shown in Figure 6-32(a) and Figure 6-32(b) respectively. However, in the case of Si-Si, the decrease in packing density with increase in melt temperature is not uniform. The reason for abnormal variation in properties of Si-Si pair of atoms may be due to the presence of less number of Si atoms in the RMC analysis compared to the number of Al-Al and Al-Si atom pairs. Addition of 0.04% Sr decreases the PD of Al-Al, Al-Si and Si-Si pair of atoms at any given melt temperature. The effect was considerably small in case of Al-Al as compared to Al-Si and Si-Si pair of atoms.



(a)



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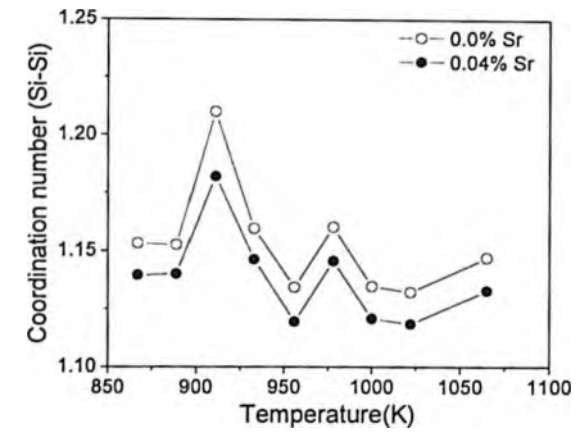
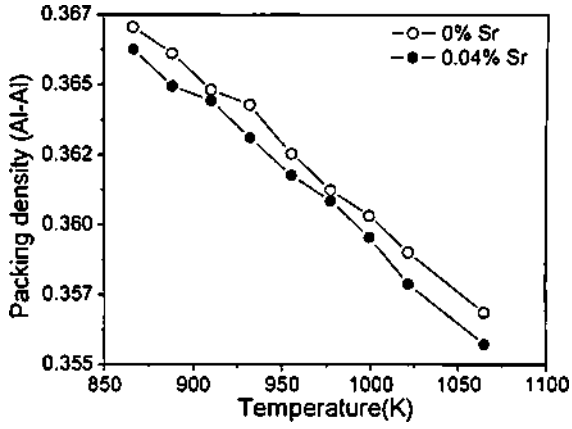
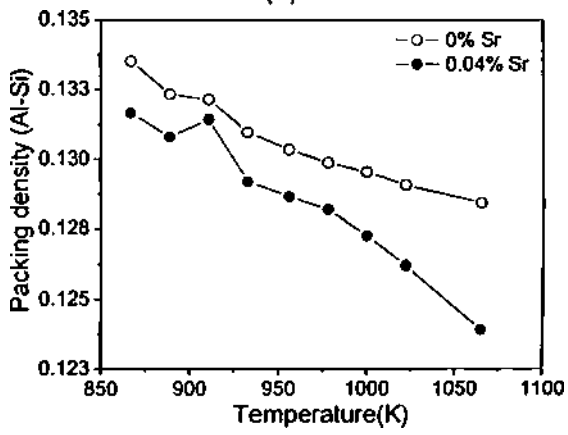


(c)

Figure 6-31: Effect of Strontium on the first shell coordination number of Al-12.5%Si alloy at various melt temperatures for (a) Al-Al, (b)Al-Si, (c) Si-Si.



(a)



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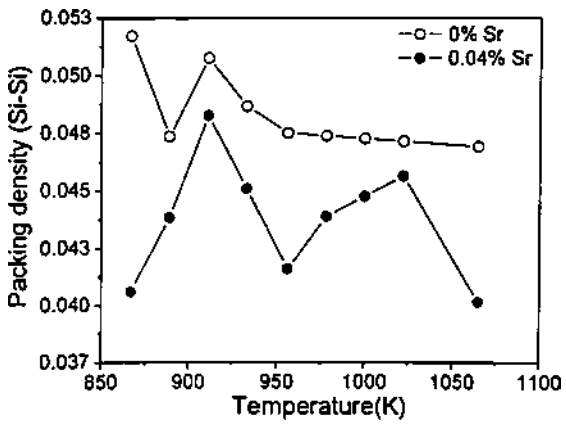


(c)

Figure 6-32: Effect of Strontium on the packing density of Al-12.5%Si alloy at various melt temperatures for (a) Al-Al, (b) Al-Si, (c) Si-Si.

Table 6-2: **The ratio of r_2/r_1 of Si-Si, Al-Si, Al-Al for Al-7%Si & Al-7%Si-0.04%Sr alloys obtained from RMC analysis (Sr in brackets represents the information for alloy with Strontium).**

	$(r)_2/(r)_1$					
Temp (K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
898	1.71	1.83	1.84	1.89	1.82	1.78
920	1.79	1.86	1.83	1.86	1.82	1.81
942	1.85	1.84	1.83	1.80	1.83	1.81
964	1.96	1.84	1.83	1.93	1.83	1.81
986	1.79	1.84	1.83	1.94	1.84	1.82
1008	1.87	1.84	1.84	1.96	1.85	1.82
1030	1.91	1.86	1.84	1.85	1.86	1.79
1052	1.91	1.87	1.85	1.94	1.84	1.83

Table 6-3: **The ratio of r_2/r_1 of Si-Si, Al-Si, Al-Al for Al-10%Si & Al-10%Si-0.04%Sr alloys obtained from RMC analysis (Sr in brackets represents the information for alloy with Strontium).**

	$(r)_2/(r)_1$					
Temp(K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
885	1.82	1.80	1.80	1.95	1.80	1.80
907	1.84	1.79	1.80	1.82	1.81	1.80
929	1.82	1.81	1.80	1.97	1.80	1.80
973	1.80	1.81	1.81	1.89	1.82	1.80
995	1.85	1.82	1.80	2.03	1.81	1.80
1017	1.81	1.81	1.80	1.87	1.81	1.80
1039	1.83	1.82	1.80	1.94	1.81	1.81

Table 6-4: **The ratio of r_2/r_1 of Si-Si, Al-Si, Al-Al for Al-12.5%Si & Al-12.5%Si-0.04%Sr alloys obtained from RMC analysis (Sr in brackets represents the information for alloy with Strontium).**

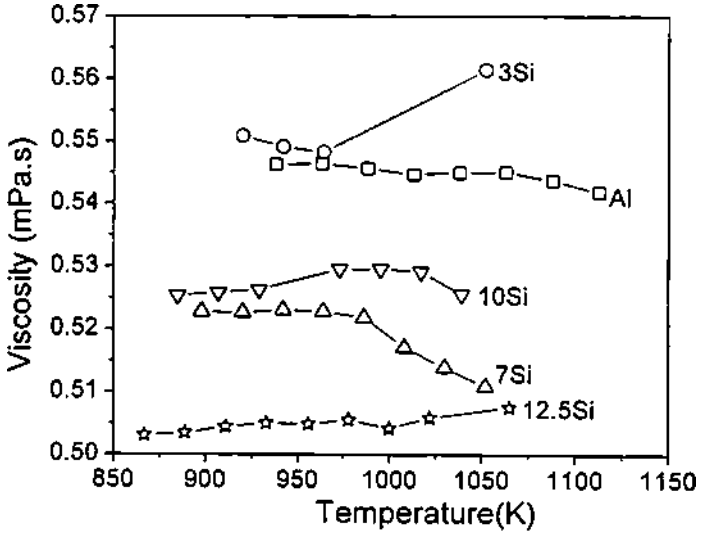
	$(r)_2/(r)_1$					
Temp (K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
867	1.79	1.81	1.79	1.89	1.82	1.81
889	1.84	1.81	1.79	1.86	1.83	1.80
911	1.80	1.80	1.81	1.79	1.82	1.82
933	1.77	1.81	1.79	1.78	1.83	1.80
956	1.86	1.81	1.79	1.91	1.83	1.80
978	1.85	1.81	1.79	1.88	1.82	1.80
1000	1.84	1.81	1.79	1.89	1.82	1.80
1022	1.84	1.81	1.79	1.82	1.82	1.80
1065	1.81	1.81	1.78	1.90	1.83	1.79

The addition of 0.04%Sr to any given alloy composition resulted in decreasing the peak height of g(r), coordination number and packing density of Al-Al, Al-Si and Si-Si atom pairs. It was also observed that Sr results in an increase in the disorder of the melt showed by the decrease in the first peak height and first peak positions of the respective PPDF. The effect of Sr was more significant on Si-Si atom pairs especially at low melt temperatures as compared to Al-Si and Al-Al pair of atoms showing that the 0.04wt% Sr addition to the Al-Si hypoeutectic alloy melt significantly alters the atom distribution and arrangement of the Si atoms causing a change to the Al-Al, Al-Si and Si-Si atom pair structures. Further the ratio of r_2/r_1 for Si-Si pair of atoms increases with Sr addition there by pushing silicon atoms farther away from the origin atom with addition of Sr to the Al-Si alloy melt. This kind of behavior represents that the Si-Si pair of atoms becomes more disordered in the Sr-modified alloy melt.

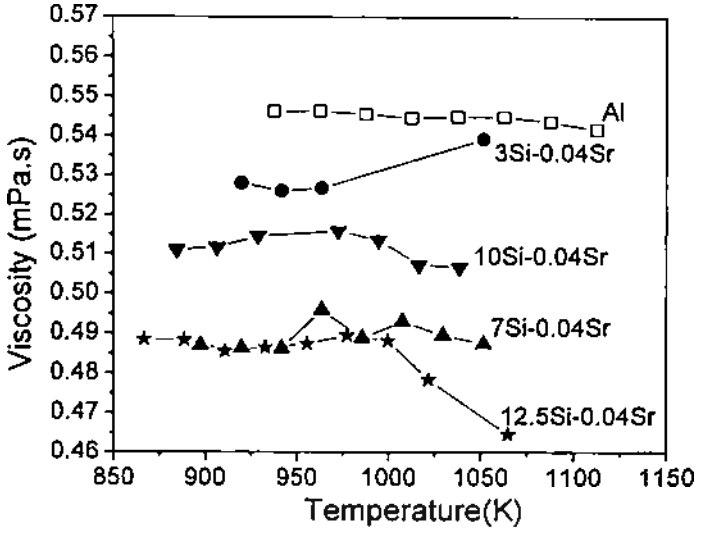
6.3 VISCOSITY OF PURE Al AND Al-Si HYPOEUTECTIC ALLOYS

In this section, the results of viscosity of pure Al and Al-Si hypoeutectic alloys evaluated by Hard Sphere theory and semi-empirical approach using atomic structure information is presented and discussed. The effect of Sr addition on the viscosity of Al-Si hypoeutectic alloys is also presented.

Figure 6-33 shows the variation of viscosity of Al and Al-Si alloys as a function of melt temperature for unmodified and modified alloys evaluated by using the hard sphere theory. It is evident from Figure 6-33 that the viscosity by the hard sphere method did not follow any trend because of competing effects of PD and molar volume factors as evaluated from Equation (1.28). Further, it can be observed that the viscosity increases with increasing melt temperature which is against the laws of physics which dictates an exponential decrease in melt viscosity with increasing temperature.



(a)



(b)

Figure 6-33 Viscosity of Al and Al-Si hypoeutectic alloys at various melt temperatures evaluated by Hard Sphere theory, (a) unmodified alloys, (b) Sr modified alloys.

Due to the lack of accuracy in the viscosity evaluated by the hard sphere theory, the semi empirical model presented in Section 1.5.5 was used to evaluate melt viscosity and is believed to be a more representative of the melt behavior.

Figure 6-34 and Figure 6-35 represents the viscosity of Al and Al-Si alloys evaluated by semi empirical approach using Equation (1.35). Figure 6-34 represents the variation of melt viscosity for pure Al and various hypoeutectic alloy compositions in unmodified and Sr-modified conditions. The alloy melt viscosity decreases with increasing temperature for all the hypoeutectic alloy compositions. Further, with increasing silicon content in Al melt, the viscosity decreases at any given temperature. Figure 6-35 shows the effect of 0.04% Sr addition on the viscosity of various Al-Si hypoeutectic alloys at various melt temperatures. It is evident from the Figure 6-35(a),(b),(c) and (d) that for any given alloy composition, the Sr addition results in decreasing the viscosity at any given temperature. Further, it can be observed that the effect of Sr addition is more pronounced at lower Si levels of 3 and 7 wt%.

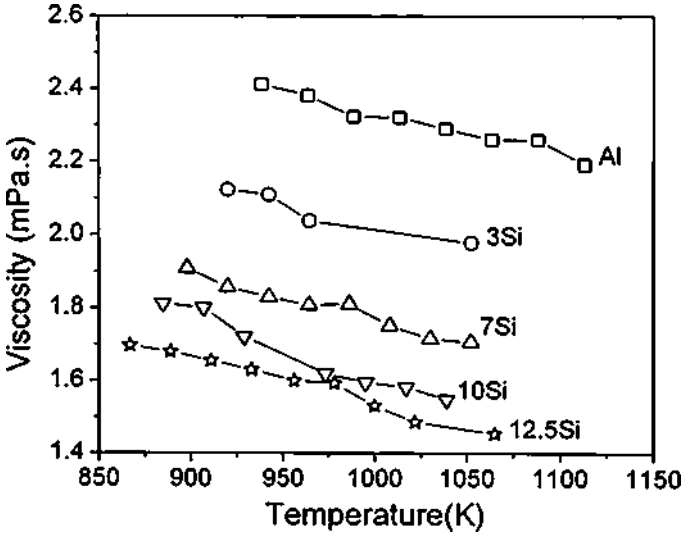
The values used for β (correction factor), V_m (Molar Volume) and v_0 (constant) are presented in Table 6-5. The β values for Al and Si were obtained from Iida et al [41]. The β-vales for alloy compositions were evaluated as a weighted average of the β for the respective pure metals.

Table 6-5: β, V_m, v_0 values for Al and Al-Si hypoeutectic alloy compositions

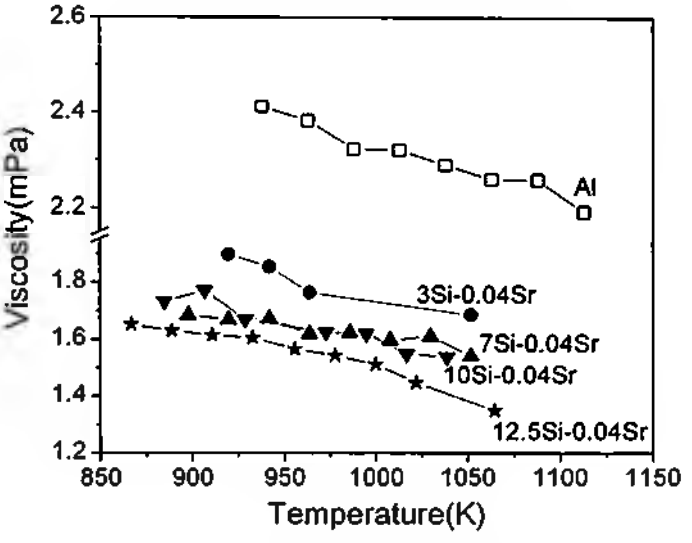
Alloy	Al	Al-3Si	Al-7Si	Al-10Si	Al-12.5Si	Si
β -values	0.52[1]	0.5159	0.5105	0.5065	0.5031	0.38[1]
V_m	9.9E-06	1.28E-05	1.21E-05	1.18E-05	1.11E-05	--
v_0	4.09E12	3.87E12	3.81E12	3.79E12	3.75E12	--

We assume that in Equation (1.35), P(A) as the P(T) of Al and P(B) as the P(T) for Si. Since P(T) is dependent on temperature, P(A) and P(B) for a particular composition of Al-Si at a given melt superheat temperature above the alloy liquidus temperature was evaluated by assuming a similar melt superheat temperature above the melting points of Al and Si, respectively.

Iida et al used the boiling point of Al, $T_{b(Al)}$ = 2333K to evaluate P(T) for pure Al using Equation (1.33). Using the same boiling point, the viscosity evaluated by the semi-empirical approach was 2.21 mPa.s at 938K and this value verifies the viscosity of 2.2 mPa.s at 943K evaluated by the Born-Green theory using the potential functions and pair distribution functions [40], thus, showing that the semi-empirical approach is fairly reliable. However, recent findings show that the boiling point of pure Al, $T_{b\ (Al)}$ = 2467.15K [105]. We have used this value for $T_{b(Al)}$ in this study to obtain the P(T) values at various superheat temperatures.



(a)



(b)

Figure 6-34: Viscosity of Al and Al-Si hypoeutectic alloys at various melt temperatures by semi empirical model, (a) unmodified alloys, (b) Sr modified alloys.

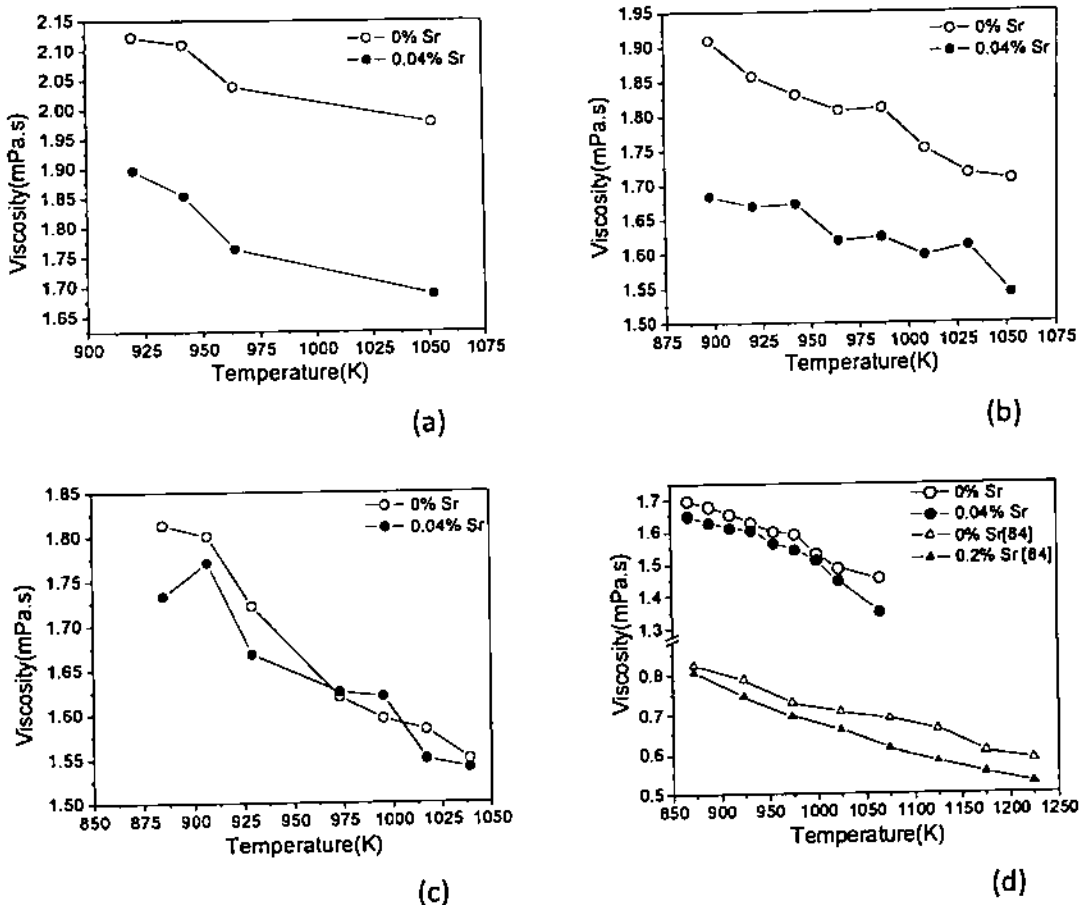


Figure 6-35: Effect of Strontium on the melt viscosity of Al-Si hypoeutectic alloys at various melt temperatures for (a) Al-3%Si, (b) Al-7%Si, (c) Al-10%Si, (d) Al-12.5%Si.

Viscosity is a structure sensitive property and the results obtained from the liquid atomic structure measurements aid in understanding the variation of viscosity of Al-Si alloys as function of melt superheat and silicon content. Similar behavior can be observed for packing density and coordination number of these hypoeutectic alloys. The free volume in the liquid alloy increases with increasing silicon content as shown by the decrease in the respective packing density and coordination number values, and thus, increasing the free mobility of atoms in the liquid resulting in a decrease in the frictional resistance between atom pairs which decreases melt viscosity. In a binary alloy systems with compound forming tendencies, viscosity increases with increasing of solute content [106,107]. Alloys with compound forming tendencies exhibit a pre-peak before the first large peak in the low Q region of the structure factor curve, S(Q) versus Q. As seen in Figure 6-7, Al-Si alloys do not exhibit such compound forming tendencies. In this study, further, we observed that the Sr addition results decreases the melt viscosity of Al-Si hypoeutectic alloys. Similar observations were found experimentally by Xigui et al

[84] and they also observed that the Sr addition decreases the viscosity of Al-Si alloys. as shown in Figure 6-35(d).

6.3.1. Limitations of Viscosity Evaluation

The following are the limitations in using the semi empirical method to evaluate the viscosity of Al-Si hypoeutectic alloys.

- The liquid alloy in this theory was treated as a Newtonian liquid. This assumption may not be true as recent research [14, 89, 90, 108] has shown that liquid metals, specifically the Al-Si alloys are non-Newtonian fluids [14,108].

- The constant factor β for all alloy compositions was calculated based on their weight fractions in the alloy. However, there is no theoretical reason to verify the validity of this assumption, yet.

- v_o is a constant and assumes that there is no net diffusion of atoms in the structure at any temperature.

- It was assumed that P(A) and P(B) as the values of P(T) for Al and Si, respectively. The validity of this assumption should be verified.

CHAPTER 7 CONCLUSIONS

This chapter presents the salient conclusions drawn from the results of this dissertation in understanding the liquid structure of Al-Si alloys in both the unmodified and Sr-modified conditions. Further, a commentary on the influence of trace levels of Sr addition to the Al-Si hypoeutectic alloy melt on the morphological modification of eutectic phases. A few recommendations for additional work on this topic has also been presented in this chapter.

7.1 CONCLUSIONS

The liquid structure of Al-Si alloys in unmodified and modified conditions was extensively studied by high energy x-ray diffraction experiments. The results obtained in this dissertation work indicate that the melt temperatures and silicon content have a significant effect on the atomic structure of Al-Si alloy melts. Increase in the melt temperature and silicon content results in higher disorder of the alloy melt. With increase in silicon content from 0% to 12.5%, it was observed that the aluminium melt changes from a close packed structure to open structure by lowering its coordination number and packing density. Further, 0.04%Sr addition to liquid Al-Si hypoeutectic alloy melt resulted in further increase in the melt disorder at any given temperature. Addition of Sr further decreases the coordination number and packing density for any given alloy composition at any given melt temperature.

Partial pair correlation functions for Al-Al, Al-Si and Si-Si pair of atoms were determined by carrying out Reverse Monte Carlo (RMC) analysis with 10,000 atoms for Al-Si hypoeutectic composition in unmodified and Sr modified conditions. The results coordination number for Al-Al and Al-Si atoms decreases with increasing melt temperature for all alloy compositions. However, this effect is unpredictable and non uniform with Si-Si pair of atoms since the number of Si atoms is small in the alloys and hence the RMC analysis lacks the resolution. Addition of 0.04%Sr further decreases the coordination number and packing density of Al-Al, Al-Si and Si-Si pair of atoms for any given alloy composition at any given melt temperature.

Viscosity of Al and Al-Si hypoeutectic alloys was evaluated using atomic structure information from diffraction experiments and RMC analysis by semi empirical approach. The viscosity decreases with increasing melt temperature for all alloy compositions.

Increasing silicon content decreases viscosity of alloy melt. Further, addition of 0.04%Sr decreases the viscosity for any given alloy composition at any given melt temperature.

Figure 7-1 presents a schematic highlighting the significant contributions from this dissertation. The definitions of the terms used in Figure 7-1 are presented in Chapter 1. Typically, simulation techniques from the fundamentals such as abintio molecular dynamics, embedded atom method (EAM) and non-equilibrium molecular dynamics (NEMD) were used to simulate atomic structures of binary metallic alloys. The independent variables of such simulations would be the potential functions, atomic densities and the dependant variables would be the g(r) from which the S(Q) could be evaluated along with the PPDF and PSF. The output from the simulations along with the potential functions and PPDF of individual atom pairs in the alloy were used to evaluate physical properties such as viscosity. This dissertation presents a method to validate the simulations from fundamentals by validation of S(Q), g(r), PSF and PPDF of the atoms pairs in addition to using the semi-empirical method and experimental data to verify the evaluated viscosity values obtained by the fundamental simulations.

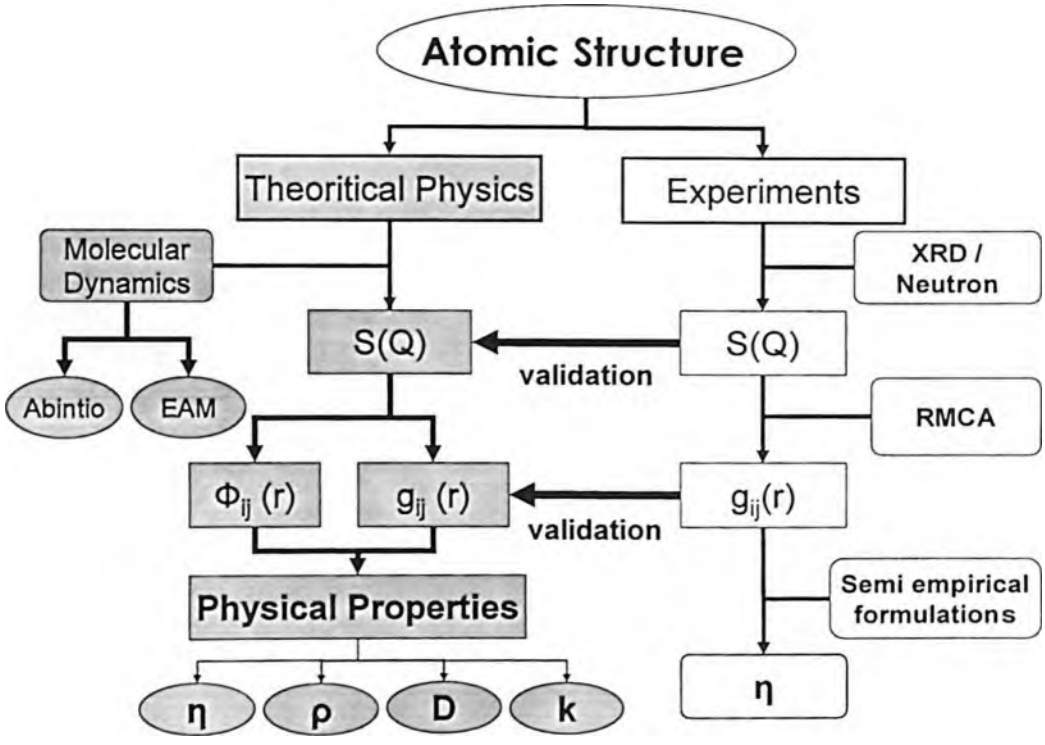


Figure 7-1: **Schematic showing the critical contributions of the present dissertation in validation the simulation studies in theoretical physics.**

This dissertation shows that the results of the partial pair distribution functions for the three individual atom pairs in a binary alloy obtained by experimental diffraction data coupled with RMC analysis, are comparable to those obtained from the abinitio modeling [104] which are derived solely from a numerical model developed on the basis of an in-depth understanding of the physics of atom behavior (shown in Figure 7-1).

7.2 COMMENTARY

As presented in the introduction section of this dissertation, the Al-Si hypoeutectic alloy is commercially one of the most important system and the topic of evolution and morphological modification of the eutectic phases in these alloys during solidification is one of the most debated topics amongst many academic researchers for nearly ninety years since the second decade of the last century [9,10,25,26 31,109,110,111, ,112,113,114,115]. Interestingly, there are still major disagreement amongst researchers on the reason and mechanism of the morphological modification of the eutectic phases in the solidified structure. A viable explanation would that the addition of Sr changes the physical properties such as melt viscosity, interfacial energy and atomic structure of the inter-dendritic liquid during the final stages of solidification, thereby, delaying the nucleation of the eutectic Si phase and leading to significant undercooling of the eutectic temperature during which the primary Al phase continues to grow and causes a super-saturation condition of Si in the inter-dendritic liquid. This super-saturation and undercooling results leads to a labile condition resulting in a spontaneous crystallization of the Si phase on the primary Al phase (heat extraction path) rendering the inter-dendritic liquid back to the eutectic composition in an under-cooled state, thus resulting the evolution of highly grain refined eutectic Al phase followed by a fibrous morphology of eutectic Si phase. A similar hypothesis has also been presented by Shankar et al [13]. Interestingly Chalmers [116], had proposed a similar theory as well to explain the modification of the eutectic phase morphologies, in the middle of the last century. Further, Gayler [109] presented a similar theory for the morphological modification by Na and Sr which was readily agreed by Gwyer [110] and Rothery [31]. The moot point of this theory is the lack of experimental evidence to support the fact that trace levels of Sr or Na additions to the Al-Si hypoeutectic alloys, specifically to the near eutectic compositions which are the final liquids to solidify before the labile condition of eutectic solidification, causes significant changes to the physical properties of the liquid to retard and/or inhibit nucleation of the eutectic phases at the solidification temperature prescribed by the equilibrium phase diagram. Hence, there were many other attempts made during the last quarter of the last century to explain these morphological modifications by solely attribution the effect of Sr on the growth of Si phase [4,25,26,117] or by physical or chemical poisoning of a heterogeneous

nucleation site for the eutectic Si phase [9,25,26,115]. None of these other attempts could fully explain all the experimental evidence that have been presented such as microstructural features and events marked by thermal data during solidification. Recently, to further strengthen our viewpoints on the mechanism of these morphological modifications, it was observed by Shankar et al [13] for the first time in the channel pattern images generated by a Ga ion beam source in a SEM on a Focused Ion Beam milled surface, that the addition of trace levels of Sr not only modified the morphology of the eutectic Si but also significantly refined the grains of the eutectic Al phase.

The theory that trace levels of Sr and Na additions alter the physical properties of the inter-dendritic liquid during the final stages of solidification of Al-Si hypoeutectic alloys [13] could be justified only by demonstrating that the atomic structure of the inter-dendritic liquid is sufficiently altered to effect a change in the physical properties. There are very few experimental techniques which have would demonstrate that such a change is viable. Recently, Bian et al [15] presented qualitative evidence to show that the atomic structure of Al-Si eutectic melt changes with Sr addition and Malik [14] showed that the Sr addition changes the rheological properties, specifically the melt viscosity of these alloys. The results of this dissertation show that Sr addition significantly alters the liquid structure of the Al-Si hypoeutectic alloys for all Si contents and alloy melt temperatures. Further, Sr addition to these alloys delay or inhibit the clustering tendencies of the atoms at temperatures close to the nucleation event. Specifically, this phenomenon is more pronounced in the eutectic alloy which mostly forms the inter-dendritic liquid compositions in contact with the primary Al dendrites during the final stages of solidification. When Sr is added to the eutectic alloy, the atom clustering may not be sufficient enough at the eutectic temperature to effect a nucleation event and thus would lead to an undercooling of the inter-dendritic liquid to reach a labile temperature at which spontaneous crystallization of the Si phase would occur on the primary Al phases which acts as a heat sink during solidification. Subsequently, the evolution of the eutectic phases will proceed as described earlier in this section. The evidence of spontaneous nucleation and subsequent evolution of the eutectic phases have been presented earlier with sufficient experimental and analytical evidences [13].

The results of RMC analysis show that the Sr addition has a significant effect on the distribution and arrangement of Si atoms in the Al-Si alloy and this change in the Si atom positions affect all the three atom pair interactions, namely Al-Al, Al-Si and Si-Si. The Si-Si atom pair interaction is affected the most by Sr addition, specifically, the ratio of second to first peak positions in the partial pair distribution function for the Si-Si pair of atoms increases with Sr addition there by pushing silicon atoms farther away from the origin atom with addition of Sr to the Al-Si alloy melt. This kind of behavior represents

that the Si-Si pair of atoms becomes more disordered in the Sr-modified alloy melt. Further, the results of viscosity show that the Sr addition decreases the viscosity of alloy melt at any given melt temperature. This substantiates the theory proposed Shankar et al [13] that the modification of the eutectic phases occurs because of the changes in the physical properties of the alloy melt. The present dissertation work on the atomic structure of liquid Al-Si hypoeutectic alloys and the effect of Sr presents emphatic evidences to support the fact that the morphological modification of the eutectic phases in Al-Si hypoeutectic alloy begin with the marked changes to the atomic structure of the alloy liquid which leads to changes in fundamental physical properties of these alloy liquids.

7.3 RECOMMENDATIONS FOR FUTURE WORK

The following are some of the recommendations for future work in this topic:

Since, partial pair correlations for Si-Si pair of atoms obtained from RMC analysis with 10,000 atoms in this study showing abnormal trend in the respective plots, it is advisable to carry out RMC analysis with 100,000 atoms to see a better definition in the Si-Si partial pair correlation functions. This may lead to a specific trend in some of the observed atom arrangement properties such as first shell coordination number and packing density.

Since, the amount of Sr added to Al-Si alloys for the modification treatment is only 0.04% (400ppm), performing EXAFS (Extended X-ray Absorption fine Spectroscopy) experiments in the liquid state would give the correlation of Sr-Al and Sr-Si in the alloy melt thereby providing more insight into the modification mechanism.

Develop a Semi empirical approach to determine the viscosity of non Newtonian liquid metals and alloys.

Determine the pair potential functions from experiment diffraction data of binary alloys along with the Hypernetted Chain (HNC) model and further, evaluate the viscosities by using Rice Allnat or Born Green theory along with the PDF and potential functions derived from experiment data.

REFERENCES

1. Davies JR, ed., "Aluminum and Aluminum Alloys", ASM International, Ohio, 1993, p627.
2. Pacz A., US patent 13810630, 1920.
3. Dash M, Makhlouf MM., J. Light. Met. 2002; 2:251.
4. Hellawell A., Progr. Mater. Sci. 1970; 15: 3.
5. Makhlouf MM, Guthy HV., J. Light. Met. 2001; 1:199.
6. Shankar S, Riddle Y, Makhlouf MM., Acta Mater. 2004; 52: 4447.
7. Gweyer AGC, Philips HWL., J. Inst. Met. 1926; 36: 283.
8. Guillet L., Rev. Mét. 1922.
9. Sigworth G., Int. J. Met. Cast. Spring 2008, 2 (2), 19-42.
10. Campbell J, Sigworth G, Jorstad J., Technical Forum: Reader and Author Dialogue, Int. J. Met. Cast. Winter 2009; 3 (1): 65.
11. Tonmukayakul N, Makhlouf MM, Shankar S., Int. J. Met. Cast .Spring 2009; 3(2), 7-16.
12. Nogita K, Mcdonald SD, Dahle Ak., Met. Mater. Trans A. 2004; 45: 323.
13. Shankar S, Makhlouf MM, Riddle Y. AFS Trans. 2005; 05: 088
14. Malik MM., MASc. Dissertation, McMaster University. 2008.
15. Bian XF, Wang W, Qin J., Mat. Sci. Forum. 2000; 331
16. Murray JJ, McAlister AJ., Bull. Alloy Phase Diagrams. 1984; 5: 74.
17. Khan S, Elliot R., J. Mater. Sci. 1994; 29: 736
18. Thall BM, Chalmers B., J. Inst. Met. 1949; 78: 79
19. Search RE., Met. Ind. 1922.
20. Schulz E., Z. Metallkunde. 1949; 39: 123.
21. Tzumara Y., Nippon Kinzoku Gakkaisi. 1957; 21: 69.
22. Edwards JD, Archer RS., Chem. Met. Eng. 1924; 31: 504
23. Jeckinson DC, Hogan LM., J. Crys. Growth. 1975; 28: 171.
24. Lu Shu-Zhu, Hellawell A., Met. Trans A. 1987; 18A: 1721.
25. Cho YH, Lee H-C, Oh Kh, Dahle AK., Met. Mater. Trans A. 2008; 39A: 2435.
26. Satyapal H, Prabhu N., J. Mater. Sci. 2008; 43(9): 3009.
27. Guillet L., Rev. Met. 1922.
28. Search RE., Met. Ind. 1922.
29. Curran J., J. Chem. Met. Engg. 1924; 31: 504.
30. Gwyer AGC, Philips HWL., J. Inst. Met. 1926; 36: 283.
31. Rothery H., J. Inst. Met. 1927; 39: 190-191.
32. Flood SC, Hunt JD., Met. Sci. 1981; 15: 287.
33. Davies VDL, West JM., J. Inst. Met. (1963-1964); 92: 175.

34. Mondolfo LF., J. Aust. Inst. Met. 1965; 10: 169.
35. Crosley PB, Mondolfo LF., Mod. Castings. 1966; 46: 89.
36. Shimoji M., Liquid Metals (Academic Press, London) 1977.
37. Krishnan S, Ansell S, Price DL., J .Non. Cryst. Sol. 1999; 250-252: 286.
38. Kitayama T, Mizutani T, Utsumi W, Shimomura O, Yamakanta M, Funakoshi K., Nature. 2000; 403: 170.
39. Waseda Y, Tamaki S., J. Phys. Soc. Japan 1977; 43: 1258.
40. Waseda Y., The Structure of Non-Crystalline Materials: Liquids and Amorphous Solids (McGraw-Hill, New York) 1980.
41. Iida T, Guthrie RIL., The Physical Properties of Liquid Metals (Clarendon Press, Oxford) 1988.
42. Bernal J., Nature. 1959; 4655: 141.
43. Hukins DWL., X-ray diffraction by Disordered and Ordered Systems (Pergamon Press, Oxford) 1981.
44. Stallard JM, Davis CM., Phys. Rev. A. 1973; 8: 368.
45. Waseda Y, Suzuki K., Z. Physik B. 1975; 20: 339.
46. Henshaw DG., Phys. Rev. 1958; 111: 1470.
47. Gingrich NS., Rev. Mod. Phys. 1943; 15: 90.
48. Thomas CD, Gingrich NS., J. Chem. Phys. 1938; 6: 411.
49. Thomas CD, Gingrich NS., J. Chem. Phys. 1938; 6: 659.
50. Waseda Y, Yokoyama K, Suzuki K., Phil. Mag. 1974; 30: 1195.
51. Waseda Y, Tamaki S., Phil. Mag. 1972; 32: 273.
52. Waseda Y, Tsuchia Y, Tamaki Y., Z. Physik B. 1979; 32: 253.
53. Davidović M, Stojić M, Jović Dj., J. Phys. C: Solid State Phys. 1983; 16: 2053.
54. Hoyer W, Jödicke R., J. Non. Cryst. Sol. 1995; 192-193: 102.
55. Mizuki J, Kakimoto K, Misawa M, Fukunaga T, Watanabe N., J. Phys.: cond. Matter. 1993; 5: 3391.
56. Lague SB, Barnes AC, Archer AD, Howells WS., J. Non. Cryst. Sol. 1996; 205-207: 89.
57. Ansell S, Krishnan S, Weber JKR, Felten JJ, Nordine PC, Beno MA, Price DL, Saboungi M., Phys. Rev. Let. 1997. 78: 464.
58. Itami T, Munejiri S, Masaki T, Aoki H, Ishii Y, Kamiyama T, Senda Y, Shimojo F, Hoshino k., Phys. Rev B. 2003; 67: 064201.
59. Mei Q, Benmore CJ, Weber JKR., Phys. Rev. Let. 2007; 98: 057802.
60. Gruner S, Marczinke J, Hennet L, Hoyer W, Cuello GJ. J. Phys.: cond. Matter. 2009; 21: 385403.
61. March NH, Tosi MP., Introduction To The Liquid State Physics (World Scientific Publishing, Singapore) 2002.
62. Brodova IG, Popel PS, Eskin GI., Liquid Metal Processing (Taylor & Francis) 2002.
63. http://www.compsoc.man.ac.uk/~lucky/Democritus/Theory/rdf.html.
64. Keating DT., J. Appl. Phys. 1963; 34: 923.

65. Faber TE, Ziman JM., Phil. Mag. 1965; 11: 153.
66. Enderby JE, North DM, Egelstaff PA., Phil. Mag. 1966; 14: 961.
67. Ramesh TG, Ramaseshan S., J. Phys. C: Solid St. Phys. 1971; 4: 3029.
68. Waseda Y, Tamaki S., Phil. Mag. 1975; 32: 951.
69. Halder NC, Wagner CNJ., J. Chem. Phys. 1967; 47: 4385.
70. Waseda Y, Tamaki S. J. Phys. F. 1977b; 7: L151.
71. Bellissent-Fune M.C, Desre P.J, Bellissent R, Tourand G., J. Phys. F: Metal Phys 1977; 7, 12:2485.
72. McGreevy RL, Pusztai L., Mol. Simul. 1988; 1: 359.
73. McGeevy RL., J. Phys. Cond. Matt. 1991; 3: F9.
74. McGreevy RL., J. Phys. Cond. Matt. 2001; 13: R877-R913.
75. Sheng HW, Luo WK, Alamgir FM, Bai JM, Ma E., Nature. 2006; 439: 419.
76. Keen DA, McGreevy RL., Nature. 1990; 344: 423.
77. Kohara S., private communication. 2001.
78. de Jong PHK, Verkerk P, van der Lugt W, de graaf LA., J. Non. Cryst. Sol. 1993; 156-158: 978.
79. Petkov V, Yunchov G., J. Phys. Cond. Matt. 1994; 6: 10885.
80. Gruner S, Kaban I, Kleinhempel R, Hoyer W, Jo´va´ri P, Delaplane RG., J. Non. Cryst. Sol. 2005; 351: 3490.
81. Takeda S, Fujii H, Kawatika Y, Kato Y, Kohara S., Mater. Sci. Eng A. 2007: 449-451: 590.
82. Bakhtiyarov SI, Overfelt RA., Acta Mater. 1999: 47: 4311.
83. Dinsdale AT, Queted PN., J. Mater. Sci. 2004; 39: 9951.
84. Xigui S, Xiufang B, Jingxiang Z, Jie Z., J. Alloys and Compounds. 2009; 479: 670.
85. Born M, Green H.S., Proc. R. Soc. A. 1947; 190: 455.
86. Rice S.A, Allnat A.R., J. Chem. Phys. 1961; 34: 2144.
87. Kitajima M, Shimoji M., Trans. Japan. Inst. Met. 1976; 17: 582.
88. Bhuiyan G.M, Ali I, Mujibur Rahman S.M., Physica B. 2003; 334: 147.
89. Qi Y, Cagin T, Kimura Y, Goddard W.A. J. Computer-Aided Materials Design. 2001; 8: 233.
90. Desgranges C, Delhommelle J., Phys. Rev. B. 2007; 76: 172102(1).
91. Shankar S, Prakash S, Jeyakumar M, Walker M, Hamed M, Kramer MJ., TMS 2009, USA, 2009.
92. Kresse G., J. Non. Crys. Sol. 2002; 312-314: 52.
93. Tangneya, Scandolo S. J. Chem. Phys 2002; 117, 19: 8898.
94. Bansal R., J. Phys C. 1973; 6: 3071.
95. Faber TE., Introduction To The Theory of Liquid Metals (Cambridge University Press) 1972.
96. Andrade EN., Phil. Mag. 1934; 17: 698.
97. Djemili B, Martin-Garin L, Martin-Garin R, Hicter P., J. de. Phys. 1980; 8: C8-363.

98. http://www.factsage.com.
99. Hammersley AP, Svensson SO, Hanfland M, Fitch AN, Hausermann D., High Press Res. 1996; 14: 235
100. http://www.ameslab.gov/news/furnace.gif
101. Qui X, Thomson J, Billinge SJL., J.Appl.Cryst. 2004; 37:678.
102. Vander Meer JPM, Konnings RJK., Nucl. Mater. 2007; 360: 16.
103. Bian X, Sun M, Xue X, Qin X., Mater. Lett. 2003; 57: 2001.
104. Wang S, Wang CZ, Feng-Chuan Chuang, Morris JR, Ho KM., J. Chem. Phys. 2005; 122: 034508.
105. http://www.chemicalelements.com/elements/al.html.,
106. Dinsdale AT, Queted PN., J. Mater. Sci. 2004; 39: 9951.
107. Hur B, Park S, Hiroshi A., Mater. Sci. Forum. 2003; 439: 51.
108. Varsani V, Fan Z., TMS Annual Meeting & Exhibition 2007; USA; 67.
109. Gayler MLV., J. Inst Met. 1927; 39: 157.
110. Gwyer AGC., J. Inst. Met. 1927; 39: 184-
111. Rosenhain W., J. Inst. Met. 1927; 39: 184.
112. Gayler MLV., J. Inst. Met. 1927; 39: 192.
113. Shankar S, Riddle YW, Makhlouf MM., Met. Mater. Trans A. 2004; 35: 3038.
114. Hillert M., Met. Mater. Trans A. 2003; 34A: 2688.
115. Shankar S, Riddle Y, Makhlouf MM., Met. Mater. Trans. A. 2005; 36A: 1613.
116. Thall BM, Chalmers B., J. Inst. Met. 1950; 77: 79.
117. Hanna MD, Zu SL, Hellawell A., Met. Mater. Trans. A. 1984; 15A: 459.

APPENDIX A TOTAL STRUCTURE INFORMATION FOR AL-SI HYPOEUTECTIC ALLOYS

Table A-1: Structural information for liquid Aluminium

Temp (K)	$S(Q)_1$	Q_1	$g(r)_1$	$g(r)_2$	$g(r)_1/g(r)_2$	r_1	r_2	r_2/r_1	CN	PD
938	2.30	2.70	2.42	1.20	2.02	2.87	5.14	1.79	11.51	0.44
963	2.27	2.70	2.40	1.19	2.02	2.87	5.14	1.79	11.47	0.43
988	2.24	2.70	2.38	1.19	2.00	2.87	5.14	1.80	11.42	0.43
1013	2.21	2.70	2.36	1.18	1.99	2.86	5.14	1.80	11.38	0.43
1038	2.19	2.70	2.35	1.18	1.98	2.86	5.14	1.79	11.34	0.43
1063	2.15	2.70	2.31	1.17	1.97	2.86	5.14	1.79	11.30	0.43
1088	2.11	2.70	2.29	1.17	1.96	2.86	5.14	1.79	11.25	0.43
1113	2.09	2.70	2.27	1.17	1.95	2.86	5.13	1.79	11.20	0.43

Table A-2: Structural information for liquid Al-3%Si alloy

Temp (K)	$S(Q)_1$	Q_1	$g(r)_1$	$g(r)_2$	$g(r)_1/g(r)_2$	r_1	r_2	r_2/r_1	CN	PD
920	2.23	2.70	2.36	1.18	1.99	2.87	5.13	1.79	11.42	0.44
942	2.20	2.69	2.35	1.18	1.99	2.87	5.13	1.79	11.37	0.44
964	2.18	2.69	2.33	1.18	1.97	2.87	5.13	1.79	11.34	0.43
1052	2.08	2.69	2.26	1.17	1.94	2.87	5.13	1.79	11.21	0.43

Table A-3: Structural information for liquid Al-3%Si-0.04%Sr alloy

Temp (K)	$S(Q)_1$	Q_1	$g(r)_1$	$g(r)_2$	$g(r)_1/g(r)_2$	r_1	r_2	r_2/r_1	CN	PD
920	2.19	2.70	2.31	1.18	1.96	2.86	5.10	1.79	11.37	0.43
942	2.18	2.70	2.29	1.18	1.95	2.86	5.11	1.79	11.32	0.43
964	2.15	2.70	2.28	1.17	1.94	2.86	5.11	1.79	11.27	0.43
1052	2.06	2.70	2.21	1.16	1.90	2.86	5.10	1.79	11.18	0.43

Table A-4: Structural information for liquid Al-7%Si alloy

Temp (K)	$S(Q)_1$	Q_1	$g(r)_1$	$g(r)_2$	$g(r)_1/g(r)_2$	r_1	r_2	r_2/r_1	CN	PD
898	2.22	2.71	2.35	1.18	1.99	2.85	5.11	1.79	11.31	0.43
920	2.19	2.71	2.33	1.18	1.98	2.85	5.11	1.79	11.31	0.43
942	2.17	2.71	2.32	1.17	1.98	2.85	5.12	1.80	11.27	0.43
964	2.14	2.70	2.30	1.17	1.97	2.85	5.12	1.80	11.22	0.43
986	2.12	2.70	2.28	1.17	1.96	2.85	5.12	1.80	11.19	0.43
1008	2.08	2.70	2.25	1.16	1.94	2.84	5.12	1.80	11.14	0.42
1030	2.05	2.70	2.23	1.16	1.93	2.84	5.11	1.80	11.10	0.42
1052	2.02	2.70	2.21	1.15	1.92	2.84	5.11	1.80	11.08	0.42

Table A-5: Structural information for liquid Al-7%Si-0.04%Sr alloy

Temp (K)	$S(Q)_1$	Q_1	$g(r)_1$	$g(r)_2$	$g(r)_1/g(r)_2$	r_1	r_2	r_2/r_1	CN	PD
898	2.17	2.71	2.32	1.18	1.97	2.83	5.11	1.81	10.88	0.42
920	2.14	2.71	2.31	1.18	1.96	2.83	5.11	1.81	10.85	0.42
942	2.12	2.71	2.29	1.17	1.95	2.83	5.12	1.81	10.80	0.42
964	2.10	2.71	2.28	1.17	1.95	2.83	5.12	1.81	10.77	0.42
986	2.07	2.71	2.26	1.17	1.94	2.83	5.11	1.80	10.74	0.42
1008	2.05	2.71	2.24	1.16	1.93	2.83	5.10	1.80	10.73	0.42
1030	2.02	2.71	2.22	1.16	1.92	2.83	5.10	1.80	10.69	0.42
1052	2.00	2.70	2.20	1.16	1.91	2.83	5.10	1.80	10.64	0.41

Table A-6: Structural information for liquid Al-10%Si alloy.

Temp (K)	$S(Q)_1$	Q_1	$g(r)_1$	$g(r)_2$	$g(r)_1/g(r)_2$	r_1	r_2	r_2/r_1	CN	PD
885	2.18	2.71	2.28	1.17	1.95	2.85	5.09	1.79	11.23	0.43
907	2.15	2.71	2.26	1.17	1.94	2.85	5.09	1.79	11.20	0.43
929	2.13	2.71	2.25	1.17	1.93	2.85	5.08	1.78	11.16	0.43
973	2.09	2.71	2.21	1.16	1.90	2.85	5.08	1.78	11.14	0.43
995	2.07	2.71	2.21	1.16	1.92	2.85	5.08	1.78	11.10	0.43
1017	2.05	2.71	2.20	1.15	1.91	2.85	5.07	1.78	11.07	0.43
1039	2.04	2.71	2.19	1.15	1.90	2.85	5.08	1.79	11.04	0.42

Table A-7: Structural information for liquid Al-10%Si-0.04% Sr alloy.

Temp (K)	$S(Q)_1$	Q_1	$g(r)_1$	$g(r)_2$	$g(r)_1/g(r)_2$	r_1	r_2	r_2/r_1	CN	PD
885	2.15	2.71	2.26	1.17	1.94	2.84	5.09	1.79	11.13	0.43
907	2.12	2.71	2.24	1.16	1.93	2.84	5.09	1.79	11.10	0.43
929	2.10	2.71	2.23	1.16	1.92	2.84	5.09	1.79	11.06	0.43
973	2.05	2.71	2.19	1.16	1.90	2.84	5.08	1.79	11.01	0.43
995	2.02	2.71	2.18	1.15	1.89	2.84	5.07	1.79	10.97	0.42
1017	1.99	2.71	2.16	1.15	1.88	2.84	5.07	1.79	10.87	0.42
1039	1.97	2.71	2.14	1.14	1.87	2.84	5.07	1.79	10.83	0.42

Table A-8: Structural information for liquid Al-12Si alloy

Temp (K)	$S(Q)_1$	Q_1	$g(r)_1$	$g(r)_2$	$g(r)_1/g(r)_2$	r_1	r_2	r_2/r_1	CN	PD
867	2.18	2.72	2.28	1.17	1.95	2.84	5.08	1.79	11.19	0.43
889	2.15	2.72	2.26	1.17	1.94	2.84	5.08	1.79	11.15	0.43
911	2.12	2.72	2.24	1.16	1.93	2.83	5.07	1.79	11.10	0.43
933	2.10	2.72	2.22	1.16	1.91	2.83	5.06	1.78	11.07	0.43
956	2.08	2.72	2.21	1.16	1.91	2.83	5.07	1.79	11.03	0.42
978	2.06	2.72	2.20	1.16	1.90	2.83	5.08	1.79	10.98	0.42
1000	2.04	2.72	2.18	1.15	1.89	2.83	5.06	1.79	10.95	0.42
1022	2.02	2.72	2.17	1.15	1.88	2.83	5.08	1.79	10.91	0.42
1065	1.97	2.71	2.13	1.14	1.87	2.83	5.07	1.79	10.86	0.42

Table A-9: Structural information for liquid Al-12Si-0.04%Sr alloy

Temp (K)	$S(Q)_1$	Q_1	$g(r)_1$	$g(r)_2$	$g(r)_1/g(r)_2$	r_1	r_2	r_2/r_1	CN	PD
867	2.14	2.72	2.24	1.16	1.92	2.83	5.10	1.80	10.76	0.43
889	2.12	2.72	2.23	1.16	1.91	2.83	5.10	1.80	10.73	0.42
911	2.09	2.72	2.21	1.16	1.90	2.82	5.09	1.80	10.69	0.42
933	2.07	2.72	2.20	1.16	1.90	2.82	5.08	1.80	10.65	0.42
956	2.05	2.72	2.18	1.16	1.89	2.82	5.09	1.80	10.61	0.42
978	2.03	2.72	2.16	1.15	1.88	2.83	5.08	1.80	10.57	0.42
1000	2.00	2.72	2.15	1.15	1.87	2.82	5.08	1.80	10.52	0.42
1022	1.97	2.71	2.13	1.15	1.86	2.82	5.08	1.80	10.47	0.41
1065	1.90	2.71	2.09	1.13	1.84	2.81	5.06	1.80	10.36	0.41

Table A-10: Numerical values of SF for Liquid Aluminium at various melt temperatures.

Q ($Å^{-1}$)	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
0.6479	0.0315	0.0322	0.0322	0.0333	0.0324	0.0328	0.0332	0.0348
0.6733	0.0328	0.0334	0.0330	0.0341	0.0335	0.0342	0.0349	0.0350
0.6987	0.0344	0.0343	0.0346	0.0353	0.0349	0.0355	0.0363	0.0362
0.7241	0.0358	0.0364	0.0362	0.0364	0.0358	0.0365	0.0370	0.0385
0.7495	0.0365	0.0379	0.0381	0.0371	0.0367	0.0378	0.0377	0.0394
0.7750	0.0380	0.0389	0.0388	0.0385	0.0384	0.0394	0.0396	0.0407
0.8004	0.0395	0.0396	0.0396	0.0399	0.0404	0.0398	0.0411	0.0412
0.8258	0.0410	0.0409	0.0404	0.0413	0.0422	0.0413	0.0419	0.0419
0.8512	0.0424	0.0425	0.0423	0.0430	0.0443	0.0434	0.0431	0.0435
0.8766	0.0437	0.0441	0.0441	0.0455	0.0464	0.0448	0.0447	0.0455
0.9020	0.0446	0.0461	0.0458	0.0477	0.0475	0.0456	0.0469	0.0473
0.9274	0.0459	0.0478	0.0477	0.0484	0.0487	0.0479	0.0487	0.0489
0.9528	0.0480	0.0491	0.0497	0.0491	0.0494	0.0496	0.0504	0.0504
0.9782	0.0506	0.0509	0.0513	0.0510	0.0508	0.0505	0.0520	0.0522
1.0036	0.0521	0.0529	0.0529	0.0531	0.0530	0.0524	0.0537	0.0542
1.0290	0.0530	0.0549	0.0548	0.0552	0.0554	0.0544	0.0555	0.0560
1.0544	0.0553	0.0568	0.0571	0.0576	0.0576	0.0560	0.0573	0.0578
1.0799	0.0582	0.0590	0.0592	0.0602	0.0600	0.0580	0.0593	0.0600
1.1053	0.0606	0.0615	0.0615	0.0626	0.0627	0.0604	0.0615	0.0630
1.1307	0.0640	0.0643	0.0644	0.0652	0.0657	0.0631	0.0642	0.0663
1.1561	0.0667	0.0668	0.0679	0.0684	0.0683	0.0657	0.0669	0.0692
1.1815	0.0694	0.0696	0.0707	0.0719	0.0710	0.0679	0.0694	0.0708
1.2069	0.0730	0.0732	0.0741	0.0760	0.0750	0.0714	0.0727	0.0734
1.2323	0.0767	0.0775	0.0780	0.0800	0.0791	0.0754	0.0765	0.0776
1.2577	0.0807	0.0813	0.0817	0.0838	0.0828	0.0788	0.0802	0.0817
1.2831	0.0846	0.0849	0.0867	0.0876	0.0873	0.0830	0.0835	0.0853
1.3085	0.0885	0.0888	0.0909	0.0918	0.0918	0.0877	0.0871	0.0896
1.3339	0.0929	0.0935	0.0954	0.0967	0.0961	0.0916	0.0918	0.0940
1.3593	0.0976	0.0989	0.1010	0.1019	0.1006	0.0958	0.0970	0.0983
1.3848	0.1018	0.1036	0.1065	0.1068	0.1053	0.1012	0.1012	0.1028
1.4102	0.1068	0.1088	0.1113	0.1119	0.1111	0.1064	0.1056	0.1077
1.4356	0.1119	0.1144	0.1163	0.1178	0.1169	0.1109	0.1107	0.1142
1.4610	0.1168	0.1194	0.1210	0.1234	0.1225	0.1161	0.1157	0.1193
1.4864	0.1210	0.1236	0.1256	0.1281	0.1274	0.1209	0.1205	0.1238
1.5118	0.1260	0.1282	0.1314	0.1333	0.1326	0.1255	0.1257	0.1289
1.5372	0.1318	0.1334	0.1371	0.1391	0.1385	0.1310	0.1317	0.1344
1.5626	0.1372	0.1395	0.1424	0.1452	0.1446	0.1369	0.1383	0.1409
1.5880	0.1424	0.1448	0.1480	0.1504	0.1503	0.1428	0.1445	0.1472
1.6134	0.1478	0.1496	0.1535	0.1555	0.1556	0.1493	0.1506	0.1529
1.6388	0.1529	0.1548	0.1586	0.1613	0.1619	0.1553	0.1571	0.1595
1.6642	0.1587	0.1607	0.1646	0.1673	0.1683	0.1631	0.1650	0.1671
1.6897	0.1652	0.1678	0.1719	0.1744	0.1751	0.1725	0.1736	0.1758
1.7151	0.1720	0.1755	0.1794	0.1822	0.1829	0.1814	0.1820	0.1854
1.7405	0.1795	0.1837	0.1874	0.1913	0.1920	0.1907	0.1920	0.1962
1.7659	0.1885	0.1924	0.1967	0.2008	0.2019	0.2005	0.2033	0.2074
1.7913	0.1982	0.2022	0.2071	0.2107	0.2131	0.2109	0.2150	0.2193
1.8167	0.2092	0.2134	0.2181	0.2223	0.2248	0.2227	0.2271	0.2318

Q ($Å^{-1}$)	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
1.8421	0.2211	0.2257	0.2310	0.2350	0.2378	0.2366	0.2404	0.2456
1.8675	0.2340	0.2390	0.2456	0.2489	0.2519	0.2518	0.2564	0.2614
1.8929	0.2483	0.2532	0.2606	0.2648	0.2684	0.2687	0.2744	0.2788
1.9183	0.2647	0.2694	0.2765	0.2825	0.2868	0.2878	0.2932	0.2985
1.9437	0.2820	0.2886	0.2947	0.3014	0.3068	0.3091	0.3137	0.3198
1.9691	0.3021	0.3096	0.3154	0.3231	0.3290	0.3327	0.3378	0.3440
1.9946	0.3246	0.3323	0.3389	0.3472	0.3529	0.3574	0.3630	0.3700
2.0200	0.3500	0.3574	0.3648	0.3733	0.3802	0.3838	0.3898	0.3984
2.0454	0.3782	0.3853	0.3937	0.4017	0.4108	0.4137	0.4203	0.4280
2.0708	0.4089	0.4166	0.4263	0.4331	0.4440	0.4478	0.4529	0.4616
2.0962	0.4436	0.4511	0.4603	0.4689	0.4792	0.4841	0.4888	0.4983
2.1216	0.4832	0.4899	0.5002	0.5096	0.5195	0.5260	0.5305	0.5407
2.1470	0.5242	0.5333	0.5446	0.5538	0.5640	0.5727	0.5778	0.5872
2.1724	0.5704	0.5822	0.5936	0.6042	0.6160	0.6245	0.6301	0.6400
2.1978	0.6233	0.6352	0.6472	0.6589	0.6712	0.6798	0.6859	0.6971
2.2232	0.6834	0.6933	0.7061	0.7179	0.7309	0.7399	0.7469	0.7574
2.2486	0.7474	0.7592	0.7706	0.7813	0.7962	0.8037	0.8119	0.8213
2.2740	0.8187	0.8306	0.8419	0.8525	0.8661	0.8732	0.8815	0.8905
2.2995	0.8975	0.9092	0.9216	0.9315	0.9443	0.9521	0.9582	0.9666
2.3249	0.9834	0.9953	1.0086	1.0192	1.0321	1.0384	1.0426	1.0510
2.3503	1.0811	1.0911	1.1040	1.1154	1.1254	1.1321	1.1340	1.1427
2.3757	1.1853	1.1952	1.2054	1.2160	1.2243	1.2302	1.2299	1.2361
2.4011	1.3004	1.3077	1.3185	1.3274	1.3322	1.3349	1.3325	1.3388
2.4265	1.4186	1.4252	1.4333	1.4406	1.4451	1.4425	1.4405	1.4430
2.4519	1.5431	1.5491	1.5537	1.5574	1.5596	1.5537	1.5448	1.5438
2.4773	1.6731	1.6744	1.6809	1.6769	1.6752	1.6664	1.6523	1.6486
2.5027	1.7980	1.7964	1.7953	1.7909	1.7846	1.7716	1.7547	1.7462
2.5281	1.9168	1.9122	1.9037	1.8963	1.8857	1.8672	1.8451	1.8336
2.5535	2.0288	2.0194	2.0055	1.9936	1.9799	1.9566	1.9304	1.9132
2.5789	2.1259	2.1094	2.0925	2.0756	2.0590	2.0341	2.0031	1.9804
2.6044	2.2087	2.1855	2.1654	2.1439	2.1225	2.0951	2.0602	2.0322
2.6298	2.2676	2.2399	2.2157	2.1908	2.1657	2.1352	2.0958	2.0652
2.6552	2.2937	2.2670	2.2395	2.2114	2.1844	2.1489	2.1074	2.0751
2.6806	2.2975	2.2702	2.2406	2.2100	2.1850	2.1447	2.1043	2.0701
2.7060	2.2821	2.2535	2.2237	2.1929	2.1687	2.1291	2.0890	2.0567
2.7314	2.2447	2.2167	2.1872	2.1589	2.1363	2.0959	2.0580	2.0302
2.7568	2.1913	2.1632	2.1370	2.1127	2.0899	2.0515	2.0156	1.9897
2.7822	2.1242	2.0979	2.0753	2.0526	2.0301	1.9945	1.9630	1.9394
2.8076	2.0444	2.0225	2.0005	1.9816	1.9615	1.9283	1.9002	1.8806
2.8330	1.9601	1.9399	1.9208	1.9061	1.8870	1.8571	1.8334	1.8180
2.8584	1.8729	1.8560	1.8395	1.8291	1.8109	1.7861	1.7683	1.7540
2.8839	1.7823	1.7705	1.7570	1.7491	1.7333	1.7123	1.6954	1.6822
2.9093	1.6989	1.6886	1.6799	1.6715	1.6594	1.6407	1.6258	1.6146
2.9347	1.6201	1.6113	1.6042	1.5969	1.5885	1.5730	1.5614	1.5530
2.9601	1.5411	1.5349	1.5296	1.5264	1.5194	1.5079	1.4977	1.4939
2.9855	1.4637	1.4596	1.4561	1.4552	1.4505	1.4406	1.4328	1.4323
3.0109	1.3921	1.3887	1.3872	1.3874	1.3830	1.3775	1.3702	1.3712

Q (Å^{-1})	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
3.0363	1.3224	1.3213	1.3219	1.3231	1.3197	1.3154	1.3104	1.3129
3.0617	1.2588	1.2604	1.2610	1.2640	1.2636	1.2596	1.2576	1.2605
3.0871	1.1985	1.2012	1.2033	1.2070	1.2098	1.2093	1.2083	1.2126
3.1125	1.1456	1.1487	1.1520	1.1558	1.1611	1.1669	1.1665	1.1722
3.1379	1.0957	1.0971	1.1029	1.1064	1.1138	1.1264	1.1254	1.1313
3.1633	1.0465	1.0491	1.0551	1.0601	1.0669	1.0811	1.0791	1.0864
3.1888	1.0019	1.0053	1.0122	1.0165	1.0226	1.0319	1.0310	1.0386
3.2142	0.9595	0.9624	0.9696	0.9740	0.9803	0.9852	0.9861	0.9934
3.2396	0.9191	0.9209	0.9274	0.9345	0.9393	0.9432	0.9439	0.9515
3.2650	0.8815	0.8839	0.8893	0.8972	0.9032	0.9064	0.9065	0.9155
3.2904	0.8463	0.8494	0.8544	0.8611	0.8693	0.8714	0.8731	0.8821
3.3158	0.8131	0.8170	0.8212	0.8281	0.8359	0.8393	0.8399	0.8490
3.3412	0.7826	0.7859	0.7911	0.7964	0.8052	0.8076	0.8102	0.8187
3.3666	0.7532	0.7565	0.7620	0.7677	0.7760	0.7794	0.7822	0.7906
3.3920	0.7266	0.7319	0.7364	0.7439	0.7503	0.7538	0.7571	0.7650
3.4174	0.7035	0.7098	0.7140	0.7235	0.7286	0.7305	0.7355	0.7444
3.4428	0.6854	0.6915	0.6948	0.7051	0.7090	0.7126	0.7170	0.7267
3.4682	0.6709	0.6756	0.6798	0.6896	0.6933	0.6983	0.7019	0.7117
3.4937	0.6593	0.6630	0.6684	0.6762	0.6802	0.6854	0.6901	0.6986
3.5191	0.6508	0.6533	0.6599	0.6654	0.6708	0.6760	0.6819	0.6875
3.5445	0.6426	0.6448	0.6505	0.6565	0.6630	0.6670	0.6725	0.6791
3.5699	0.6342	0.6375	0.6437	0.6495	0.6574	0.6600	0.6638	0.6713
3.5953	0.6274	0.6338	0.6384	0.6447	0.6519	0.6562	0.6576	0.6652
3.6207	0.6236	0.6310	0.6339	0.6418	0.6471	0.6539	0.6534	0.6610
3.6461	0.6231	0.6283	0.6321	0.6399	0.6443	0.6506	0.6516	0.6595
3.6715	0.6233	0.6282	0.6331	0.6407	0.6457	0.6496	0.6521	0.6586
3.6969	0.6241	0.6294	0.6358	0.6425	0.6477	0.6521	0.6545	0.6598
3.7223	0.6257	0.6325	0.6391	0.6456	0.6515	0.6573	0.6570	0.6653
3.7477	0.6311	0.6363	0.6432	0.6495	0.6551	0.6603	0.6596	0.6671
3.7731	0.6365	0.6394	0.6460	0.6519	0.6572	0.6613	0.6617	0.6681
3.7986	0.6409	0.6452	0.6499	0.6557	0.6621	0.6637	0.6665	0.6722
3.8240	0.6475	0.6521	0.6557	0.6619	0.6695	0.6707	0.6739	0.6792
3.8494	0.6551	0.6603	0.6634	0.6693	0.6775	0.6802	0.6842	0.6884
3.8748	0.6644	0.6691	0.6729	0.6787	0.6864	0.6903	0.6922	0.6964
3.9002	0.6755	0.6792	0.6830	0.6887	0.6945	0.6979	0.6976	0.7036
3.9256	0.6863	0.6901	0.6949	0.6997	0.7037	0.7069	0.7063	0.7118
3.9510	0.6977	0.7010	0.7078	0.7104	0.7158	0.7187	0.7178	0.7223
3.9764	0.7102	0.7137	0.7208	0.7240	0.7285	0.7316	0.7305	0.7349
4.0018	0.7253	0.7292	0.7342	0.7401	0.7430	0.7458	0.7442	0.7487
4.0272	0.7417	0.7462	0.7488	0.7555	0.7588	0.7646	0.7594	0.7641
4.0526	0.7577	0.7628	0.7652	0.7701	0.7738	0.7816	0.7743	0.7804
4.0780	0.7739	0.7787	0.7827	0.7860	0.7889	0.7964	0.7914	0.7959
4.1035	0.7912	0.7951	0.8008	0.8040	0.8050	0.8097	0.8077	0.8110
4.1289	0.8121	0.8130	0.8192	0.8225	0.8232	0.8256	0.8227	0.8259
4.1543	0.8333	0.8334	0.8379	0.8403	0.8415	0.8438	0.8378	0.8408
4.1797	0.8531	0.8536	0.8571	0.8600	0.8610	0.8595	0.8556	0.8568
4.2051	0.8733	0.8754	0.8783	0.8804	0.8812	0.8791	0.8759	0.8757
4.2305	0.8932	0.8968	0.8981	0.8994	0.8999	0.8975	0.8937	0.8937
4.2559	0.9162	0.9193	0.9208	0.9212	0.9218	0.9172	0.9135	0.9133
4.2813	0.9404	0.9428	0.9434	0.9433	0.9442	0.9380	0.9337	0.9343
4.3067	0.9659	0.9647	0.9654	0.9652	0.9643	0.9586	0.9545	0.9529

Q (Å^{-1})	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
4.3321	0.9912	0.9883	0.9886	0.9875	0.9857	0.9819	0.9763	0.9750
4.3575	1.0132	1.0104	1.0117	1.0084	1.0090	1.0044	0.9977	0.9985
4.3829	1.0375	1.0348	1.0351	1.0304	1.0327	1.0323	1.0243	1.0288
4.4084	1.0625	1.0599	1.0577	1.0540	1.0586	1.0667	1.0590	1.0630
4.4338	1.0837	1.0820	1.0786	1.0760	1.0844	1.0898	1.0935	1.0942
4.4592	1.1064	1.1047	1.1008	1.0981	1.1072	1.1205	1.1168	1.1145
4.4846	1.1294	1.1273	1.1218	1.1187	1.1226	1.1273	1.1241	1.1208
4.5100	1.1531	1.1490	1.1415	1.1386	1.1386	1.1344	1.1286	1.1234
4.5354	1.1732	1.1690	1.1609	1.1577	1.1550	1.1460	1.1363	1.1302
4.5608	1.1894	1.1867	1.1801	1.1747	1.1694	1.1599	1.1466	1.1411
4.5862	1.2078	1.2039	1.1993	1.1924	1.1863	1.1755	1.1629	1.1559
4.6116	1.2266	1.2210	1.2171	1.2099	1.2031	1.1912	1.1783	1.1718
4.6370	1.2424	1.2366	1.2326	1.2249	1.2181	1.2045	1.1919	1.1848
4.6624	1.2556	1.2504	1.2461	1.2380	1.2307	1.2175	1.2041	1.1962
4.6878	1.2664	1.2616	1.2557	1.2467	1.2396	1.2266	1.2123	1.2045
4.7133	1.2781	1.2767	1.2672	1.2578	1.2539	1.2400	1.2235	1.2171
4.7387	1.2854	1.2882	1.2769	1.2660	1.2646	1.2447	1.2300	1.2250
4.7641	1.2915	1.2907	1.2809	1.2716	1.2664	1.2480	1.2340	1.2308
4.7895	1.2945	1.2898	1.2810	1.2761	1.2700	1.2533	1.2391	1.2347
4.8149	1.2917	1.2887	1.2820	1.2757	1.2701	1.2560	1.2419	1.2356
4.8403	1.2898	1.2880	1.2826	1.2749	1.2715	1.2563	1.2431	1.2363
4.8657	1.2880	1.2847	1.2788	1.2716	1.2727	1.2528	1.2421	1.23
4.8911	1.2846	1.2827	1.2766	1.2698	1.2708	1.2514	1.2409	1.2
4.9165	1.2812	1.2786	1.2734	1.2678	1.2650	1.2497	1.2371	1.2
4.9419	1.2777	1.2729	1.2703	1.2655	1.2617	1.2461	1.2360	1.22
4.9673	1.2705	1.2645	1.2645	1.2592	1.2548	1.2403	1.2315	1.2254
4.9927	1.2640	1.2597	1.2571	1.2527	1.2480	1.2360	1.2262	1.2219
5.0182	1.2557	1.2523	1.2485	1.2446	1.2412	1.2303	1.2205	1.2151
5.0436	1.2434	1.2412	1.2385	1.2365	1.2324	1.2207	1.2111	1.2051
5.0690	1.2331	1.2307	1.2292	1.2265	1.2207	1.2114	1.2020	1.1953
5.0944	1.2218	1.2209	1.2179	1.2162	1.2118	1.2016	1.1925	1.1856
5.1198	1.2101	1.2079	1.2059	1.2024	1.2023	1.1910	1.1821	1.1777
5.1452	1.1998	1.1980	1.1980	1.1933	1.1927	1.1819	1.1739	1.1695
5.1706	1.1897	1.1879	1.1867	1.1838	1.1823	1.1717	1.1641	1.1590
5.1960	1.1760	1.1729	1.1722	1.1710	1.1699	1.1568	1.1493	1.1464
5.2214	1.1653	1.1606	1.1597	1.1586	1.1567	1.1446	1.1371	1.1370
5.2468	1.1503	1.1473	1.1471	1.1443	1.1431	1.1339	1.1255	1.1258
5.2722	1.1360	1.1333	1.1342	1.1311	1.1301	1.1214	1.1129	1.1112
5.2976	1.1228	1.1208	1.1204	1.1182	1.1177	1.1097	1.1003	1.0973
5.3231	1.1094	1.1084	1.1059	1.1046	1.1037	1.0955	1.0881	1.0845
5.3485	1.0963	1.0933	1.0909	1.0909	1.0900	1.0811	1.0765	1.0743
5.3739	1.0805	1.0778	1.0754	1.0762	1.0762	1.0675	1.0626	1.0627
5.3993	1.0664	1.0643	1.0627	1.0634	1.0633	1.0550	1.0515	1.0523
5.4247	1.0512	1.0520	1.0492	1.0495	1.0504	1.0421	1.0402	1.0401
5.4501	1.0372	1.0393	1.0341	1.0364	1.0364	1.0313	1.0287	1.0302
5.4755	1.0204	1.0228	1.0202	1.0219	1.0223	1.0194	1.0163	1.0163
5.5009	1.0080	1.0088	1.0097	1.0099	1.0109	1.0092	1.0031	1.0043
5.5263	0.9952	0.9957	0.9974	0.9988	0.9990	0.9939	0.9904	0.9935
5.5517	0.9821	0.9830	0.9835	0.9839	0.9841	0.9800	0.9767	0.9799
5.5771	0.9708	0.9694	0.9712	0.9707	0.9728	0.9686	0.9666	0.9685
5.6025	0.9575	0.9548	0.9575	0.9593	0.9625	0.9591	0.9569	0.9587

Q ($Å^{-1}$)	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
5.6280	0.9445	0.9439	0.9453	0.9489	0.9516	0.9493	0.9460	0.9489
5.6534	0.9301	0.9318	0.9334	0.9373	0.9376	0.9373	0.9341	0.9374
5.6788	0.9192	0.9215	0.9228	0.9259	0.9262	0.9248	0.9252	0.9267
5.7042	0.9072	0.9097	0.9112	0.9132	0.9157	0.9137	0.9144	0.9165
5.7296	0.8980	0.8998	0.9001	0.9023	0.9060	0.9056	0.9044	0.9075
5.7550	0.8878	0.8917	0.8911	0.8943	0.8975	0.8983	0.8948	0.8989
5.7804	0.8784	0.8829	0.8829	0.8863	0.8882	0.8890	0.8861	0.8914
5.8058	0.8705	0.8749	0.8754	0.8796	0.8805	0.8828	0.8791	0.8859
5.8312	0.8627	0.8658	0.8672	0.8732	0.8734	0.8757	0.8724	0.8780
5.8566	0.8565	0.8590	0.8607	0.8665	0.8686	0.8685	0.8678	0.8719
5.8820	0.8488	0.8515	0.8538	0.8579	0.8625	0.8618	0.8618	0.8655
5.9074	0.8416	0.8448	0.8481	0.8515	0.8566	0.8559	0.8560	0.8600
5.9329	0.8354	0.8391	0.8435	0.8465	0.8517	0.8504	0.8536	0.8560
5.9583	0.8312	0.8332	0.8383	0.8407	0.8478	0.8453	0.8506	0.8522
5.9837	0.8280	0.8304	0.8333	0.8356	0.8437	0.8438	0.8459	0.8479
6.0091	0.8227	0.8272	0.8292	0.8314	0.8379	0.8399	0.8395	0.8420
6.0345	0.8223	0.8267	0.8290	0.8314	0.8375	0.8392	0.8389	0.8416
6.0599	0.8222	0.8263	0.8290	0.8316	0.8374	0.8387	0.8385	0.8415
6.0853	0.8224	0.8262	0.8292	0.8321	0.8373	0.8386	0.8385	0.8416
6.1107	0.8231	0.8265	0.8298	0.8330	0.8376	0.8390	0.8387	0.8420
1361	0.8244	0.8273	0.8308	0.8344	0.8384	0.8398	0.8394	0.8429
15	0.8262	0.8286	0.8323	0.8361	0.8398	0.8408	0.8405	0.8442
69	0.8286	0.8306	0.8344	0.8383	0.8416	0.8422	0.8420	0.8459
23	0.8315	0.8333	0.8370	0.8410	0.8439	0.8441	0.8439	0.8479
2378	0.8349	0.8365	0.8401	0.8443	0.8467	0.8466	0.8463	0.8504
6.2632	0.8389	0.8404	0.8438	0.8478	0.8499	0.8497	0.8491	0.8533
6.2886	0.8437	0.8449	0.8481	0.8519	0.8538	0.8534	0.8524	0.8566
6.3140	0.8490	0.8498	0.8529	0.8564	0.8581	0.8573	0.8561	0.8601
6.3394	0.8545	0.8550	0.8581	0.8612	0.8628	0.8615	0.8601	0.8639
6.3648	0.8602	0.8608	0.8636	0.8661	0.8679	0.8661	0.8644	0.8680
6.3902	0.8665	0.8668	0.8696	0.8715	0.8735	0.8714	0.8691	0.8723
6.4156	0.8732	0.8732	0.8757	0.8773	0.8794	0.8767	0.8740	0.8766
6.4410	0.8801	0.8798	0.8820	0.8832	0.8852	0.8821	0.8789	0.8810
6.4664	0.8870	0.8865	0.8884	0.8893	0.8912	0.8879	0.8841	0.8857
6.4918	0.8941	0.8932	0.8951	0.8959	0.8975	0.8938	0.8896	0.8906
6.5172	0.9017	0.9003	0.9020	0.9027	0.9041	0.8999	0.8953	0.8959
6.5427	0.9095	0.9075	0.9091	0.9096	0.9110	0.9062	0.9013	0.9016
6.5681	0.9173	0.9150	0.9163	0.9168	0.9180	0.9129	0.9076	0.9075
6.5935	0.9254	0.9226	0.9236	0.9242	0.9250	0.9198	0.9140	0.9137
6.6189	0.9336	0.9302	0.9310	0.9316	0.9321	0.9270	0.9207	0.9201
6.6443	0.9417	0.9379	0.9384	0.9387	0.9393	0.9339	0.9275	0.9269
6.6697	0.9498	0.9455	0.9459	0.9459	0.9463	0.9406	0.9343	0.9336
6.6951	0.9576	0.9532	0.9531	0.9529	0.9531	0.9472	0.9408	0.9401
6.7205	0.9652	0.9606	0.9602	0.9597	0.9594	0.9535	0.9470	0.9464
6.7459	0.9728	0.9679	0.9671	0.9663	0.9656	0.9600	0.9531	0.9526
6.7713	0.9799	0.9750	0.9737	0.9728	0.9716	0.9660	0.9592	0.9586
6.7967	0.9867	0.9820	0.9803	0.9791	0.9776	0.9718	0.9651	0.9646
6.8221	0.9934	0.9888	0.9868	0.9853	0.9834	0.9777	0.9710	0.9705
6.8476	0.9998	0.9955	0.9929	0.9914	0.9892	0.9837	0.9769	0.9763
6.8730	1.0059	1.0020	0.9987	0.9973	0.9948	0.9896	0.9826	0.9818
6.8984	1.0120	1.0081	1.0044	1.0031	1.0002	0.9953	0.9882	0.9872

Q ($Å^{-1}$)	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
6.9238	1.0178	1.0138	1.0099	1.0086	1.0053	1.0005	0.9934	0.9923
6.9492	1.0229	1.0190	1.0150	1.0137	1.0099	1.0055	0.9982	0.9969
6.9746	1.0274	1.0238	1.0197	1.0185	1.0144	1.0102	1.0030	1.0010
7.0000	1.0317	1.0283	1.0241	1.0231	1.0189	1.0146	1.0074	1.0049
7.0254	1.0357	1.0324	1.0283	1.0272	1.0232	1.0186	1.0112	1.0085
7.0508	1.0392	1.0360	1.0320	1.0310	1.0272	1.0222	1.0147	1.0120
7.0762	1.0422	1.0389	1.0354	1.0343	1.0305	1.0255	1.0178	1.0151
7.1016	1.0449	1.0412	1.0382	1.0371	1.0334	1.0284	1.0206	1.0179
7.1270	1.0469	1.0428	1.0405	1.0391	1.0357	1.0303	1.0229	1.0200
7.1525	1.0486	1.0440	1.0423	1.0404	1.0374	1.0315	1.0248	1.0216
7.1779	1.0497	1.0449	1.0434	1.0414	1.0387	1.0324	1.0260	1.0227
7.2033	1.0502	1.0454	1.0441	1.0418	1.0395	1.0330	1.0268	1.0234
7.2287	1.0500	1.0453	1.0444	1.0417	1.0400	1.0333	1.0273	1.0240
7.2541	1.0495	1.0452	1.0445	1.0418	1.0405	1.0335	1.0279	1.0247
7.2795	1.0487	1.0450	1.0444	1.0420	1.0408	1.0335	1.0283	1.0255
7.3049	1.0477	1.0447	1.0439	1.0419	1.0409	1.0337	1.0285	1.0264
7.3303	1.0467	1.0439	1.0431	1.0414	1.0408	1.0339	1.0286	1.0268
7.3557	1.0455	1.0431	1.0420	1.0409	1.0407	1.0340	1.0285	1.0272
7.3811	1.0442	1.0421	1.0407	1.0402	1.0401	1.0337	1.0283	1.0274
7.4065	1.0429	1.0410	1.0394	1.0393	1.0393	1.0330	1.0279	1.0274
7.4319	1.0413	1.0396	1.0378	1.0380	1.0381	1.0319	1.0273	1.0270
7.4574	1.0393	1.0380	1.0361	1.0365	1.0366	1.0308	1.0268	1.0266
7.4828	1.0371	1.0362	1.0345	1.0349	1.0352	1.0301	1.0263	1.0264
7.5082	1.0350	1.0344	1.0328	1.0333	1.0337	1.0298	1.0260	1.0263
7.5336	1.0330	1.0325	1.0311	1.0317	1.0320	1.0295	1.0255	1.0259
7.5590	1.0308	1.0304	1.0293	1.0300	1.0300	1.0289	1.0248	1.0257
7.5844	1.0285	1.0279	1.0272	1.0278	1.0278	1.0279	1.0240	1.0252
7.6098	1.0260	1.0253	1.0249	1.0254	1.0254	1.0264	1.0229	1.0241
7.6352	1.0232	1.0225	1.0223	1.0227	1.0227	1.0244	1.0213	1.0223
7.6606	1.0202	1.0196	1.0197	1.0198	1.0199	1.0222	1.0194	1.0203
7.6860	1.0168	1.0166	1.0168	1.0167	1.0172	1.0200	1.0173	1.0180
7.7114	1.0129	1.0134	1.0135	1.0135	1.0144	1.0175	1.0148	1.0156
7.7368	1.0091	1.0102	1.0100	1.0103	1.0116	1.0147	1.0120	1.0130
7.7623	1.0055	1.0070	1.0067	1.0076	1.0089	1.0116	1.0087	1.0101
7.7877	1.0018	1.0038	1.0032	1.0046	1.0062	1.0084	1.0053	1.0071
7.8131	0.9977	1.0002	0.9994	1.0013	1.0031	1.0047	1.0012	1.0036
7.8385	0.9938	0.9965	0.9956	0.9979	1.0000	1.0006	0.9970	0.9997
7.8639	0.9901	0.9929	0.9917	0.9945	0.9969	0.9965	0.9927	0.9957
7.8893	0.9867	0.9894	0.9880	0.9912	0.9937	0.9919	0.9886	0.9918
7.9147	0.9834	0.9859	0.9847	0.9877	0.9904	0.9877	0.9846	0.9879
7.9401	0.9799	0.9826	0.9818	0.9841	0.9873	0.9839	0.9806	0.9841
7.9655	0.9763	0.9793	0.9790	0.9808	0.9842	0.9808	0.9771	0.9809
7.9909	0.9730	0.9758	0.9763	0.9775	0.9811	0.9781	0.9740	0.9778
8.0163	0.9698	0.9725	0.9735	0.9744	0.9781	0.9754	0.9711	0.9746
8.0417	0.9668	0.9694	0.9709	0.9715	0.9750	0.9726	0.9682	0.9716
8.0672	0.9639	0.9665	0.9684	0.9688	0.9721	0.9700	0.9658	0.9692
8.0926	0.9610	0.9635	0.9659	0.9661	0.9692	0.9676	0.9635	0.9666
8.1180	0.9582	0.9607	0.9616	0.9636	0.9664	0.9651	0.9611	0.9639
8.1434	0.9555	0.9580	0.9578	0.9611	0.9635	0.9623	0.9586	0.9613
8.1688	0.9531	0.9553	0.9564	0.9587	0.9607	0.9595	0.9562	0.9589
8.1942	0.9507	0.9525	0.9563	0.9563	0.9582	0.9570	0.9540	0.9567

Q (Å^{-1})	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
8.2196	0.9485	0.9500	0.9558	0.9541	0.9557	0.9546	0.9518	0.9548
8.2450	0.9465	0.9477	0.9554	0.9523	0.9533	0.9523	0.9499	0.9529
8.2704	0.9447	0.9456	0.9549	0.9506	0.9511	0.9501	0.9481	0.9512
8.2958	0.9429	0.9436	0.9541	0.9489	0.9490	0.9481	0.9465	0.9496
8.3212	0.9415	0.9418	0.9533	0.9471	0.9473	0.9461	0.9447	0.9478
8.3466	0.9404	0.9403	0.9525	0.9456	0.9460	0.9444	0.9432	0.9461
8.3721	0.9395	0.9390	0.9517	0.9444	0.9448	0.9430	0.9419	0.9448
8.3975	0.9388	0.9379	0.9511	0.9433	0.9437	0.9417	0.9409	0.9437
8.4229	0.9381	0.9371	0.9503	0.9422	0.9427	0.9410	0.9401	0.9427
8.4483	0.9375	0.9367	0.9495	0.9414	0.9423	0.9407	0.9395	0.9421
8.4737	0.9372	0.9363	0.9482	0.9408	0.9420	0.9404	0.9392	0.9414
8.4991	0.9372	0.9360	0.9468	0.9403	0.9418	0.9401	0.9390	0.9406
8.5245	0.9374	0.9362	0.9454	0.9400	0.9417	0.9398	0.9388	0.9400
8.5499	0.9378	0.9368	0.9442	0.9402	0.9421	0.9398	0.9391	0.9398
8.5753	0.9384	0.9378	0.9428	0.9406	0.9427	0.9401	0.9397	0.9399
8.6007	0.9390	0.9389	0.9412	0.9411	0.9435	0.9406	0.9400	0.9403
8.6261	0.9399	0.9403	0.9396	0.9418	0.9445	0.9412	0.9403	0.9408
8.6515	0.9414	0.9418	0.9408	0.9428	0.9459	0.9419	0.9411	0.9417
8.6770	0.9434	0.9436	0.9440	0.9443	0.9475	0.9434	0.9423	0.9430
8.7024	0.9454	0.9457	0.9467	0.9464	0.9491	0.9451	0.9438	0.9446
8.7278	0.9475	0.9479	0.9486	0.9488	0.9509	0.9469	0.9454	0.9464
8.7532	0.9497	0.9502	0.9506	0.9513	0.9527	0.9492	0.9471	0.9480
8.7786	0.9522	0.9524	0.9526	0.9537	0.9548	0.9516	0.9489	0.9498
8.8040	0.9548	0.9547	0.9548	0.9560	0.9569	0.9543	0.9506	0.9515
8.8294	0.9576	0.9571	0.9570	0.9583	0.9590	0.9567	0.9522	0.9532
8.8548	0.9601	0.9595	0.9594	0.9609	0.9609	0.9590	0.9539	0.9553
8.8802	0.9626	0.9619	0.9621	0.9635	0.9629	0.9613	0.9559	0.9577
8.9056	0.9654	0.9645	0.9647	0.9663	0.9654	0.9637	0.9584	0.9602
8.9310	0.9686	0.9673	0.9675	0.9691	0.9680	0.9663	0.9608	0.9627
8.9565	0.9719	0.9699	0.9701	0.9719	0.9707	0.9689	0.9633	0.9649
8.9819	0.9752	0.9726	0.9726	0.9745	0.9734	0.9712	0.9655	0.9669
9.0073	0.9782	0.9757	0.9754	0.9772	0.9760	0.9735	0.9679	0.9692
9.0327	0.9814	0.9789	0.9785	0.9799	0.9785	0.9756	0.9705	0.9717
9.0581	0.9847	0.9820	0.9815	0.9827	0.9812	0.9777	0.9733	0.9743
9.0835	0.9877	0.9850	0.9842	0.9854	0.9838	0.9799	0.9762	0.9769
9.1089	0.9911	0.9881	0.9873	0.9883	0.9869	0.9822	0.9790	0.9794
9.1343	0.9947	0.9913	0.9905	0.9912	0.9905	0.9845	0.9820	0.9819
9.1597	0.9986	0.9946	0.9935	0.9942	0.9938	0.9870	0.9852	0.9846
9.1851	1.0023	0.9980	0.9963	0.9974	0.9968	0.9897	0.9884	0.9873
9.2105	1.0058	1.0016	0.9992	1.0007	0.9997	0.9923	0.9914	0.9897
9.2359	1.0090	1.0050	1.0019	1.0039	1.0026	0.9953	0.9944	0.9921
9.2614	1.0123	1.0086	1.0045	1.0072	1.0056	0.9987	0.9973	0.9947
9.2868	1.0155	1.0120	1.0074	1.0103	1.0086	1.0019	1.0000	0.9974
9.3122	1.0184	1.0151	1.0102	1.0133	1.0113	1.0046	1.0025	1.0000
9.3376	1.0208	1.0178	1.0130	1.0158	1.0136	1.0069	1.0045	1.0025
9.3630	1.0227	1.0203	1.0156	1.0183	1.0160	1.0091	1.0065	1.0050
9.3884	1.0245	1.0226	1.0179	1.0207	1.0184	1.0113	1.0086	1.0073
9.4138	1.0262	1.0248	1.0201	1.0226	1.0205	1.0134	1.0103	1.0094
9.4392	1.0276	1.0266	1.0220	1.0241	1.0222	1.0153	1.0116	1.0110
9.4646	1.0283	1.0280	1.0238	1.0251	1.0236	1.0173	1.0128	1.0124
9.4900	1.0290	1.0292	1.0256	1.0260	1.0249	1.0191	1.0139	1.0139

Q (Å^{-1})	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
9.5154	1.0297	1.0301	1.0271	1.0266	1.0257	1.0204	1.0148	1.0156
9.5408	1.0304	1.0302	1.0279	1.0269	1.0265	1.0214	1.0157	1.0168
9.5663	1.0309	1.0302	1.0286	1.0270	1.0272	1.0224	1.0166	1.0178
9.5917	1.0316	1.0301	1.0292	1.0271	1.0279	1.0231	1.0174	1.0188
9.6171	1.0327	1.0301	1.0300	1.0273	1.0289	1.0237	1.0180	1.0196
9.6425	1.0336	1.0300	1.0302	1.0273	1.0296	1.0242	1.0187	1.0205
9.6679	1.0344	1.0300	1.0300	1.0273	1.0299	1.0249	1.0193	1.0212
9.6933	1.0347	1.0300	1.0295	1.0271	1.0299	1.0254	1.0199	1.0214
9.7187	1.0347	1.0302	1.0287	1.0270	1.0300	1.0256	1.0207	1.0216
9.7441	1.0344	1.0301	1.0281	1.0272	1.0300	1.0261	1.0214	1.0221
9.7695	1.0342	1.0302	1.0282	1.0276	1.0300	1.0264	1.0219	1.0227
9.7949	1.0340	1.0302	1.0285	1.0276	1.0300	1.0262	1.0221	1.0230
9.8203	1.0333	1.0302	1.0283	1.0273	1.0296	1.0254	1.0223	1.0231
9.8457	1.0325	1.0300	1.0276	1.0271	1.0292	1.0247	1.0223	1.0231
9.8712	1.0315	1.0297	1.0266	1.0269	1.0288	1.0242	1.0223	1.0228
9.8966	1.0303	1.0292	1.0262	1.0267	1.0282	1.0240	1.0225	1.0225
9.9220	1.0287	1.0285	1.0258	1.0260	1.0275	1.0237	1.0221	1.0222
9.9474	1.0268	1.0278	1.0254	1.0252	1.0270	1.0233	1.0217	1.0215
9.9728	1.0253	1.0265	1.0247	1.0245	1.0266	1.0227	1.0212	1.0211
9.9982	1.0244	1.0252	1.0240	1.0238	1.0259	1.0219	1.0206	1.0209
10.0236	1.0234	1.0239	1.0229	1.0227	1.0250	1.0209	1.0197	1.020
10.0490	1.0221	1.0225	1.0216	1.0214	1.0238	1.0199	1.0188	1
10.0744	1.0211	1.0209	1.0205	1.0204	1.0224	1.0188	1.0178	
10.0998	1.0204	1.0192	1.0197	1.0195	1.0212	1.0176	1.0166	
10.1252	1.0196	1.0175	1.0187	1.0183	1.0200	1.0167	1.0154	1.
10.1506	1.0187	1.0160	1.0175	1.0169	1.0189	1.0160	1.0143	1.013
10.1761	1.0176	1.0145	1.0161	1.0156	1.0178	1.0154	1.0131	1.0162
10.2015	1.0162	1.0130	1.0146	1.0142	1.0165	1.0147	1.0116	1.0152
10.2269	1.0148	1.0116	1.0136	1.0132	1.0152	1.0142	1.0105	1.0141
10.2523	1.0136	1.0102	1.0131	1.0124	1.0136	1.0139	1.0095	1.0132
10.2777	1.0126	1.0093	1.0128	1.0117	1.0123	1.0136	1.0086	1.0125
10.3031	1.0120	1.0089	1.0126	1.0110	1.0116	1.0138	1.0081	1.0118
10.3285	1.0114	1.0085	1.0119	1.0101	1.0112	1.0139	1.0079	1.0113
10.3539	1.0110	1.0081	1.0109	1.0098	1.0109	1.0138	1.0079	1.0108
10.3793	1.0105	1.0075	1.0102	1.0095	1.0107	1.0140	1.0080	1.0102
10.4047	1.0098	1.0066	1.0100	1.0094	1.0107	1.0144	1.0084	1.0097
10.4301	1.0090	1.0059	1.0094	1.0094	1.0108	1.0144	1.0084	1.0091
10.4555	1.0086	1.0056	1.0090	1.0096	1.0113	1.0145	1.0087	1.0085
10.4810	1.0085	1.0053	1.0085	1.0096	1.0116	1.0144	1.0090	1.0085
10.5064	1.0085	1.0052	1.0085	1.0100	1.0117	1.0145	1.0095	1.0084
10.5318	1.0084	1.0051	1.0082	1.0102	1.0115	1.0145	1.0100	1.0080
10.5572	1.0081	1.0051	1.0082	1.0106	1.0111	1.0138	1.0105	1.0080
10.5826	1.0079	1.0050	1.0081	1.0108	1.0109	1.0131	1.0110	1.0083
10.6080	1.0079	1.0052	1.0080	1.0108	1.0106	1.0124	1.0112	1.0086
10.6334	1.0078	1.0053	1.0078	1.0104	1.0105	1.0124	1.0113	1.0089
10.6588	1.0079	1.0052	1.0074	1.0101	1.0103	1.0130	1.0112	1.0092
10.6842	1.0080	1.0053	1.0069	1.0100	1.0099	1.0148	1.0105	1.0093
10.7096	1.0080	1.0052	1.0064	1.0098	1.0094	1.0143	1.0096	1.0094
10.7350	1.0078	1.0048	1.0060	1.0092	1.0086	1.0135	1.0088	1.0095
10.7604	1.0078	1.0045	1.0054	1.0085	1.0079	1.0123	1.0081	1.0096
10.7859	1.0078	1.0046	1.0049	1.0080	1.0076	1.0112	1.0075	1.0097

Q ($Å^{-1}$)	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
10.8113	1.0079	1.0048	1.0044	1.0072	1.0075	1.0103	1.0074	1.0099
10.8367	1.0076	1.0051	1.0035	1.0063	1.0076	1.0092	1.0072	1.0101
10.8621	1.0072	1.0053	1.0029	1.0059	1.0077	1.0081	1.0070	1.0106
10.8875	1.0069	1.0054	1.0025	1.0059	1.0079	1.0075	1.0070	1.0111
10.9129	1.0067	1.0055	1.0025	1.0061	1.0079	1.0070	1.0069	1.0112
10.9383	1.0064	1.0060	1.0026	1.0064	1.0078	1.0064	1.0065	1.0112
10.9637	1.0061	1.0062	1.0029	1.0066	1.0077	1.0059	1.0062	1.0111
10.9891	1.0056	1.0062	1.0034	1.0068	1.0076	1.0056	1.0061	1.0112
11.0145	1.0053	1.0064	1.0041	1.0073	1.0075	1.0054	1.0061	1.0112
11.0399	1.0049	1.0065	1.0050	1.0075	1.0074	1.0058	1.0063	1.0111
11.0654	1.0046	1.0068	1.0060	1.0081	1.0075	1.0064	1.0058	1.0108
11.0908	1.0048	1.0069	1.0067	1.0084	1.0081	1.0069	1.0072	1.0101
11.1162	1.0052	1.0069	1.0073	1.0084	1.0087	1.0071	1.0071	1.0094
11.1416	1.0057	1.0067	1.0078	1.0083	1.0091	1.0069	1.0069	1.0088
11.1670	1.0062	1.0063	1.0080	1.0078	1.0093	1.0073	1.0067	1.0082
11.1924	1.0070	1.0060	1.0086	1.0073	1.0095	1.0078	1.0062	1.0073
11.2178	1.0079	1.0056	1.0093	1.0066	1.0096	1.0079	1.0057	1.0065
11.2432	1.0091	1.0053	1.0096	1.0058	1.0096	1.0081	1.0057	1.0056
11.2686	1.0104	1.0056	1.0101	1.0053	1.0098	1.0086	1.0060	1.0049
11.2940	1.0111	1.0060	1.0107	1.0051	1.0102	1.0092	1.0064	1.0047
11.3194	1.0116	1.0065	1.0110	1.0052	1.0105	1.0095	1.0070	1.0052
11.3448	1.0123	1.0072	1.0113	1.0059	1.0109	1.0099	1.0075	1.0063
11.3703	1.0133	1.0077	1.0118	1.0067	1.0116	1.0107	1.0078	1.0077
11.3957	1.0141	1.0082	1.0122	1.0074	1.0117	1.0116	1.0080	1.0086
11.4211	1.0146	1.0087	1.0127	1.0081	1.0115	1.0123	1.0083	1.0091
11.4465	1.0147	1.0091	1.0127	1.0090	1.0112	1.0124	1.0081	1.0096
11.4719	1.0148	1.0091	1.0126	1.0097	1.0112	1.0125	1.0078	1.0103
11.4973	1.0148	1.0095	1.0127	1.0110	1.0117	1.0131	1.0077	1.0109
11.5227	1.0150	1.0102	1.0129	1.0124	1.0124	1.0135	1.0078	1.0114
11.5481	1.0151	1.0107	1.0134	1.0141	1.0136	1.0143	1.0082	1.0118
11.5735	1.0156	1.0116	1.0143	1.0160	1.0150	1.0150	1.0087	1.0120
11.5989	1.0167	1.0129	1.0153	1.0176	1.0165	1.0155	1.0094	1.0127
11.6243	1.0173	1.0137	1.0162	1.0191	1.0176	1.0156	1.0098	1.0137
11.6497	1.0182	1.0146	1.0172	1.0198	1.0185	1.0162	1.0104	1.0143
11.6752	1.0196	1.0154	1.0183	1.0198	1.0191	1.0176	1.0111	1.0146
11.7006	1.0212	1.0167	1.0200	1.0203	1.0198	1.0189	1.0118	1.0151
11.7260	1.0228	1.0182	1.0216	1.0210	1.0205	1.0201	1.0127	1.0156
11.7514	1.0242	1.0195	1.0230	1.0217	1.0211	1.0214	1.0138	1.0161
11.7768	1.0255	1.0212	1.0247	1.0224	1.0218	1.0221	1.0152	1.0174
11.8022	1.0267	1.0223	1.0261	1.0233	1.0226	1.0220	1.0168	1.0188
11.8276	1.0279	1.0234	1.0271	1.0244	1.0234	1.0222	1.0182	1.0203
11.8530	1.0290	1.0245	1.0280	1.0253	1.0240	1.0231	1.0195	1.0214
11.8784	1.0298	1.0255	1.0288	1.0259	1.0245	1.0242	1.0205	1.0222
11.9038	1.0306	1.0263	1.0294	1.0266	1.0247	1.0253	1.0214	1.0228
11.9292	1.0312	1.0272	1.0296	1.0274	1.0249	1.0260	1.0225	1.0234
11.9546	1.0314	1.0279	1.0295	1.0282	1.0256	1.0262	1.0230	1.0240
11.9801	1.0313	1.0286	1.0295	1.0290	1.0268	1.0268	1.0232	1.0246
12.0055	1.0309	1.0293	1.0295	1.0299	1.0280	1.0277	1.0234	1.0250
12.0309	1.0308	1.0298	1.0297	1.0308	1.0290	1.0284	1.0238	1.0251
12.0563	1.0309	1.0301	1.0304	1.0318	1.0301	1.0290	1.0241	1.0253
12.0817	1.0315	1.0305	1.0314	1.0327	1.0312	1.0293	1.0246	1.0258

Q ($Å^{-1}$)	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
12.1071	1.0313	1.0307	1.0323	1.0333	1.0325	1.0294	1.0253	1.0263
12.1325	1.0327	1.0309	1.0331	1.0337	1.0333	1.0301	1.0255	1.0264
12.1579	1.0339	1.0319	1.0342	1.0336	1.0338	1.0314	1.0258	1.0265
12.1833	1.0349	1.0328	1.0349	1.0334	1.0343	1.0323	1.0262	1.0271
12.2087	1.0357	1.0337	1.0352	1.0336	1.0351	1.0327	1.0265	1.0276
12.2341	1.0362	1.0344	1.0354	1.0335	1.0361	1.0324	1.0266	1.0279
12.2595	1.0370	1.0345	1.0358	1.0332	1.0370	1.0317	1.0271	1.0283
12.2850	1.0381	1.0350	1.0366	1.0336	1.0381	1.0310	1.0281	1.0291
12.3104	1.0388	1.0346	1.0367	1.0343	1.0389	1.0305	1.0287	1.0299
12.3358	1.0390	1.0348	1.0369	1.0351	1.0395	1.0306	1.0296	1.0308
12.3612	1.0397	1.0354	1.0373	1.0359	1.0396	1.0307	1.0308	1.0314
12.3866	1.0409	1.0357	1.0375	1.0365	1.0395	1.0308	1.0318	1.0323
12.4120	1.0417	1.0361	1.0375	1.0367	1.0398	1.0316	1.0331	1.0337
12.4374	1.0419	1.0370	1.0373	1.0373	1.0402	1.0325	1.0345	1.0347
12.4628	1.0416	1.0380	1.0368	1.0377	1.0406	1.0328	1.0350	1.0352
12.4882	1.0410	1.0387	1.0367	1.0377	1.0406	1.0338	1.0350	1.0357
12.5136	1.0406	1.0391	1.0374	1.0375	1.0403	1.0348	1.0354	1.0359
12.5390	1.0412	1.0396	1.0380	1.0374	1.0398	1.0356	1.0358	1.0358
12.5644	1.0413	1.0402	1.0386	1.0373	1.0396	1.0365	1.0360	1.0355
12.5899	1.0407	1.0405	1.0390	1.0370	1.0394	1.0377	1.0361	1.0350
12.6153	1.0400	1.0412	1.0395	1.0367	1.0390	1.0388	1.0360	1.0343
12.6407	1.0394	1.0421	1.0398	1.0361	1.0385	1.0398	1.0357	1.0337
12.6661	1.0388	1.0423	1.0396	1.0354	1.0383	1.0400	1.0350	1.0335
12.6915	1.0373	1.0414	1.0382	1.0345	1.0381	1.0394	1.0338	1.0329
12.7169	1.0358	1.0400	1.0369	1.0335	1.0379	1.0386	1.0326	1.0320
12.7423	1.0342	1.0387	1.0361	1.0330	1.0377	1.0374	1.0316	1.0312
12.7677	1.0335	1.0376	1.0360	1.0333	1.0377	1.0370	1.0315	1.0315
12.7931	1.0320	1.0354	1.0348	1.0325	1.0363	1.0362	1.0307	1.0310
12.8185	1.0298	1.0322	1.0320	1.0309	1.0338	1.0345	1.0293	1.0294
12.8439	1.0277	1.0295	1.0293	1.0292	1.0313	1.0323	1.0279	1.0274
12.8693	1.0263	1.0270	1.0269	1.0273	1.0287	1.0303	1.0266	1.0255
12.8948	1.0247	1.0243	1.0242	1.0254	1.0264	1.0282	1.0251	1.0239
12.9202	1.0232	1.0221	1.0217	1.0240	1.0245	1.0264	1.0240	1.0229
12.9456	1.0219	1.0200	1.0190	1.0228	1.0225	1.0244	1.0230	1.0209
12.9710	1.0206	1.0177	1.0167	1.0209	1.0203	1.0220	1.0210	1.0191
12.9964	1.0199	1.0155	1.0150	1.0190	1.0185	1.0206	1.0190	1.0178
13.0218	1.0195	1.0141	1.0134	1.0172	1.0174	1.0193	1.0173	1.0167
13.0472	1.0187	1.0130	1.0115	1.0156	1.0165	1.0183	1.0153	1.0154
13.0726	1.0168	1.0116	1.0098	1.0141	1.0149	1.0170	1.0132	1.0134
13.0980	1.0144	1.0102	1.0087	1.0130	1.0131	1.0154	1.0108	1.0118
13.1234	1.0124	1.0087	1.0078	1.0114	1.0117	1.0136	1.0084	1.0108
13.1488	1.0106	1.0072	1.0064	1.0097	1.0105	1.0123	1.0064	1.0103
13.1742	1.0083	1.0056	1.0048	1.0081	1.0093	1.0110	1.0046	1.0098
13.1997	1.0058	1.0044	1.0032	1.0070	1.0076	1.0097	1.0031	1.0091
13.2251	1.0033	1.0030	1.0017	1.0059	1.0056	1.0085	1.0019	1.0081
13.2505	1.0011	1.0018	1.0006	1.0049	1.0036	1.0075	1.0010	1.0072
13.2759	0.9985	1.0008	0.9993	1.0035	1.0014	1.0070	1.0000	1.0064
13.3013	0.9948	0.9986	0.9967	1.0008	0.9979	1.0054	0.9980	1.0041
13.3267	0.9915	0.9966	0.9943	0.9987	0.9945	1.0034	0.9961	1.0015
13.3521	0.9884	0.9948	0.9927	0.9971	0.9918	1.0007	0.9943	0.9990
13.3775	0.9862	0.9934	0.9918	0.9953	0.9895	0.9983	0.9931	0.9970

Q ($Å^{-1}$)	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
13.4029	0.9842	0.9916	0.9905	0.9932	0.9873	0.9955	0.9919	0.9945
13.4283	0.9830	0.9898	0.9896	0.9917	0.9855	0.9933	0.9907	0.9918
13.4537	0.9822	0.9880	0.9891	0.9900	0.9843	0.9918	0.9897	0.9889
13.4791	0.9816	0.9867	0.9885	0.9889	0.9834	0.9903	0.9883	0.9871
13.5046	0.9816	0.9857	0.9876	0.9886	0.9832	0.9892	0.9870	0.9854
13.5300	0.9820	0.9849	0.9863	0.9881	0.9830	0.9882	0.9855	0.9840
13.5554	0.9830	0.9844	0.9857	0.9881	0.9830	0.9877	0.9843	0.9833
13.5808	0.9842	0.9836	0.9859	0.9878	0.9831	0.9867	0.9833	0.9829
13.6062	0.9852	0.9831	0.9862	0.9874	0.9841	0.9864	0.9824	0.9832
13.6316	0.9864	0.9830	0.9865	0.9869	0.9853	0.9865	0.9821	0.9834
13.6570	0.9879	0.9840	0.9866	0.9871	0.9865	0.9868	0.9825	0.9839
13.6824	0.9894	0.9854	0.9867	0.9879	0.9880	0.9874	0.9835	0.9846
13.7078	0.9912	0.9864	0.9875	0.9896	0.9899	0.9881	0.9846	0.9855
13.7332	0.9929	0.9871	0.9880	0.9907	0.9920	0.9889	0.9857	0.9862
13.7586	0.9946	0.9887	0.9893	0.9918	0.9935	0.9903	0.9874	0.9878
13.7840	0.9963	0.9906	0.9908	0.9933	0.9950	0.9924	0.9893	0.9897
13.8095	0.9980	0.9926	0.9923	0.9957	0.9962	0.9945	0.9919	0.9918
13.8349	1.0001	0.9946	0.9940	0.9983	0.9973	0.9967	0.9950	0.9940
13.8603	1.0020	0.9966	0.9956	1.0004	0.9989	0.9984	0.9975	0.9957
13.8857	1.0035	0.9987	0.9966	1.0018	1.0010	1.0001	1.0004	0.9975
13.9111	1.0044	1.0009	0.9977	1.0034	1.0027	1.0016	1.0035	0.9991
13.9365	1.0056	1.0031	0.9995	1.0053	1.0045	1.0030	1.0061	1.0006
13.9619	1.0072	1.0053	1.0013	1.0070	1.0060	1.0039	1.0084	1.0024
13.9873	1.0085	1.0070	1.0021	1.0086	1.0068	1.0042	1.0100	1.0040
14.0127	1.0098	1.0085	1.0024	1.0096	1.0070	1.0048	1.0109	1.0051
14.0381	1.0114	1.0097	1.0025	1.0101	1.0074	1.0060	1.0116	1.0067
14.0635	1.0127	1.0110	1.0031	1.0102	1.0084	1.0070	1.0122	1.0086
14.0889	1.0130	1.0116	1.0038	1.0095	1.0094	1.0067	1.0122	1.0093
14.1144	1.0126	1.0116	1.0041	1.0082	1.0095	1.0060	1.0114	1.0089
14.1398	1.0118	1.0114	1.0046	1.0066	1.0089	1.0046	1.0104	1.0080
14.1652	1.0105	1.0112	1.0043	1.0048	1.0083	1.0030	1.0091	1.0075
14.1906	1.0088	1.0107	1.0043	1.0027	1.0080	1.0016	1.0081	1.0070
14.2160	1.0068	1.0093	1.0046	1.0008	1.0081	1.0000	1.0065	1.0060
14.2414	1.0051	1.0075	1.0044	0.9991	1.0074	0.9980	1.0046	1.0049
14.2668	1.0029	1.0052	1.0042	0.9981	1.0059	0.9966	1.0027	1.0037
14.2922	1.0008	1.0028	1.0039	0.9980	1.0042	0.9963	1.0008	1.0027
14.3176	0.9983	1.0001	1.0032	0.9974	1.0021	0.9955	0.9990	1.0015
14.3430	0.9963	0.9979	1.0024	0.9965	1.0005	0.9948	0.9977	1.0004
14.3684	0.9942	0.9953	1.0014	0.9955	0.9991	0.9947	0.9962	0.9996
14.3938	0.9920	0.9928	1.0001	0.9943	0.9973	0.9940	0.9951	0.9990
14.4193	0.9900	0.9912	0.9991	0.9932	0.9958	0.9928	0.9938	0.9985
14.4447	0.9895	0.9901	0.9984	0.9923	0.9945	0.9921	0.9925	0.9976
14.4701	0.9890	0.9891	0.9981	0.9914	0.9934	0.9922	0.9917	0.9968
14.4955	0.9887	0.9886	0.9973	0.9909	0.9922	0.9930	0.9915	0.9964
14.5209	0.9888	0.9889	0.9965	0.9912	0.9918	0.9939	0.9916	0.9965
14.5463	0.9895	0.9898	0.9957	0.9913	0.9919	0.9952	0.9922	0.9967
14.5717	0.9906	0.9915	0.9949	0.9918	0.9925	0.9963	0.9927	0.9969
14.5971	0.9926	0.9933	0.9943	0.9926	0.9929	0.9971	0.9931	0.9969
14.6225	0.9949	0.9954	0.9945	0.9932	0.9934	0.9981	0.9940	0.9977
14.6479	0.9966	0.9981	0.9954	0.9938	0.9945	0.9996	0.9957	0.9987
14.6733	0.9984	1.0013	0.9973	0.9951	0.9967	1.0012	0.9980	1.0004

Q ($Å^{-1}$)	S(Q) 938K	S(Q) 963K	S(Q) 988K	S(Q) 1013K	S(Q) 1038K	S(Q) 1063K	S(Q) 1088K	S(Q) 1113K
14.6987	1.0011	1.0042	1.0002	0.9970	0.9997	1.0029	1.0008	1.0025
14.7242	1.0044	1.0066	1.0032	1.0000	1.0029	1.0045	1.0035	1.0049
14.7496	1.0077	1.0090	1.0059	1.0039	1.0056	1.0059	1.0060	1.0073
14.7750	1.0103	1.0115	1.0089	1.0078	1.0080	1.0083	1.0088	1.0098
14.8004	1.0132	1.0143	1.0123	1.0115	1.0105	1.0115	1.0119	1.0124
14.8258	1.0159	1.0168	1.0157	1.0144	1.0131	1.0145	1.0152	1.0149
14.8512	1.0185	1.0194	1.0191	1.0177	1.0160	1.0183	1.0188	1.0179
14.8766	1.0208	1.0216	1.0223	1.0208	1.0188	1.0225	1.0222	1.0209
14.9020	1.0225	1.0238	1.0251	1.0232	1.0216	1.0256	1.0250	1.0233
14.9274	1.0241	1.0263	1.0275	1.0254	1.0247	1.0288	1.0277	1.0252
14.9528	1.0256	1.0284	1.0298	1.0276	1.0275	1.0326	1.0306	1.0269
14.9782	1.0262	1.0301	1.0319	1.0294	1.0299	1.0360	1.0332	1.0283

Table A-11: Numerical values of SF for Liquid Al-3%Si alloy at various melt temperatures.

Q ($Å^{-1}$)	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 1052K
0.6479	0.0323	0.0326	0.0325	0.0321
0.6733	0.0318	0.0342	0.0334	0.0316
0.6987	0.0334	0.0355	0.0351	0.0317
0.7241	0.0351	0.0369	0.0362	0.0335
0.7495	0.0371	0.0373	0.0379	0.0358
0.7750	0.0395	0.0384	0.0396	0.0373
0.8004	0.0409	0.0406	0.0411	0.0386
0.8258	0.0413	0.0419	0.0427	0.0394
0.8512	0.0431	0.0432	0.0435	0.0403
0.8766	0.0444	0.0454	0.0452	0.0417
0.9020	0.0452	0.0470	0.0474	0.0436
0.9274	0.0469	0.0481	0.0487	0.0458
0.9528	0.0488	0.0494	0.0501	0.0474
0.9782	0.0508	0.0515	0.0523	0.0489
1.0036	0.0532	0.0545	0.0548	0.0521
1.0290	0.0562	0.0573	0.0571	0.0560
1.0544	0.0591	0.0599	0.0603	0.0603
1.0799	0.0625	0.0618	0.0637	0.0607
1.1053	0.0661	0.0645	0.0665	0.0608
1.1307	0.0692	0.0673	0.0695	0.0634
1.1561	0.0724	0.0709	0.0721	0.0666
1.1815	0.0754	0.0746	0.0747	0.0692
1.2069	0.0799	0.0799	0.0797	0.0733
1.2323	0.0851	0.0856	0.0863	0.0781
1.2577	0.0899	0.0898	0.0923	0.0814
1.2831	0.0945	0.0947	0.0971	0.0838
1.3085	0.0992	0.1004	0.1016	0.0887
1.3339	0.1046	0.1068	0.1057	0.0962
1.3593	0.1105	0.1126	0.1108	0.1020
1.3848	0.1160	0.1185	0.1173	0.1054
1.4102	0.1223	0.1251	0.1239	0.1091
1.4356	0.1283	0.1313	0.1298	0.1137
1.4610	0.1335	0.1366	0.1367	0.1187
1.4864	0.1388	0.1414	0.1430	0.1235
1.5118	0.1447	0.1468	0.1480	0.1288
1.5372	0.1498	0.1525	0.1532	0.1347
1.5626	0.1542	0.1574	0.1588	0.1406
1.5880	0.1585	0.1614	0.1628	0.1467
1.6134	0.1631	0.1652	0.1667	0.1534
1.6388	0.1676	0.1703	0.1716	0.1598
1.6642	0.1722	0.1762	0.1774	0.1670
1.6897	0.1785	0.1824	0.1845	0.1760
1.7151	0.1858	0.1894	0.1919	0.1860
1.7405	0.1933	0.1976	0.1995	0.1958
1.7659	0.2009	0.2057	0.2082	0.2073
1.7913	0.2105	0.2150	0.2181	0.2207
1.8167	0.2220	0.2255	0.2294	0.2339
1.8421	0.2341	0.2371	0.2417	0.2470
1.8675	0.2464	0.2499	0.2548	0.2625
1.8929	0.2602	0.2653	0.2706	0.2808
1.9183	0.2760	0.2821	0.2887	0.3016
1.9437	0.2933	0.3004	0.3057	0.3230
1.9691	0.3132	0.3208	0.3245	0.3463
1.9946	0.3361	0.3433	0.3481	0.3741
2.0200	0.3617	0.3691	0.3759	0.4096
2.0454	0.3901	0.3985	0.4057	0.4642
2.0708	0.4211	0.4303	0.4379	0.5499
2.0962	0.4555	0.4655	0.4743	0.6199
2.1216	0.4968	0.5050	0.5161	0.6288
2.1470	0.5412	0.5487	0.5615	0.6298
2.1724	0.5900	0.6012	0.6138	0.6652
2.1978	0.6448	0.6555	0.6682	0.7150
2.2232	0.7039	0.7154	0.7265	0.7695
2.2486	0.7686	0.7801	0.7918	0.8320
2.2740	0.8383	0.8503	0.8629	0.9024
2.2995	0.9156	0.9286	0.9415	0.9792
2.3249	1.0030	1.0160	1.0284	1.0646
2.3503	1.1000	1.1120	1.1269	1.1569
2.3757	1.2038	1.2151	1.2294	1.2554
2.4011	1.3183	1.3291	1.3394	1.3679
2.4265	1.4385	1.4457	1.4520	1.4922
2.4519	1.5590	1.5664	1.5688	1.6097
2.4773	1.6853	1.6891	1.6889	1.6992
2.5027	1.8050	1.8038	1.8000	1.7815
2.5281	1.9177	1.9103	1.9029	1.8632
2.5535	2.0227	2.0091	1.9977	1.9416
2.5789	2.1109	2.0942	2.0751	2.0087
2.6044	2.1821	2.1610	2.1399	2.0589
2.6298	2.2293	2.2032	2.1807	2.0901
2.6552	2.2476	2.2204	2.1956	2.0981
2.6806	2.2472	2.2151	2.1913	2.0898
2.7060	2.2259	2.1937	2.1696	2.0728
2.7314	2.1848	2.1554	2.1329	2.0383
2.7568	2.1322	2.1066	2.0845	1.9908
2.7822	2.0661	2.0436	2.0253	1.9357
2.8076	1.9887	1.9692	1.9557	1.8751
2.8330	1.9087	1.8930	1.8861	1.8119
2.8584	1.8293	1.8140	1.8078	1.7466
2.8839	1.7441	1.7312	1.7243	1.6785
2.9093	1.6631	1.6528	1.6476	1.6137
2.9347	1.5889	1.5813	1.5774	1.5544
2.9601	1.5179	1.5121	1.5079	1.5004
2.9855	1.4469	1.4438	1.4392	1.4561
3.0109	1.3784	1.3784	1.3753	1.4102
3.0363	1.3162	1.3151	1.3131	1.3501
3.0617	1.2593	1.2594	1.2587	1.2847
3.0871	1.2030	1.2047	1.2070	1.2252
3.1125	1.1533	1.1556	1.1602	1.1781
3.1379	1.1066	1.1084	1.1139	1.1356
3.1633	1.0621	1.0623	1.0686	1.0909
3.1888	1.0199	1.0196	1.0254	1.0458
3.2142	0.9788	0.9800	0.9855	1.0015
3.2396	0.9373	0.9423	0.9461	0.9605
3.2650	0.8998	0.9072	0.9104	0.9246
3.2904	0.8678	0.8758	0.8781	0.8915
3.3158	0.8363	0.8436	0.8457	0.8599
3.3412	0.8045	0.8109	0.8140	0.8304
3.3666	0.7741	0.7800	0.7839	0.8019
3.3920	0.7484	0.7528	0.7572	0.7761
3.4174	0.7261	0.7290	0.7368	0.7536
3.4428	0.7066	0.7101	0.7169	0.7368
3.4682	0.6900	0.6952	0.7007	0.7210
3.4937	0.6754	0.6820	0.6878	0.7075
3.5191	0.6639	0.6702	0.6766	0.6967
3.5445	0.6545	0.6599	0.6653	0.6855
3.5699	0.6468	0.6527	0.6564	0.6794
3.5953	0.6415	0.6474	0.6505	0.6770
3.6207	0.6360	0.6418	0.6482	0.6710
3.6461	0.6340	0.6391	0.6457	0.6649
3.6715	0.6349	0.6396	0.6469	0.6647
3.6969	0.6370	0.6424	0.6499	0.6666
3.7223	0.6406	0.6454	0.6527	0.6700
3.7477	0.6430	0.6475	0.6545	0.6731
3.7731	0.6444	0.6502	0.6550	0.6762
3.7986	0.6501	0.6542	0.6592	0.6791
3.8240	0.6565	0.6598	0.6665	0.6875

Q ($Å^{-1}$)	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 1052K
3.8494	0.6632	0.6685	0.6752	0.7046
3.8748	0.6719	0.6787	0.6842	0.7344
3.9002	0.6809	0.6883	0.6920	0.7556
3.9256	0.6922	0.6988	0.7007	0.7506
3.9510	0.7053	0.7098	0.7143	0.7489
3.9764	0.7195	0.7230	0.7297	0.7633
4.0018	0.7347	0.7390	0.7438	0.7892
4.0272	0.7519	0.7572	0.7599	0.8105
4.0526	0.7656	0.7704	0.7723	0.8181
4.0780	0.7819	0.7869	0.7883	0.8273
4.1035	0.7995	0.8031	0.8064	0.8375
4.1289	0.8172	0.8200	0.8237	0.8462
4.1543	0.8362	0.8393	0.8415	0.8542
4.1797	0.8566	0.8589	0.8606	0.8667
4.2051	0.8783	0.8806	0.8807	0.8835
4.2305	0.8988	0.9006	0.9012	0.9001
4.2559	0.9206	0.9236	0.9244	0.9197
4.2813	0.9449	0.9464	0.9444	0.9407
4.3067	0.9676	0.9683	0.9669	0.9610
4.3321	0.9921	0.9909	0.9898	0.9827
4.3575	1.0149	1.0132	1.0128	1.0029
4.3829	1.0428	1.0384	1.0382	1.0271
4.4084	1.0679	1.0631	1.0613	1.0547
4.4338	1.0890	1.0853	1.0834	1.0842
4.4592	1.1094	1.1072	1.1047	1.1071
4.4846	1.1319	1.1260	1.1242	1.1178
4.5100	1.1514	1.1473	1.1431	1.1268
4.5354	1.1694	1.1665	1.1623	1.1398
4.5608	1.1875	1.1820	1.1808	1.1541
4.5862	1.2082	1.2005	1.1988	1.1705
4.6116	1.2254	1.2192	1.2181	1.1883
4.6370	1.2396	1.2353	1.2329	1.2043
4.6624	1.2536	1.2484	1.2462	1.2181
4.6878	1.2641	1.2586	1.2543	1.2263
4.7133	1.2766	1.2712	1.2646	1.2354
4.7387	1.2828	1.2790	1.2722	1.2412
4.7641	1.2867	1.2819	1.2776	1.2466
4.7895	1.2917	1.2844	1.2799	1.2495
4.8149	1.2911	1.2858	1.2800	1.2503
4.8403	1.2887	1.2848	1.2794	1.2504
4.8657	1.2844	1.2798	1.2763	1.2496
4.8911	1.2808	1.2762	1.2726	1.2503
4.9165	1.2758	1.2732	1.2681	1.2500
4.9419	1.2717	1.2681	1.2625	1.2463
4.9673	1.2656	1.2611	1.2583	1.2400
4.9927	1.2585	1.2538	1.2515	1.2371
5.0182	1.2493	1.2450	1.2417	1.2357
5.0436	1.2386	1.2341	1.2322	1.2291
5.0690	1.2287	1.2242	1.2226	1.2162
5.0944	1.2148	1.2134	1.2106	1.2022
5.1198	1.2024	1.2003	1.1974	1.1886
5.1452	1.1941	1.1904	1.1881	1.1765
5.1706	1.1841	1.1776	1.1798	1.1641
5.1960	1.1679	1.1632	1.1667	1.1489
5.2214	1.1533	1.1518	1.1554	1.1376
5.2468	1.1399	1.1409	1.1417	1.1251
5.2722	1.1275	1.1269	1.1261	1.1124
5.2976	1.1146	1.1132	1.1122	1.1008
5.3231	1.1010	1.1003	1.0970	1.0876
5.3485	1.0866	1.0851	1.0826	1.0735
5.3739	1.0707	1.0692	1.0679	1.0605
5.3993	1.0573	1.0559	1.0552	1.0484
5.4247	1.0416	1.0426	1.0429	1.0359
5.4501	1.0288	1.0301	1.0289	1.0245
5.4755	1.0123	1.0161	1.0160	1.0100

Q ($Å^{-1}$)	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 1052K
5.5009	0.9998	1.0048	1.0047	1.0005
5.5263	0.9883	0.9908	0.9906	0.9913
5.5517	0.9749	0.9762	0.9752	0.9773
5.5771	0.9626	0.9645	0.9626	0.9644
5.6025	0.9505	0.9531	0.9527	0.9551
5.6280	0.9376	0.9408	0.9424	0.9476
5.6534	0.9266	0.9294	0.9309	0.9412
5.6788	0.9166	0.9192	0.9196	0.9324
5.7042	0.9067	0.9073	0.9081	0.9176
5.7296	0.8954	0.8966	0.8962	0.9041
5.7550	0.8852	0.8885	0.8894	0.8954
5.7804	0.8762	0.8819	0.8826	0.8879
5.8058	0.8702	0.8747	0.8752	0.8815
5.8312	0.8630	0.8658	0.8689	0.8757
5.8566	0.8566	0.8588	0.8644	0.8715
5.8820	0.8500	0.8534	0.8581	0.8665
5.9074	0.8449	0.8477	0.8506	0.8633
5.9329	0.8405	0.8438	0.8450	0.8614
5.9583	0.8360	0.8395	0.8413	0.8570
5.9837	0.8324	0.8367	0.8380	0.8551
6.0091	0.8311	0.8356	0.8349	0.8527
6.0345	0.8294	0.8328	0.8328	0.8500
6.0599	0.8270	0.8298	0.8331	0.8466
6.0853	0.8264	0.8292	0.8341	0.8475
6.1107	0.8276	0.8298	0.8347	0.8467
6.1361	0.8297	0.8308	0.8367	0.8451
6.1615	0.8289	0.8310	0.8378	0.8456
6.1869	0.8317	0.8342	0.8403	0.8485
6.2123	0.8374	0.8373	0.8405	0.8523
6.2378	0.8404	0.8409	0.8418	0.8588
6.2632	0.8444	0.8463	0.8484	0.8646
6.2886	0.8485	0.8510	0.8538	0.8648
6.3140	0.8540	0.8569	0.8584	0.8640
6.3394	0.8595	0.8620	0.8651	0.8665
6.3648	0.8646	0.8682	0.8701	0.8713
6.3902	0.8695	0.8722	0.8728	0.8744
6.4156	0.8745	0.8770	0.8789	0.8790
6.4410	0.8791	0.8818	0.8853	0.8862
6.4664	0.8848	0.8887	0.8904	0.8916
6.4918	0.8928	0.8955	0.8950	0.8944
6.5172	0.9016	0.9042	0.9029	0.9012
6.5427	0.9083	0.9099	0.9080	0.9060
6.5681	0.9167	0.9177	0.9160	0.9104
6.5935	0.9240	0.9250	0.9248	0.9174
6.6189	0.9319	0.9331	0.9320	0.9248
6.6443	0.9381	0.9398	0.9376	0.9310
6.6697	0.9439	0.9458	0.9441	0.9383
6.6951	0.9520	0.9526	0.9504	0.9469
6.7205	0.9602	0.9595	0.9576	0.9547
6.7459	0.9674	0.9657	0.9675	0.9599
6.7713	0.9749	0.9731	0.9732	0.9661
6.7967	0.9835	0.9796	0.9778	0.9717
6.8221	0.9862	0.9862	0.9832	0.9746
6.8476	0.9924	0.9934	0.9871	0.9810
6.8730	0.9995	0.9981	0.9921	0.9872
6.8984	1.0058	1.0041	0.9995	0.9917
6.9238	1.0090	1.0094	1.0051	0.9976
6.9492	1.0146	1.0149	1.0096	1.0049
6.9746	1.0230	1.0207	1.0178	1.0120
7.0000	1.0280	1.0243	1.0191	1.0145
7.0254	1.0327	1.0293	1.0228	1.0198
7.0508	1.0354	1.0327	1.0277	1.0235
7.0762	1.0371	1.0327	1.0290	1.0237
7.1016	1.0404	1.0342	1.0309	1.0248
7.1270	1.0422	1.0383	1.0342	1.0266

Q ($Å^{-1}$)	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 1052K
7.1525	1.0459	1.0393	1.0360	1.0300
7.1779	1.0510	1.0420	1.0360	1.0341
7.2033	1.0458	1.0404	1.0362	1.0338
7.2287	1.0405	1.0393	1.0346	1.0325
7.2541	1.0392	1.0392	1.0362	1.0335
7.2795	1.0389	1.0391	1.0393	1.0344
7.3049	1.0385	1.0396	1.0394	1.0358
7.3303	1.0396	1.0405	1.0402	1.0384
7.3557	1.0383	1.0417	1.0382	1.0385
7.3811	1.0392	1.0418	1.0385	1.0374
7.4065	1.0395	1.0395	1.0370	1.0373
7.4319	1.0391	1.0390	1.0362	1.0355
7.4574	1.0383	1.0372	1.0358	1.0345
7.4828	1.0369	1.0346	1.0337	1.0339
7.5082	1.0345	1.0337	1.0330	1.0336
7.5336	1.0303	1.0294	1.0310	1.0314
7.5590	1.0272	1.0282	1.0280	1.0281
7.5844	1.0252	1.0273	1.0259	1.0253
7.6098	1.0216	1.0241	1.0240	1.0240
7.6352	1.0228	1.0236	1.0221	1.0241
7.6606	1.0199	1.0216	1.0191	1.0268
7.6860	1.0175	1.0194	1.0175	1.0271
7.7114	1.0163	1.0155	1.0156	1.0236
7.7368	1.0129	1.0127	1.0111	1.0179
7.7623	1.0103	1.0097	1.0061	1.0139
7.7877	1.0064	1.0056	1.0032	1.0113
7.8131	1.0036	1.0042	0.9999	1.0123
7.8385	0.9996	1.0005	0.9934	1.0084
7.8639	0.9968	0.9951	0.9894	1.0005
7.8893	0.9937	0.9909	0.9882	0.9930
7.9147	0.9876	0.9885	0.9871	0.9870
7.9401	0.9842	0.9859	0.9860	0.9854
7.9655	0.9805	0.9847	0.9853	0.9856
7.9909	0.9738	0.9778	0.9784	0.9807
8.0163	0.9721	0.9762	0.9765	0.9792
8.0417	0.9703	0.9742	0.9745	0.9776
8.0672	0.9683	0.9719	0.9723	0.9763
8.0926	0.9660	0.9692	0.9699	0.9747
8.1180	0.9635	0.9662	0.9670	0.9728
8.1434	0.9613	0.9634	0.9641	0.9705
8.1688	0.9589	0.9605	0.9612	0.9681
8.1942	0.9565	0.9577	0.9583	0.9656
8.2196	0.9543	0.9550	0.9556	0.9631
8.2450	0.9524	0.9527	0.9530	0.9608
8.2704	0.9507	0.9508	0.9510	0.9588
8.2958	0.9490	0.9490	0.9491	0.9568
8.3212	0.9477	0.9477	0.9474	0.9545
8.3466	0.9464	0.9466	0.9460	0.9522
8.3721	0.9453	0.9456	0.9448	0.9498
8.3975	0.9443	0.9448	0.9440	0.9474
8.4229	0.9436	0.9443	0.9436	0.9454
8.4483	0.9432	0.9441	0.9433	0.9443
8.4737	0.9426	0.9439	0.9429	0.9435
8.4991	0.9420	0.9438	0.9424	0.9427
8.5245	0.9419	0.9438	0.9422	0.9421
8.5499	0.9423	0.9436	0.9427	0.9424
8.5753	0.9426	0.9435	0.9434	0.9431
8.6007	0.9429	0.9436	0.9442	0.9440
8.6261	0.9436	0.9443	0.9452	0.9449
8.6515	0.9448	0.9456	0.9469	0.9458
8.6770	0.9462	0.9472	0.9487	0.9472
8.7024	0.9480	0.9490	0.9505	0.9487
8.7278	0.9500	0.9511	0.9526	0.9505
8.7532	0.9521	0.9535	0.9547	0.9523
8.7786	0.9543	0.9560	0.9569	0.9540

Q ($Å^{-1}$)	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 1052K
8.8040	0.9565	0.9588	0.9590	0.9557
8.8294	0.9589	0.9613	0.9606	0.9572
8.8548	0.9612	0.9638	0.9623	0.9587
8.8802	0.9637	0.9662	0.9642	0.9606
8.9056	0.9663	0.9687	0.9663	0.9627
8.9310	0.9690	0.9714	0.9683	0.9653
8.9565	0.9719	0.9737	0.9701	0.9679
8.9819	0.9748	0.9764	0.9719	0.9705
9.0073	0.9778	0.9792	0.9741	0.9730
9.0327	0.9809	0.9816	0.9766	0.9753
9.0581	0.9837	0.9838	0.9794	0.9777
9.0835	0.9864	0.9861	0.9821	0.9798
9.1089	0.9893	0.9888	0.9853	0.9820
9.1343	0.9925	0.9915	0.9891	0.9842
9.1597	0.9955	0.9943	0.9929	0.9862
9.1851	0.9983	0.9970	0.9962	0.9884
9.2105	1.0011	0.9995	0.9995	0.9905
9.2359	1.0036	1.0020	1.0027	0.9927
9.2614	1.0061	1.0051	1.0057	0.9948
9.2868	1.0086	1.0083	1.0082	0.9971
9.3122	1.0109	1.0115	1.0106	0.9996
9.3376	1.0130	1.0143	1.0129	1.0022
9.3630	1.0155	1.0171	1.0152	1.0050
9.3884	1.0182	1.0197	1.0171	1.0077
9.4138	1.0204	1.0218	1.0185	1.0100
9.4392	1.0220	1.0237	1.0196	1.0119
9.4646	1.0237	1.0252	1.0208	1.0133
9.4900	1.0254	1.0269	1.0221	1.0147
9.5154	1.0269	1.0280	1.0233	1.0163
9.5408	1.0279	1.0286	1.0240	1.0178
9.5663	1.0287	1.0290	1.0244	1.0191
9.5917	1.0295	1.0293	1.0252	1.0204
9.6171	1.0300	1.0293	1.0260	1.0218
9.6425	1.0302	1.0288	1.0265	1.0231
9.6679	1.0298	1.0282	1.0267	1.0236
9.6933	1.0293	1.0275	1.0269	1.0239
9.7187	1.0285	1.0268	1.0269	1.0242
9.7441	1.0277	1.0264	1.0269	1.0244
9.7695	1.0269	1.0266	1.0271	1.0248
9.7949	1.0263	1.0266	1.0274	1.0251
9.8203	1.0254	1.0263	1.0277	1.0254
9.8457	1.0252	1.0260	1.0279	1.0255
9.8712	1.0254	1.0255	1.0273	1.0255
9.8966	1.0254	1.0249	1.0269	1.0251
9.9220	1.0248	1.0241	1.0266	1.0239
9.9474	1.0240	1.0236	1.0263	1.0232
9.9728	1.0233	1.0230	1.0254	1.0224
9.9982	1.0226	1.0218	1.0241	1.0219
10.0236	1.0216	1.0203	1.0227	1.0216
10.0490	1.0201	1.0188	1.0210	1.0214
10.0744	1.0190	1.0178	1.0195	1.0210
10.0998	1.0184	1.0165	1.0178	1.0202
10.1252	1.0174	1.0152	1.0159	1.0189
10.1506	1.0161	1.0142	1.0143	1.0175
10.1761	1.0145	1.0132	1.0130	1.0160
10.2015	1.0130	1.0125	1.0119	1.0147
10.2269	1.0118	1.0120	1.0108	1.0135
10.2523	1.0106	1.0113	1.0098	1.0123
10.2777	1.0095	1.0107	1.0090	1.0116
10.3031	1.0088	1.0105	1.0087	1.0114
10.3285	1.0086	1.0104	1.0087	1.0117
10.3539	1.0092	1.0104	1.0089	1.0123
10.3793	1.0097	1.0103	1.0092	1.0128
10.4047	1.0098	1.0102	1.0097	1.0133
10.4301	1.0097	1.0101	1.0100	1.0138

Q ($Å^{-1}$)	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 1052K
10.4555	1.0097	1.0098	1.0101	1.0151
10.4810	1.0095	1.0092	1.0098	1.0157
10.5064	1.0093	1.0081	1.0098	1.0161
10.5318	1.0088	1.0073	1.0099	1.0165
10.5572	1.0084	1.0073	1.0097	1.0169
10.5826	1.0080	1.0074	1.0092	1.0169
10.6080	1.0076	1.0071	1.0090	1.0166
10.6334	1.0069	1.0070	1.0093	1.0161
10.6588	1.0060	1.0070	1.0094	1.0154
10.6842	1.0054	1.0069	1.0092	1.0146
10.7096	1.0052	1.0068	1.0089	1.0138
10.7350	1.0050	1.0062	1.0085	1.0127
10.7604	1.0047	1.0055	1.0078	1.0113
10.7859	1.0047	1.0055	1.0068	1.0103
10.8113	1.0049	1.0061	1.0062	1.0096
10.8367	1.0057	1.0066	1.0057	1.0095
10.8621	1.0065	1.0071	1.0054	1.0094
10.8875	1.0072	1.0073	1.0054	1.0093
10.9129	1.0077	1.0072	1.0053	1.0096
10.9383	1.0078	1.0071	1.0057	1.0095
10.9637	1.0078	1.0066	1.0061	1.0092
10.9891	1.0079	1.0067	1.0064	1.0091
11.0145	1.0079	1.0069	1.0065	1.0096
11.0399	1.0079	1.0073	1.0064	1.0099
11.0654	1.0085	1.0078	1.0065	1.0097
11.0908	1.0091	1.0078	1.0070	1.0096
11.1162	1.0094	1.0074	1.0074	1.0094
11.1416	1.0095	1.0071	1.0077	1.0089
11.1670	1.0095	1.0069	1.0079	1.0081
11.1924	1.0096	1.0069	1.0080	1.0078
11.2178	1.0100	1.0068	1.0083	1.0076
11.2432	1.0108	1.0066	1.0086	1.0075
11.2686	1.0116	1.0073	1.0085	1.0074
11.2940	1.0122	1.0085	1.0084	1.0078
11.3194	1.0123	1.0095	1.0089	1.0082
11.3448	1.0127	1.0104	1.0101	1.0089
11.3703	1.0131	1.0110	1.0117	1.0096
11.3957	1.0132	1.0110	1.0127	1.0103
11.4211	1.0132	1.0112	1.0132	1.0110
11.4465	1.0131	1.0113	1.0133	1.0112
11.4719	1.0135	1.0115	1.0134	1.0118
11.4973	1.0144	1.0120	1.0134	1.0126
11.5227	1.0150	1.0121	1.0124	1.0128
11.5481	1.0158	1.0125	1.0117	1.0124
11.5735	1.0169	1.0130	1.0120	1.0123
11.5989	1.0175	1.0132	1.0124	1.0129
11.6243	1.0176	1.0135	1.0123	1.0135
11.6497	1.0181	1.0142	1.0126	1.0141
11.6752	1.0188	1.0150	1.0138	1.0146
11.7006	1.0193	1.0163	1.0148	1.0158
11.7260	1.0202	1.0174	1.0152	1.0167
11.7514	1.0215	1.0187	1.0158	1.0175
11.7768	1.0228	1.0208	1.0167	1.0183
11.8022	1.0234	1.0231	1.0181	1.0190
11.8276	1.0236	1.0249	1.0202	1.0196
11.8530	1.0243	1.0266	1.0225	1.0202
11.8784	1.0258	1.0284	1.0247	1.0213
11.9038	1.0275	1.0302	1.0261	1.0223
11.9292	1.0296	1.0317	1.0270	1.0231
11.9546	1.0314	1.0326	1.0280	1.0237
11.9801	1.0328	1.0335	1.0288	1.0243
12.0055	1.0338	1.0344	1.0294	1.0244
12.0309	1.0342	1.0351	1.0303	1.0249
12.0563	1.0348	1.0359	1.0318	1.0262
12.0817	1.0353	1.0369	1.0335	1.0281

Q ($Å^{-1}$)	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 1052K
12.1071	1.0357	1.0378	1.0352	1.0295
12.1325	1.0362	1.0386	1.0363	1.0305
12.1579	1.0367	1.0395	1.0374	1.0313
12.1833	1.0366	1.0401	1.0388	1.0314
12.2087	1.0364	1.0407	1.0396	1.0313
12.2341	1.0363	1.0409	1.0397	1.0308
12.2595	1.0361	1.0416	1.0399	1.0309
12.2850	1.0363	1.0426	1.0405	1.0316
12.3104	1.0355	1.0433	1.0411	1.0319
12.3358	1.0351	1.0442	1.0418	1.0324
12.3612	1.0354	1.0450	1.0422	1.0331
12.3866	1.0365	1.0454	1.0422	1.0340
12.4120	1.0378	1.0458	1.0421	1.0348
12.4374	1.0393	1.0464	1.0417	1.0357
12.4628	1.0401	1.0467	1.0415	1.0364
12.4882	1.0404	1.0465	1.0409	1.0373
12.5136	1.0407	1.0459	1.0406	1.0385
12.5390	1.0413	1.0450	1.0404	1.0398
12.5644	1.0419	1.0442	1.0399	1.0412
12.5899	1.0427	1.0436	1.0396	1.0420
12.6153	1.0436	1.0429	1.0394	1.0421
12.6407	1.0443	1.0424	1.0391	1.0419
12.6661	1.0444	1.0414	1.0391	1.0413
12.6915	1.0437	1.0394	1.0387	1.0401
12.7169	1.0429	1.0373	1.0378	1.0390
12.7423	1.0423	1.0355	1.0367	1.0382
12.7677	1.0423	1.0348	1.0363	1.0382
12.7931	1.0409	1.0335	1.0349	1.0369
12.8185	1.0380	1.0316	1.0321	1.0340
12.8439	1.0349	1.0296	1.0295	1.0314
12.8693	1.0319	1.0276	1.0269	1.0294
12.8948	1.0291	1.0256	1.0245	1.0272
12.9202	1.0269	1.0243	1.0228	1.0253
12.9456	1.0244	1.0231	1.0209	1.0235
12.9710	1.0216	1.0216	1.0189	1.0214
12.9964	1.0193	1.0205	1.0171	1.0197
13.0218	1.0174	1.0192	1.0153	1.0179
13.0472	1.0155	1.0179	1.0137	1.0162
13.0726	1.0134	1.0167	1.0126	1.0145
13.0980	1.0115	1.0154	1.0114	1.0130
13.1234	1.0093	1.0135	1.0104	1.0114
13.1488	1.0071	1.0115	1.0095	1.0097
13.1742	1.0053	1.0089	1.0081	1.0082
13.1997	1.0042	1.0065	1.0058	1.0068
13.2251	1.0031	1.0045	1.0040	1.0061
13.2505	1.0023	1.0028	1.0027	1.0056
13.2759	1.0015	1.0016	1.0014	1.0051
13.3013	0.9992	0.9989	0.9986	1.0027
13.3267	0.9971	0.9960	0.9961	1.0005
13.3521	0.9954	0.9934	0.9940	0.9989
13.3775	0.9942	0.9915	0.9920	0.9975
13.4029	0.9933	0.9899	0.9899	0.9954
13.4283	0.9925	0.9886	0.9879	0.9937
13.4537	0.9921	0.9875	0.9863	0.9916
13.4791	0.9924	0.9871	0.9851	0.9894
13.5046	0.9925	0.9869	0.9843	0.9879
13.5300	0.9918	0.9859	0.9835	0.9862
13.5554	0.9910	0.9851	0.9838	0.9848
13.5808	0.9903	0.9846	0.9848	0.9834
13.6062	0.9898	0.9843	0.9852	0.9825
13.6316	0.9890	0.9839	0.9861	0.9820
13.6570	0.9891	0.9843	0.9874	0.9824
13.6824	0.9895	0.9849	0.9883	0.9834
13.7078	0.9897	0.9858	0.9892	0.9851
13.7332	0.9898	0.9872	0.9912	0.9873

13.7586	0.9904	0.9892	0.9943	0.9895
13.7840	0.9912	0.9911	0.9967	0.9917
13.8095	0.9920	0.9927	0.9982	0.9931
13.8349	0.9929	0.9944	0.9999	0.9948
13.8603	0.9939	0.9965	1.0011	0.9962
13.8857	0.9949	0.9986	1.0015	0.9972
13.9111	0.9965	1.0008	1.0015	0.9981
13.9365	0.9984	1.0027	1.0021	0.9990
13.9619	1.0005	1.0040	1.0033	0.9998
13.9873	1.0019	1.0048	1.0041	1.0002
14.0127	1.0026	1.0052	1.0049	1.0007
14.0381	1.0031	1.0058	1.0057	1.0009
14.0635	1.0038	1.0071	1.0065	1.0012
14.0889	1.0039	1.0081	1.0064	1.0015
14.1144	1.0038	1.0081	1.0056	1.0020
14.1398	1.0037	1.0077	1.0052	1.0025
14.1652	1.0036	1.0072	1.0047	1.0028
14.1906	1.0029	1.0067	1.0039	1.0024
14.2160	1.0015	1.0065	1.0032	1.0018
14.2414	1.0003	1.0060	1.0029	1.0009
14.2668	0.9991	1.0045	1.0016	0.9991
14.2922	0.9977	1.0025	0.9996	0.9977
14.3176	0.9964	0.9996	0.9977	0.9961
14.3430	0.9956	0.9976	0.9973	0.9952
14.3684	0.9956	0.9966	0.9968	0.9951
14.3938	0.9954	0.9955	0.9953	0.9948
14.4193	0.9956	0.9944	0.9939	0.9946
14.4447	0.9951	0.9934	0.9936	0.9948
14.4701	0.9947	0.9928	0.9934	0.9950
14.4955	0.9946	0.9928	0.9932	0.9945
14.5209	0.9950	0.9936	0.9938	0.9952
14.5463	0.9954	0.9951	0.9947	0.9968
14.5717	0.9960	0.9966	0.9954	0.9989
14.5971	0.9970	0.9980	0.9964	1.0013
14.6225	0.9987	0.9996	0.9980	1.0036
14.6479	1.0008	1.0016	1.0001	1.0062
14.6733	1.0029	1.0047	1.0026	1.0088
14.6987	1.0054	1.0083	1.0058	1.0106
14.7242	1.0080	1.0111	1.0094	1.0124
14.7496	1.0109	1.0130	1.0124	1.0139
14.7750	1.0138	1.0146	1.0148	1.0155
14.8004	1.0166	1.0168	1.0180	1.0180
14.8258	1.0193	1.0188	1.0210	1.0207
14.8512	1.0223	1.0216	1.0240	1.0235
14.8766	1.0250	1.0246	1.0259	1.0266
14.9020	1.0265	1.0267	1.0264	1.0288
14.9274	1.0276	1.0286	1.0268	1.0307
14.9528	1.0285	1.0308	1.0278	1.0324
14.9782	1.0296	1.0329	1.0279	1.0335

Table A-12: Numerical values of SF for Liquid Al-7%Si alloy at various melt temperatures.

Q ($Å^{-1}$)	S(Q) 898K	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 986K	S(Q) 1008K	S(Q) 1030K	S(Q) 1052K
0.6479	0.0426	0.0413	0.0429	0.0426	0.0439	0.0437	0.0434	0.0461
0.6733	0.0437	0.0434	0.0442	0.0443	0.0450	0.0451	0.0454	0.0463
0.6987	0.0441	0.0447	0.0459	0.0460	0.0463	0.0461	0.0470	0.0471
0.7241	0.0454	0.0469	0.0475	0.0474	0.0491	0.0466	0.0481	0.0496
0.7495	0.0463	0.0491	0.0488	0.0484	0.0502	0.0478	0.0499	0.0516
0.7750	0.0483	0.0504	0.0505	0.0495	0.0520	0.0509	0.0517	0.0535
0.8004	0.0500	0.0508	0.0508	0.0512	0.0530	0.0525	0.0535	0.0541
0.8258	0.0510	0.0517	0.0518	0.0527	0.0538	0.0535	0.0549	0.0561
0.8512	0.0526	0.0535	0.0536	0.0540	0.0554	0.0544	0.0559	0.0582
0.8766	0.0549	0.0544	0.0558	0.0552	0.0571	0.0574	0.0579	0.0594
0.9020	0.0564	0.0548	0.0571	0.0569	0.0585	0.0596	0.0607	0.0608
0.9274	0.0574	0.0572	0.0581	0.0593	0.0605	0.0609	0.0634	0.0623
0.9528	0.0586	0.0591	0.0598	0.0604	0.0614	0.0620	0.0648	0.0641
0.9782	0.0606	0.0603	0.0619	0.0613	0.0627	0.0635	0.0660	0.0657
1.0036	0.0632	0.0623	0.0642	0.0634	0.0648	0.0663	0.0673	0.0673
1.0290	0.0654	0.0647	0.0659	0.0662	0.0671	0.0684	0.0685	0.0690
1.0544	0.0675	0.0668	0.0681	0.0687	0.0697	0.0709	0.0709	0.0715
1.0799	0.0694	0.0695	0.0706	0.0712	0.0718	0.0739	0.0740	0.0747
1.1053	0.0726	0.0727	0.0735	0.0742	0.0747	0.0768	0.0763	0.0782
1.1307	0.0755	0.0753	0.0771	0.0767	0.0776	0.0797	0.0788	0.0816
1.1561	0.0773	0.0779	0.0805	0.0794	0.0805	0.0832	0.0824	0.0851
1.1815	0.0801	0.0809	0.0830	0.0823	0.0834	0.0866	0.0853	0.0877
1.2069	0.0844	0.0843	0.0862	0.0865	0.0871	0.0902	0.0894	0.0908
1.2323	0.0877	0.0883	0.0901	0.0906	0.0910	0.0942	0.0945	0.0953
1.2577	0.0909	0.0925	0.0942	0.0946	0.0954	0.0985	0.0991	0.1007
1.2831	0.0952	0.0970	0.0980	0.0991	0.1000	0.1025	0.1032	0.1062
1.3085	0.1000	0.1015	0.1020	0.1037	0.1050	0.1064	0.1072	0.1107
1.3339	0.1041	0.1058	0.1062	0.1079	0.1102	0.1108	0.1119	0.1150
1.3593	0.1084	0.1095	0.1113	0.1119	0.1157	0.1160	0.1175	0.1202
1.3848	0.1129	0.1139	0.1160	0.1166	0.1207	0.1214	0.1229	0.1257
1.4102	0.1181	0.1201	0.1217	0.1226	0.1260	0.1275	0.1288	0.1320
1.4356	0.1231	0.1258	0.1276	0.1286	0.1311	0.1335	0.1348	0.1382
1.4610	0.1283	0.1309	0.1329	0.1344	0.1363	0.1393	0.1406	0.1438
1.4864	0.1334	0.1358	0.1373	0.1397	0.1417	0.1442	0.1457	0.1487
1.5118	0.1384	0.1403	0.1423	0.1448	0.1467	0.1489	0.1510	0.1547
1.5372	0.1435	0.1452	0.1476	0.1500	0.1517	0.1544	0.1566	0.1611
1.5626	0.1489	0.1507	0.1527	0.1548	0.1574	0.1604	0.1629	0.1674
1.5880	0.1535	0.1563	0.1577	0.1601	0.1632	0.1657	0.1692	0.1728
1.6134	0.1577	0.1618	0.1630	0.1659	0.1689	0.1712	0.1752	0.1788
1.6388	0.1634	0.1663	0.1681	0.1719	0.1747	0.1775	0.1811	0.1850
1.6642	0.1695	0.1717	0.1743	0.1781	0.1813	0.1839	0.1879	0.1919
1.6897	0.1754	0.1787	0.1819	0.1852	0.1883	0.1917	0.1954	0.1997
1.7151	0.1823	0.1864	0.1898	0.1933	0.1961	0.2005	0.2037	0.2086
1.7405	0.1907	0.1949	0.1982	0.2016	0.2057	0.2094	0.2131	0.2188
1.7659	0.2002	0.2032	0.2075	0.2100	0.2156	0.2189	0.2226	0.2288
1.7913	0.2099	0.2126	0.2174	0.2205	0.2254	0.2299	0.2330	0.2397
1.8167	0.2199	0.2232	0.2279	0.2324	0.2363	0.2415	0.2456	0.2519
1.8421	0.2309	0.2351	0.2401	0.2458	0.2488	0.2540	0.2595	0.2651
1.8675	0.2439	0.2482	0.2540	0.2598	0.2632	0.2683	0.2752	0.2802
1.8929	0.2582	0.2629	0.2696	0.2746	0.2797	0.2847	0.2922	0.2976

Q ($Å^{-1}$)	S(Q) 898K	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 986K	S(Q) 1008K	S(Q) 1030K	S(Q) 1052K
1.9183	0.2749	0.2801	0.2869	0.2923	0.2979	0.3033	0.3107	0.3171
1.9437	0.2928	0.2986	0.3056	0.3109	0.3178	0.3233	0.3306	0.3371
1.9691	0.3128	0.3185	0.3257	0.3315	0.3386	0.3450	0.3533	0.3595
1.9946	0.3345	0.3400	0.3477	0.3548	0.3618	0.3680	0.3779	0.3849
2.0200	0.3587	0.3658	0.3728	0.3807	0.3884	0.3947	0.4045	0.4131
2.0454	0.3863	0.3941	0.4010	0.4096	0.4174	0.4253	0.4338	0.4427
2.0708	0.4166	0.4240	0.4336	0.4421	0.4495	0.4579	0.4680	0.4756
2.0962	0.4492	0.4578	0.4675	0.4765	0.4845	0.4929	0.5037	0.5132
2.1216	0.4873	0.4970	0.5053	0.5157	0.5248	0.5339	0.5437	0.5544
2.1470	0.5288	0.5398	0.5487	0.5588	0.5690	0.5793	0.5883	0.5982
2.1724	0.5767	0.5877	0.5967	0.6071	0.6184	0.6283	0.6388	0.6488
2.1978	0.6286	0.6393	0.6495	0.6613	0.6725	0.6817	0.6940	0.7038
2.2232	0.6861	0.6971	0.7074	0.7203	0.7320	0.7411	0.7537	0.7630
2.2486	0.7494	0.7607	0.7724	0.7847	0.7969	0.8069	0.8167	0.8280
2.2740	0.8194	0.8290	0.8421	0.8549	0.8660	0.8781	0.8871	0.8979
2.2995	0.8956	0.9065	0.9181	0.9329	0.9426	0.9543	0.9629	0.9737
2.3249	0.9808	0.9930	1.0040	1.0179	1.0283	1.0344	1.0455	1.0553
2.3503	1.0728	1.0873	1.0966	1.1074	1.1195	1.1233	1.1340	1.1432
2.3757	1.1733	1.1855	1.1969	1.2034	1.2157	1.2175	1.2252	1.2339
2.4011	1.2846	1.2940	1.3045	1.3109	1.3194	1.3180	1.3239	1.3303
2.4265	1.4004	1.4065	1.4139	1.4218	1.4271	1.4223	1.4247	1.4299
2.4519	1.5189	1.5215	1.5260	1.5332	1.5337	1.5272	1.5259	1.5282
2.4773	1.6422	1.6399	1.6403	1.6451	1.6433	1.6313	1.6269	1.6275
2.5027	1.7597	1.7551	1.7515	1.7523	1.7467	1.7300	1.7220	1.7
2.5281	1.8685	1.8619	1.8548	1.8512	1.8419	1.8196	1.8049	
2.5535	1.9728	1.9609	1.9509	1.9408	1.9292	1.9012	1.8812	
2.5789	2.0613	2.0450	2.0306	2.0157	2.0030	1.9675	1.9468	
2.6044	2.1358	2.1136	2.0955	2.0787	2.0611	2.0208	1.9987	1.9
2.6298	2.1878	2.1619	2.1443	2.1215	2.1008	2.0591	2.0337	2.011
2.6552	2.2129	2.1860	2.1651	2.1411	2.1189	2.0766	2.0477	2.0246
2.6806	2.2160	2.1886	2.1657	2.1426	2.1184	2.0778	2.0453	2.0235
2.7060	2.2025	2.1762	2.1535	2.1280	2.1049	2.0645	2.0323	2.0126
2.7314	2.1704	2.1442	2.1229	2.0974	2.0759	2.0372	2.0052	1.9876
2.7568	2.1250	2.0968	2.0785	2.0558	2.0354	1.9979	1.9696	1.9515
2.7822	2.0656	2.0407	2.0246	2.0027	1.9878	1.9493	1.9259	1.9088
2.8076	1.9970	1.9752	1.9598	1.9383	1.9270	1.8920	1.8722	1.8572
2.8330	1.9202	1.9033	1.8894	1.8705	1.8603	1.8300	1.8133	1.8003
2.8584	1.8426	1.8299	1.8171	1.8044	1.7935	1.7667	1.7536	1.7421
2.8839	1.7647	1.7533	1.7440	1.7344	1.7238	1.7011	1.6916	1.6818
2.9093	1.6901	1.6809	1.6747	1.6660	1.6567	1.6398	1.6316	1.6258
2.9347	1.6184	1.6216	1.6076	1.5990	1.5940	1.5802	1.5722	1.5701
2.9601	1.5486	1.5432	1.5415	1.5354	1.5308	1.5205	1.5149	1.5133
2.9855	1.4786	1.4744	1.4725	1.4707	1.4669	1.4595	1.4577	1.4574
3.0109	1.4132	1.4105	1.4075	1.4093	1.4065	1.4020	1.4022	1.4032
3.0363	1.3500	1.3502	1.3480	1.3504	1.3491	1.3477	1.3482	1.3503
3.0617	1.2938	1.2949	1.2936	1.2960	1.2964	1.2976	1.2995	1.3014
3.0871	1.2403	1.2417	1.2407	1.2429	1.2463	1.2466	1.2512	1.2542
3.1125	1.1914	1.1930	1.1934	1.1963	1.2011	1.2009	1.2087	1.2121
3.1379	1.1442	1.1458	1.1482	1.1502	1.1559	1.1579	1.1672	1.1710
3.1633	1.0994	1.1018	1.1044	1.1081	1.1125	1.1172	1.1244	1.1311

Q ($Å^{-1}$)	S(Q) 898K	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 986K	S(Q) 1008K	S(Q) 1030K	S(Q) 1052K
3.2142	1.0179	1.0197	1.0255	1.0288	1.0324	1.0399	1.0472	1.0569
3.2396	0.9784	0.9800	0.9880	0.9894	0.9942	1.0025	1.0117	1.0196
3.2650	0.9426	0.9437	0.9506	0.9531	0.9589	0.9678	0.9772	0.9834
3.2904	0.9108	0.9110	0.9158	0.9218	0.9266	0.9358	0.9450	0.9503
3.3158	0.8777	0.8789	0.8850	0.8907	0.8939	0.9039	0.9137	0.9191
3.3412	0.8463	0.8479	0.8547	0.8582	0.8619	0.8726	0.8825	0.8900
3.3666	0.8153	0.8176	0.8240	0.8265	0.8330	0.8432	0.8520	0.8612
3.3920	0.7866	0.7904	0.7952	0.7975	0.8055	0.8167	0.8237	0.8338
3.4174	0.7607	0.7650	0.7693	0.7731	0.7804	0.7904	0.7977	0.8082
3.4428	0.7380	0.7421	0.7475	0.7510	0.7591	0.7676	0.7754	0.7851
3.4682	0.7185	0.7220	0.7287	0.7314	0.7408	0.7484	0.7558	0.7659
3.4937	0.7009	0.7049	0.7118	0.7151	0.7244	0.7323	0.7393	0.7502
3.5191	0.6871	0.6915	0.6988	0.7017	0.7100	0.7193	0.7259	0.7363
3.5445	0.6748	0.6790	0.6860	0.6899	0.6979	0.7069	0.7131	0.7230
3.5699	0.6642	0.6705	0.6759	0.6813	0.6883	0.6967	0.7026	0.7121
3.5953	0.6568	0.6630	0.6683	0.6731	0.6793	0.6875	0.6934	0.7043
3.6207	0.6500	0.6550	0.6620	0.6667	0.6727	0.6798	0.6866	0.6973
3.6461	0.6462	0.6493	0.6574	0.6637	0.6685	0.6760	0.6830	0.6924
3.6715	0.6451	0.6480	0.6549	0.6607	0.6662	0.6737	0.6803	0.6892
3.6969	0.6420	0.6470	0.6529	0.6603	0.6643	0.6703	0.6778	0.6864
3.7223	0.6414	0.6476	0.6536	0.6604	0.6635	0.6697	0.6766	0.6850
3.7477	0.6436	0.6503	0.6559	0.6609	0.6662	0.6725	0.6775	0.6857
3.7731	0.6474	0.6521	0.6573	0.6623	0.6685	0.6750	0.6798	0.6872
3.7986	0.6511	0.6549	0.6605	0.6653	0.6719	0.6777	0.6832	0.6890
3.8240	0.6559	0.6606	0.6655	0.6717	0.6775	0.6832	0.6874	0.6938
3.8494	0.6629	0.6679	0.6727	0.6785	0.6837	0.6887	0.6918	0.7001
3.8748	0.6715	0.6750	0.6801	0.6872	0.6922	0.6951	0.6993	0.7073
3.9002	0.6792	0.6825	0.6881	0.6948	0.6998	0.7032	0.7068	0.7144
3.9256	0.6886	0.6927	0.6970	0.7034	0.7087	0.7129	0.7138	0.7220
3.9510	0.6989	0.7032	0.7077	0.7139	0.7176	0.7231	0.7235	0.7314
3.9764	0.7095	0.7149	0.7195	0.7251	0.7283	0.7328	0.7348	0.7409
4.0018	0.7223	0.7270	0.7325	0.7369	0.7408	0.7436	0.7478	0.7521
4.0272	0.7360	0.7415	0.7459	0.7502	0.7554	0.7564	0.7615	0.7644
4.0526	0.7510	0.7565	0.7610	0.7648	0.7704	0.7697	0.7740	0.7765
4.0780	0.7676	0.7725	0.7756	0.7806	0.7850	0.7838	0.7869	0.7896
4.1035	0.7845	0.7879	0.7891	0.7955	0.7985	0.7980	0.8001	0.8041
4.1289	0.8016	0.8046	0.8064	0.8116	0.8144	0.8142	0.8150	0.8200
4.1543	0.8190	0.8234	0.8256	0.8295	0.8314	0.8311	0.8314	0.8350
4.1797	0.8389	0.8422	0.8439	0.8467	0.8487	0.8477	0.8481	0.8504
4.2051	0.8589	0.8618	0.8641	0.8651	0.8679	0.8657	0.8661	0.8683
4.2305	0.8784	0.8807	0.8827	0.8839	0.8858	0.8828	0.8819	0.8853
4.2559	0.9012	0.9019	0.9024	0.9065	0.9064	0.9027	0.9005	0.9038
4.2813	0.9226	0.9231	0.9245	0.9269	0.9271	0.9231	0.9194	0.9237
4.3067	0.9422	0.9431	0.9467	0.9475	0.9474	0.9421	0.9382	0.9429
4.3321	0.9649	0.9650	0.9688	0.9679	0.9678	0.9619	0.9596	0.9620
4.3575	0.9877	0.9872	0.9897	0.9879	0.9874	0.9813	0.9796	0.9798
4.3829	1.0117	1.0102	1.0106	1.0088	1.0080	1.0013	0.9988	0.9989
4.4084	1.0354	1.0326	1.0322	1.0317	1.0298	1.0205	1.0191	1.0198
4.4338	1.0585	1.0552	1.0535	1.0529	1.0498	1.0407	1.0391	1.0410
4.4592	1.0803	1.0773	1.0754	1.0727	1.0702	1.0617	1.0578	1.0597
4.4846	1.1017	1.0967	1.0961	1.0937	1.0911	1.0810	1.0743	1.0761

Q ($Å^{-1}$)	S(Q) 898K	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 986K	S(Q) 1008K	S(Q) 1030K	S(Q) 1052K
4.5354	1.1447	1.1397	1.1370	1.1345	1.1318	1.1201	1.1126	1.1109
4.5608	1.1625	1.1580	1.1545	1.1499	1.1488	1.1362	1.1300	1.1266
4.5862	1.1817	1.1762	1.1726	1.1665	1.1655	1.1533	1.1472	1.1428
4.6116	1.1998	1.1947	1.1905	1.1834	1.1833	1.1704	1.1634	1.1592
4.6370	1.2154	1.2120	1.2066	1.1992	1.1984	1.1865	1.1781	1.1747
4.6624	1.2296	1.2250	1.2209	1.2140	1.2129	1.2006	1.1916	1.1895
4.6878	1.2394	1.2339	1.2303	1.2248	1.2216	1.2091	1.2015	1.1993
4.7133	1.2537	1.2477	1.2414	1.2374	1.2327	1.2205	1.2128	1.2113
4.7387	1.2630	1.2568	1.2493	1.2468	1.2411	1.2295	1.2198	1.2204
4.7641	1.2687	1.2613	1.2548	1.2534	1.2475	1.2351	1.2263	1.2259
4.7895	1.2738	1.2666	1.2614	1.2578	1.2530	1.2394	1.2326	1.2302
4.8149	1.2756	1.2706	1.2656	1.2602	1.2549	1.2427	1.2356	1.2335
4.8403	1.2758	1.2724	1.2683	1.2621	1.2569	1.2453	1.2382	1.2366
4.8657	1.2743	1.2700	1.2670	1.2597	1.2550	1.2459	1.2370	1.2355
4.8911	1.2759	1.2704	1.2658	1.2592	1.2561	1.2457	1.2378	1.2371
4.9165	1.2736	1.2691	1.2658	1.2598	1.2563	1.2459	1.2398	1.2387
4.9419	1.2712	1.2684	1.2636	1.2596	1.2556	1.2449	1.2411	1.2366
4.9673	1.2654	1.2637	1.2586	1.2562	1.2517	1.2408	1.2369	1.2326
4.9927	1.2586	1.2582	1.2527	1.2525	1.2466	1.2361	1.2331	1.2296
5.0182	1.2520	1.2518	1.2465	1.2469	1.2405	1.2316	1.2271	1.2250
5.0436	1.2452	1.2430	1.2384	1.2375	1.2317	1.2233	1.2209	1.2181
5.0690	1.2381	1.2336	1.2303	1.2277	1.2249	1.2168	1.2135	1.2124
5.0944	1.2284	1.2233	1.2210	1.2176	1.2179	1.2085	1.2065	1.2064
5.1198	1.2177	1.2140	1.2128	1.2088	1.2087	1.1983	1.1978	1.1982
5.1452	1.2094	1.2039	1.2031	1.2013	1.2004	1.1912	1.1907	1.1898
5.1706	1.1993	1.1943	1.1930	1.1909	1.1903	1.1829	1.1827	1.1827
5.1960	1.1851	1.1819	1.1804	1.1778	1.1790	1.1702	1.1710	1.1731
5.2214	1.1732	1.1700	1.1710	1.1682	1.1681	1.1614	1.1593	1.1618
5.2468	1.1618	1.1585	1.1588	1.1545	1.1561	1.1503	1.1482	1.1510
5.2722	1.1484	1.1475	1.1455	1.1440	1.1436	1.1388	1.1366	1.1396
5.2976	1.1360	1.1339	1.1329	1.1317	1.1317	1.1268	1.1251	1.1290
5.3231	1.1236	1.1195	1.1197	1.1173	1.1197	1.1154	1.1124	1.1183
5.3485	1.1085	1.1059	1.1068	1.1055	1.1060	1.1033	1.1010	1.1067
5.3739	1.0925	1.0921	1.0927	1.0909	1.0913	1.0884	1.0875	1.0925
5.3993	1.0785	1.0799	1.0804	1.0792	1.0773	1.0762	1.0774	1.0805
5.4247	1.0653	1.0673	1.0678	1.0651	1.0653	1.0641	1.0655	1.0687
5.4501	1.0520	1.0533	1.0551	1.0514	1.0541	1.0525	1.0528	1.0581
5.4755	1.0383	1.0382	1.0401	1.0386	1.0403	1.0390	1.0402	1.0452
5.5009	1.0277	1.0270	1.0285	1.0286	1.0292	1.0278	1.0318	1.0350
5.5263	1.0157	1.0153	1.0165	1.0169	1.0184	1.0163	1.0208	1.0240
5.5517	1.0009	1.0004	1.0023	1.0022	1.0038	1.0043	1.0071	1.0095
5.5771	0.9880	0.9881	0.9892	0.9910	0.9904	0.9936	0.9957	0.9972
5.6025	0.9754	0.9760	0.9768	0.9798	0.9808	0.9829	0.9848	0.9854
5.6280	0.9640	0.9642	0.9677	0.9678	0.9712	0.9713	0.9742	0.9766
5.6534	0.9506	0.9523	0.9562	0.9565	0.9597	0.9589	0.9628	0.9662
5.6788	0.9397	0.9419	0.9453	0.9457	0.9502	0.9499	0.9538	0.9571
5.7042	0.9282	0.9314	0.9334	0.9354	0.9394	0.9392	0.9429	0.9465
5.7296	0.9178	0.9211	0.9234	0.9269	0.9289	0.9294	0.9317	0.9365
5.7550	0.9094	0.9109	0.9155	0.9185	0.9185	0.9212	0.9218	0.9290
5.7804	0.9011	0.9028	0.9055	0.9092	0.9090	0.9135	0.9143	0.9217
5.8058	0.8922	0.8953	0.8965	0.9006	0.9015	0.9064	0.9075	0.9145

Q (Å^{-1})	S(Q) 898K	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 986K	S(Q) 1008K	S(Q) 1030K	S(Q) 1052K
5.8566	0.8803	0.8787	0.8838	0.8854	0.8869	0.8911	0.8964	0.8993
5.8820	0.8732	0.8708	0.8768	0.8775	0.8807	0.8842	0.8898	0.8925
5.9074	0.8660	0.8645	0.8696	0.8707	0.8761	0.8789	0.8831	0.8870
5.9329	0.8583	0.8594	0.8625	0.8650	0.8704	0.8729	0.8785	0.8822
5.9583	0.8520	0.8539	0.8573	0.8590	0.8647	0.8672	0.8730	0.8768
5.9837	0.8490	0.8496	0.8549	0.8543	0.8608	0.8623	0.8674	0.8728
6.0091	0.8461	0.8479	0.8521	0.8519	0.8583	0.8596	0.8632	0.8706
6.0345	0.8438	0.8459	0.8479	0.8502	0.8552	0.8560	0.8615	0.8680
6.0599	0.8413	0.8429	0.8437	0.8478	0.8527	0.8533	0.8590	0.8669
6.0853	0.8392	0.8413	0.8434	0.8486	0.8519	0.8537	0.8576	0.8662
6.1107	0.8384	0.8407	0.8440	0.8506	0.8530	0.8530	0.8562	0.8645
6.1361	0.8385	0.8404	0.8448	0.8501	0.8527	0.8514	0.8552	0.8631
6.1615	0.8372	0.8401	0.8442	0.8475	0.8499	0.8504	0.8550	0.8612
6.1869	0.8381	0.8417	0.8449	0.8473	0.8501	0.8522	0.8572	0.8619
6.2123	0.8405	0.8422	0.8468	0.8493	0.8518	0.8555	0.8586	0.8628
6.2378	0.8442	0.8453	0.8495	0.8523	0.8553	0.8584	0.8606	0.8644
6.2632	0.8487	0.8510	0.8539	0.8563	0.8592	0.8600	0.8646	0.8683
6.2886	0.8536	0.8548	0.8570	0.8594	0.8621	0.8608	0.8672	0.8711
6.3140	0.8567	0.8572	0.8604	0.8623	0.8648	0.8637	0.8694	0.8735
6.3394	0.8609	0.8614	0.8655	0.8655	0.8693	0.8675	0.8725	0.8777
6.3648	0.8663	0.8658	0.8706	0.8691	0.8724	0.8722	0.8767	0.8802
6.3902	0.8704	0.8710	0.8742	0.8732	0.8764	0.8761	0.8794	0.8821
6.4156	0.8750	0.8765	0.8773	0.8788	0.8824	0.8797	0.8820	0.8853
6.4410	0.8809	0.8818	0.8823	0.8854	0.8875	0.8852	0.8864	0.8900
6.4664	0.8868	0.8875	0.8882	0.8909	0.8930	0.8912	0.8913	0.8936
6.4918	0.8930	0.8922	0.8929	0.8951	0.8976	0.8943	0.8952	0.8975
6.5172	0.9014	0.8994	0.9021	0.9007	0.9043	0.9009	0.8997	0.9025
6.5427	0.9071	0.9049	0.9080	0.9067	0.9096	0.9064	0.9054	0.9073
6.5681	0.9142	0.9117	0.9130	0.9142	0.9161	0.9111	0.9120	0.9143
6.5935	0.9216	0.9182	0.9213	0.9213	0.9214	0.9154	0.9184	0.9210
6.6189	0.9278	0.9263	0.9283	0.9273	0.9277	0.9220	0.9250	0.9270
6.6443	0.9332	0.9325	0.9331	0.9331	0.9339	0.9290	0.9300	0.9320
6.6697	0.9419	0.9388	0.9381	0.9399	0.9390	0.9351	0.9350	0.9351
6.6951	0.9488	0.9469	0.9449	0.9455	0.9455	0.9414	0.9395	0.9417
6.7205	0.9552	0.9542	0.9534	0.9511	0.9523	0.9482	0.9439	0.9482
6.7459	0.9638	0.9618	0.9608	0.9596	0.9594	0.9536	0.9517	0.9539
6.7713	0.9718	0.9688	0.9662	0.9670	0.9667	0.9605	0.9576	0.9604
6.7967	0.9778	0.9751	0.9730	0.9728	0.9721	0.9679	0.9613	0.9654
6.8221	0.9832	0.9789	0.9792	0.9772	0.9770	0.9717	0.9669	0.9688
6.8476	0.9897	0.9848	0.9844	0.9825	0.9833	0.9750	0.9722	0.9738
6.8730	0.9951	0.9922	0.9894	0.9876	0.9884	0.9798	0.9770	0.9791
6.8984	1.0002	0.9982	0.9945	0.9939	0.9939	0.9861	0.9809	0.9856
6.9238	1.0051	1.0047	0.9985	0.9989	0.9974	0.9899	0.9850	0.9907
6.9492	1.0112	1.0116	1.0032	1.0039	1.0021	0.9942	0.9918	0.9950
6.9746	1.0168	1.0178	1.0101	1.0108	1.0079	1.0001	1.0013	1.0022
7.0000	1.0220	1.0211	1.0156	1.0154	1.0110	1.0040	1.0043	1.0043
7.0254	1.0271	1.0234	1.0201	1.0197	1.0161	1.0095	1.0105	1.0077
7.0508	1.0302	1.0261	1.0243	1.0229	1.0228	1.0134	1.0123	1.0115
7.0762	1.0340	1.0287	1.0296	1.0252	1.0255	1.0180	1.0153	1.0170
7.1016	1.0360	1.0306	1.0331	1.0287	1.0258	1.0224	1.0181	1.0215
7.1270	1.0374	1.0345	1.0342	1.0322	1.0283	1.0248	1.0208	1.0240

Q (Å^{-1})	S(Q) 898K	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 986K	S(Q) 1008K	S(Q) 1030K	S(Q) 1052K
7.1779	1.0421	1.0373	1.0367	1.0368	1.0358	1.0272	1.0256	1.0271
7.2033	1.0453	1.0396	1.0394	1.0389	1.0373	1.0283	1.0285	1.0287
7.2287	1.0468	1.0420	1.0392	1.0400	1.0368	1.0290	1.0293	1.0310
7.2541	1.0474	1.0427	1.0410	1.0405	1.0392	1.0300	1.0290	1.0317
7.2795	1.0458	1.0428	1.0403	1.0417	1.0386	1.0306	1.0300	1.0317
7.3049	1.0470	1.0412	1.0399	1.0415	1.0389	1.0315	1.0298	1.0319
7.3303	1.0476	1.0413	1.0419	1.0419	1.0398	1.0341	1.0320	1.0352
7.3557	1.0456	1.0417	1.0415	1.0394	1.0396	1.0339	1.0317	1.0348
7.3811	1.0458	1.0421	1.0407	1.0386	1.0404	1.0346	1.0325	1.0336
7.4065	1.0465	1.0424	1.0397	1.0390	1.0419	1.0362	1.0349	1.0354
7.4319	1.0458	1.0415	1.0404	1.0391	1.0421	1.0360	1.0366	1.0367
7.4574	1.0447	1.0413	1.0417	1.0418	1.0420	1.0368	1.0368	1.0382
7.4828	1.0430	1.0419	1.0404	1.0431	1.0416	1.0379	1.0352	1.0383
7.5082	1.0421	1.0414	1.0387	1.0417	1.0402	1.0375	1.0360	1.0380
7.5336	1.0381	1.0395	1.0360	1.0381	1.0377	1.0341	1.0364	1.0374
7.5590	1.0353	1.0370	1.0344	1.0359	1.0361	1.0326	1.0345	1.0366
7.5844	1.0355	1.0353	1.0351	1.0349	1.0384	1.0319	1.0336	1.0360
7.6098	1.0355	1.0328	1.0328	1.0330	1.0368	1.0292	1.0324	1.0349
7.6352	1.0343	1.0306	1.0310	1.0321	1.0352	1.0282	1.0322	1.0349
7.6606	1.0310	1.0253	1.0285	1.0301	1.0312	1.0273	1.0291	1.0332
7.6860	1.0294	1.0241	1.0271	1.0282	1.0288	1.0271	1.0263	1.0331
7.7114	1.0271	1.0240	1.0253	1.0275	1.0272	1.0268	1.0255	1.0307
7.7368	1.0238	1.0234	1.0244	1.0251	1.0254	1.0242	1.0229	1.0279
7.7623	1.0198	1.0213	1.0207	1.0214	1.0216	1.0214	1.0210	1.0263
7.7877	1.0162	1.0167	1.0157	1.0154	1.0198	1.0176	1.0179	1.0252
7.8131	1.0141	1.0123	1.0130	1.0127	1.0175	1.0164	1.0161	1.0
7.8385	1.0126	1.0089	1.0126	1.0110	1.0144	1.0154	1.0149	1.
7.8639	1.0113	1.0063	1.0096	1.0075	1.0111	1.0130	1.0118	1.
7.8893	1.0072	1.0034	1.0041	1.0041	1.0080	1.0074	1.0085	1.0
7.9147	1.0019	0.9980	0.9989	1.0003	1.0041	1.0034	1.0058	1.0118
7.9401	0.9985	0.9933	0.9955	0.9981	1.0008	1.0016	1.0037	1.0106
7.9655	0.9960	0.9937	0.9941	0.9969	0.9992	0.9996	1.0013	1.0093
7.9909	0.9889	0.9889	0.9888	0.9913	0.9926	0.9936	0.9948	1.0027
8.0163	0.9870	0.9872	0.9872	0.9894	0.9910	0.9921	0.9933	1.0008
8.0417	0.9849	0.9852	0.9854	0.9872	0.9892	0.9905	0.9918	0.9987
8.0672	0.9827	0.9830	0.9835	0.9849	0.9872	0.9887	0.9901	0.9965
8.0926	0.9802	0.9805	0.9814	0.9824	0.9852	0.9866	0.9882	0.9941
8.1180	0.9777	0.9777	0.9791	0.9798	0.9829	0.9843	0.9861	0.9913
8.1434	0.9751	0.9747	0.9766	0.9772	0.9805	0.9818	0.9838	0.9885
8.1688	0.9723	0.9719	0.9739	0.9745	0.9778	0.9793	0.9813	0.9859
8.1942	0.9696	0.9691	0.9712	0.9720	0.9752	0.9767	0.9790	0.9835
8.2196	0.9671	0.9666	0.9686	0.9694	0.9727	0.9740	0.9768	0.9812
8.2450	0.9648	0.9644	0.9663	0.9671	0.9704	0.9715	0.9746	0.9790
8.2704	0.9628	0.9624	0.9644	0.9651	0.9684	0.9691	0.9727	0.9771
8.2958	0.9609	0.9602	0.9626	0.9633	0.9666	0.9670	0.9707	0.9752
8.3212	0.9588	0.9582	0.9608	0.9615	0.9649	0.9650	0.9685	0.9732
8.3466	0.9571	0.9566	0.9594	0.9596	0.9634	0.9631	0.9670	0.9712
8.3721	0.9555	0.9554	0.9581	0.9579	0.9620	0.9614	0.9653	0.9694
8.3975	0.9541	0.9543	0.9566	0.9567	0.9609	0.9599	0.9636	0.9677
8.4229	0.9528	0.9533	0.9553	0.9558	0.9600	0.9584	0.9620	0.9663
8.4483	0.9517	0.9525	0.9544	0.9552	0.9591	0.9571	0.9605	0.9653

Q (Å^{-1})	S(Q) 898K	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 986K	S(Q) 1008K	S(Q) 1030K	S(Q) 1052K
8.4991	0.9497	0.9513	0.9529	0.9536	0.9573	0.9553	0.9577	0.9631
8.5245	0.9490	0.9508	0.9525	0.9531	0.9565	0.9546	0.9564	0.9620
8.5499	0.9487	0.9505	0.9524	0.9530	0.9562	0.9543	0.9558	0.9613
8.5753	0.9486	0.9503	0.9526	0.9530	0.9559	0.9542	0.9553	0.9608
8.6007	0.9489	0.9503	0.9530	0.9532	0.9559	0.9543	0.9551	0.9604
8.6261	0.9495	0.9507	0.9534	0.9536	0.9559	0.9547	0.9553	0.9604
8.6515	0.9504	0.9516	0.9540	0.9543	0.9561	0.9554	0.9559	0.9610
8.6770	0.9515	0.9529	0.9548	0.9551	0.9566	0.9562	0.9569	0.9622
8.7024	0.9531	0.9541	0.9559	0.9561	0.9575	0.9571	0.9580	0.9635
8.7278	0.9551	0.9555	0.9573	0.9570	0.9587	0.9580	0.9593	0.9647
8.7532	0.9569	0.9570	0.9591	0.9580	0.9601	0.9591	0.9606	0.9659
8.7786	0.9588	0.9584	0.9608	0.9591	0.9617	0.9604	0.9622	0.9673
8.8040	0.9610	0.9602	0.9623	0.9605	0.9632	0.9618	0.9637	0.9686
8.8294	0.9632	0.9622	0.9638	0.9619	0.9646	0.9633	0.9651	0.9697
8.8548	0.9656	0.9644	0.9657	0.9636	0.9661	0.9647	0.9666	0.9707
8.8802	0.9681	0.9666	0.9677	0.9655	0.9680	0.9663	0.9681	0.9720
8.9056	0.9706	0.9688	0.9697	0.9675	0.9700	0.9681	0.9695	0.9736
8.9310	0.9732	0.9711	0.9720	0.9697	0.9721	0.9701	0.9710	0.9753
8.9565	0.9756	0.9734	0.9744	0.9723	0.9742	0.9719	0.9728	0.9772
8.9819	0.9779	0.9755	0.9767	0.9746	0.9764	0.9736	0.9744	0.9789
9.0073	0.9803	0.9776	0.9791	0.9771	0.9787	0.9755	0.9761	0.9805
9.0327	0.9827	0.9801	0.9817	0.9797	0.9808	0.9777	0.9780	0.9821
9.0581	0.9852	0.9829	0.9845	0.9826	0.9832	0.9801	0.9804	0.9841
.0835	0.9877	0.9859	0.9873	0.9857	0.9854	0.9826	0.9829	0.9858
.1089	0.9906	0.9890	0.9902	0.9888	0.9881	0.9852	0.9856	0.9877
9.1343	0.9938	0.9924	0.9930	0.9920	0.9912	0.9877	0.9882	0.9901
9.1597	0.9967	0.9958	0.9960	0.9951	0.9944	0.9901	0.9908	0.9926
9.1851	0.9993	0.9987	0.9991	0.9981	0.9975	0.9926	0.9934	0.9953
9.2105	1.0021	1.0014	1.0023	1.0010	1.0007	0.9949	0.9957	0.9979
9.2359	1.0048	1.0041	1.0054	1.0038	1.0035	0.9972	0.9981	1.0003
9.2614	1.0074	1.0072	1.0084	1.0066	1.0062	0.9997	1.0007	1.0027
9.2868	1.0103	1.0106	1.0112	1.0093	1.0086	1.0022	1.0033	1.0052
9.3122	1.0132	1.0139	1.0139	1.0119	1.0107	1.0048	1.0058	1.0072
9.3376	1.0157	1.0165	1.0162	1.0142	1.0131	1.0073	1.0080	1.0093
9.3630	1.0181	1.0186	1.0184	1.0164	1.0156	1.0097	1.0103	1.0117
9.3884	1.0205	1.0205	1.0204	1.0181	1.0179	1.0118	1.0122	1.0138
9.4138	1.0227	1.0222	1.0223	1.0196	1.0199	1.0138	1.0140	1.0157
9.4392	1.0245	1.0235	1.0239	1.0212	1.0217	1.0155	1.0157	1.0174
9.4646	1.0261	1.0246	1.0253	1.0224	1.0233	1.0169	1.0171	1.0188
9.4900	1.0275	1.0255	1.0265	1.0236	1.0248	1.0182	1.0184	1.0202
9.5154	1.0289	1.0265	1.0274	1.0248	1.0258	1.0196	1.0199	1.0213
9.5408	1.0299	1.0276	1.0282	1.0258	1.0265	1.0210	1.0211	1.0224
9.5663	1.0308	1.0283	1.0290	1.0270	1.0273	1.0225	1.0221	1.0236
9.5917	1.0318	1.0287	1.0297	1.0282	1.0281	1.0237	1.0229	1.0245
9.6171	1.0326	1.0292	1.0305	1.0290	1.0292	1.0248	1.0234	1.0256
9.6425	1.0334	1.0299	1.0315	1.0298	1.0302	1.0258	1.0238	1.0265
9.6679	1.0338	1.0301	1.0322	1.0303	1.0308	1.0263	1.0242	1.0272
9.6933	1.0339	1.0301	1.0328	1.0307	1.0312	1.0266	1.0247	1.0279
9.7187	1.0340	1.0304	1.0333	1.0308	1.0312	1.0269	1.0250	1.0286
9.7441	1.0340	1.0308	1.0336	1.0312	1.0310	1.0272	1.0253	1.0291
9.7695	1.0341	1.0315	1.0339	1.0316	1.0308	1.0274	1.0259	1.0297

Q (Å^{-1})	S(Q) 898K	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 986K	S(Q) 1008K	S(Q) 1030K	S(Q) 1052K
9.8203	1.0343	1.0322	1.0340	1.0316	1.0305	1.0278	1.0266	1.0307
9.8457	1.0340	1.0321	1.0335	1.0316	1.0306	1.0279	1.0270	1.0310
9.8712	1.0337	1.0321	1.0329	1.0313	1.0306	1.0278	1.0273	1.0313
9.8966	1.0333	1.0320	1.0325	1.0312	1.0305	1.0276	1.0274	1.0313
9.9220	1.0330	1.0315	1.0319	1.0309	1.0303	1.0274	1.0271	1.0311
9.9474	1.0326	1.0309	1.0311	1.0305	1.0300	1.0272	1.0267	1.0309
9.9728	1.0321	1.0303	1.0303	1.0299	1.0296	1.0265	1.0264	1.0305
9.9982	1.0314	1.0296	1.0296	1.0292	1.0291	1.0258	1.0262	1.0302
10.0236	1.0307	1.0288	1.0288	1.0286	1.0283	1.0251	1.0258	1.0298
10.0490	1.0297	1.0276	1.0278	1.0277	1.0274	1.0246	1.0253	1.0296
10.0744	1.0287	1.0264	1.0268	1.0272	1.0267	1.0242	1.0246	1.0294
10.0998	1.0278	1.0253	1.0260	1.0265	1.0260	1.0236	1.0239	1.0290
10.1252	1.0267	1.0244	1.0254	1.0257	1.0256	1.0228	1.0231	1.0286
10.1506	1.0260	1.0234	1.0248	1.0248	1.0253	1.0219	1.0223	1.0283
10.1761	1.0253	1.0221	1.0239	1.0238	1.0247	1.0208	1.0218	1.0278
10.2015	1.0242	1.0210	1.0229	1.0229	1.0239	1.0197	1.0213	1.0271
10.2269	1.0230	1.0201	1.0220	1.0225	1.0232	1.0191	1.0206	1.0264
10.2523	1.0220	1.0195	1.0210	1.0223	1.0226	1.0186	1.0200	1.0257
10.2777	1.0212	1.0190	1.0203	1.0219	1.0220	1.0182	1.0197	1.0252
10.3031	1.0207	1.0189	1.0199	1.0216	1.0216	1.0184	1.0198	1.0251
10.3285	1.0206	1.0188	1.0193	1.0215	1.0215	1.0186	1.0199	1.0248
10.3539	1.0203	1.0188	1.0188	1.0213	1.0216	1.0188	1.0201	1.0248
10.3793	1.0199	1.0186	1.0182	1.0210	1.0218	1.0188	1.0201	1.0249
10.4047	1.0197	1.0183	1.0179	1.0208	1.0220	1.0190	1.0199	1.0251
10.4301	1.0199	1.0180	1.0178	1.0207	1.0221	1.0191	1.0196	1.0253
10.4555	1.0201	1.0180	1.0180	1.0204	1.0219	1.0195	1.0198	1.0257
10.4810	1.0202	1.0178	1.0182	1.0198	1.0219	1.0195	1.0200	1.0262
10.5064	1.0201	1.0178	1.0184	1.0193	1.0219	1.0197	1.0203	1.0266
10.5318	1.0198	1.0178	1.0183	1.0189	1.0216	1.0200	1.0204	1.0267
10.5572	1.0194	1.0176	1.0180	1.0185	1.0214	1.0200	1.0204	1.0268
10.5826	1.0191	1.0172	1.0180	1.0182	1.0211	1.0197	1.0202	1.0266
10.6080	1.0188	1.0167	1.0182	1.0177	1.0207	1.0190	1.0198	1.0264
10.6334	1.0184	1.0163	1.0184	1.0173	1.0205	1.0182	1.0194	1.0260
10.6588	1.0182	1.0157	1.0185	1.0171	1.0200	1.0176	1.0189	1.0253
10.6842	1.0178	1.0149	1.0185	1.0170	1.0196	1.0171	1.0185	1.0241
10.7096	1.0171	1.0142	1.0184	1.0171	1.0192	1.0167	1.0180	1.0230
10.7350	1.0165	1.0135	1.0180	1.0172	1.0185	1.0162	1.0171	1.0222
10.7604	1.0161	1.0130	1.0175	1.0169	1.0179	1.0156	1.0164	1.0216
10.7859	1.0158	1.0126	1.0174	1.0163	1.0172	1.0153	1.0156	1.0212
10.8113	1.0157	1.0121	1.0171	1.0158	1.0170	1.0150	1.0147	1.0210
10.8367	1.0157	1.0116	1.0164	1.0151	1.0171	1.0142	1.0139	1.0209
10.8621	1.0154	1.0110	1.0158	1.0145	1.0175	1.0133	1.0137	1.0211
10.8875	1.0138	1.0107	1.0152	1.0142	1.0181	1.0125	1.0136	1.0212
10.9129	1.0118	1.0103	1.0150	1.0141	1.0182	1.0116	1.0133	1.0213
10.9383	1.0108	1.0097	1.0150	1.0142	1.0181	1.0111	1.0129	1.0213
10.9637	1.0127	1.0094	1.0147	1.0135	1.0178	1.0109	1.0127	1.0213
10.9891	1.0161	1.0093	1.0143	1.0127	1.0176	1.0103	1.0128	1.0212
11.0145	1.0194	1.0096	1.0143	1.0125	1.0173	1.0098	1.0129	1.0208
11.0399	1.0221	1.0097	1.0143	1.0119	1.0167	1.0092	1.0129	1.0204
11.0654	1.0244	1.0099	1.0140	1.0116	1.0160	1.0089	1.0130	1.0199
11.0908	1.0263	1.0100	1.0138	1.0116	1.0152	1.0088	1.0130	1.0191

Q (Å^{-1})	S(Q) 898K	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 986K	S(Q) 1008K	S(Q) 1030K	S(Q) 1052K
11.1416	1.0283	1.0103	1.0194	1.0114	1.0139	1.0087	1.0125	1.0166
11.1670	1.0288	1.0104	1.0129	1.0118	1.0132	1.0086	1.0120	1.0152
11.1924	1.0285	1.0106	1.0124	1.0119	1.0128	1.0080	1.0117	1.0141
11.2178	1.0277	1.0108	1.0121	1.0123	1.0122	1.0077	1.0111	1.0131
11.2432	1.0264	1.0111	1.0119	1.0125	1.0115	1.0075	1.0106	1.0124
11.2686	1.0250	1.0118	1.0118	1.0130	1.0116	1.0076	1.0099	1.0119
11.2940	1.0231	1.0127	1.0120	1.0138	1.0118	1.0079	1.0094	1.0116
11.3194	1.0207	1.0131	1.0120	1.0147	1.0124	1.0079	1.0094	1.0113
11.3448	1.0181	1.0139	1.0123	1.0152	1.0132	1.0078	1.0100	1.0115
11.3703	1.0148	1.0145	1.0127	1.0157	1.0141	1.0076	1.0104	1.0119
11.3957	1.0110	1.0146	1.0129	1.0162	1.0144	1.0071	1.0103	1.0120
11.4211	1.0091	1.0142	1.0133	1.0166	1.0145	1.0066	1.0101	1.0125
11.4465	1.0099	1.0139	1.0138	1.0164	1.0150	1.0065	1.0100	1.0129
11.4719	1.0129	1.0140	1.0141	1.0161	1.0154	1.0065	1.0103	1.0132
11.4973	1.0151	1.0145	1.0147	1.0165	1.0160	1.0067	1.0107	1.0137
11.5227	1.0159	1.0151	1.0157	1.0168	1.0165	1.0070	1.0104	1.0144
11.5481	1.0164	1.0157	1.0165	1.0166	1.0173	1.0073	1.0104	1.0151
11.5735	1.0171	1.0166	1.0170	1.0167	1.0181	1.0080	1.0102	1.0156
11.5989	1.0178	1.0175	1.0182	1.0170	1.0189	1.0091	1.0102	1.0159
11.6243	1.0183	1.0183	1.0192	1.0171	1.0197	1.0098	1.0100	1.0159
11.6497	1.0187	1.0193	1.0200	1.0177	1.0205	1.0104	1.0097	1.0162
11.6752	1.0192	1.0201	1.0204	1.0183	1.0214	1.0108	1.0093	1.0163
11.7006	1.0195	1.0209	1.0209	1.0188	1.0222	1.0116	1.0092	1.0168
11.7260	1.0200	1.0216	1.0218	1.0196	1.0228	1.0126	1.0091	1.0171
11.7514	1.0202	1.0223	1.0228	1.0204	1.0234	1.0134	1.0093	1.0173
11.7768	1.0208	1.0234	1.0241	1.0221	1.0241	1.0145	1.0097	1.0179
11.8022	1.0216	1.0243	1.0252	1.0239	1.0247	1.0158	1.0108	1.0188
11.8276	1.0226	1.0251	1.0266	1.0251	1.0253	1.0171	1.0121	1.0198
11.8530	1.0238	1.0259	1.0277	1.0260	1.0261	1.0181	1.0131	1.0212
11.8784	1.0252	1.0261	1.0285	1.0269	1.0269	1.0188	1.0143	1.0228
11.9038	1.0271	1.0259	1.0293	1.0275	1.0276	1.0197	1.0161	1.0243
11.9292	1.0287	1.0257	1.0303	1.0281	1.0285	1.0205	1.0181	1.0257
11.9546	1.0297	1.0256	1.0311	1.0284	1.0295	1.0210	1.0195	1.0264
11.9801	1.0303	1.0263	1.0317	1.0291	1.0304	1.0217	1.0207	1.0270
12.0055	1.0309	1.0273	1.0322	1.0298	1.0313	1.0224	1.0216	1.0275
12.0309	1.0317	1.0284	1.0328	1.0301	1.0320	1.0230	1.0223	1.0283
12.0563	1.0327	1.0295	1.0334	1.0305	1.0329	1.0237	1.0233	1.0291
12.0817	1.0338	1.0308	1.0342	1.0312	1.0341	1.0247	1.0244	1.0297
12.1071	1.0349	1.0322	1.0351	1.0317	1.0357	1.0258	1.0255	1.0303
12.1325	1.0358	1.0332	1.0356	1.0321	1.0370	1.0264	1.0264	1.0307
12.1579	1.0366	1.0342	1.0356	1.0325	1.0382	1.0268	1.0269	1.0315
12.1833	1.0373	1.0348	1.0351	1.0326	1.0392	1.0268	1.0273	1.0322
12.2087	1.0381	1.0357	1.0351	1.0330	1.0395	1.0268	1.0272	1.0328
12.2341	1.0385	1.0368	1.0354	1.0335	1.0392	1.0268	1.0271	1.0331
12.2595	1.0387	1.0379	1.0356	1.0341	1.0390	1.0269	1.0275	1.0335
12.2850	1.0394	1.0392	1.0361	1.0354	1.0388	1.0278	1.0283	1.0343
12.3104	1.0401	1.0398	1.0366	1.0367	1.0386	1.0287	1.0291	1.0351
12.3358	1.0408	1.0400	1.0372	1.0379	1.0388	1.0295	1.0298	1.0360
12.3612	1.0415	1.0395	1.0380	1.0392	1.0393	1.0301	1.0304	1.0372
12.3866	1.0427	1.0390	1.0388	1.0402	1.0396	1.0304	1.0312	1.0381
12.4120	1.0433	1.0390	1.0401	1.0413	1.0394	1.0306	1.0317	1.0393

Q (Å^{-1})	S(Q) 898K	S(Q) 920K	S(Q) 942K	S(Q) 964K	S(Q) 986K	S(Q) 1008K	S(Q) 1030K	S(Q) 1052K
12.4628	1.0431	1.0390	1.0422	1.0428	1.0390	1.0308	1.0325	1.0404
12.4882	1.0435	1.0394	1.0426	1.0430	1.0392	1.0312	1.0327	1.0406
12.5136	1.0437	1.0398	1.0425	1.0430	1.0396	1.0317	1.0333	1.0407
12.5390	1.0435	1.0398	1.0424	1.0428	1.0401	1.0323	1.0338	1.0408
12.5644	1.0431	1.0394	1.0426	1.0423	1.0407	1.0326	1.0342	1.0407
12.5899	1.0428	1.0393	1.0427	1.0416	1.0413	1.0328	1.0341	1.0405
12.6153	1.0425	1.0387	1.0423	1.0402	1.0417	1.0328	1.0342	1.0404
12.6407	1.0419	1.0382	1.0419	1.0386	1.0419	1.0326	1.0342	1.0406
12.6661	1.0412	1.0378	1.0415	1.0370	1.0416	1.0320	1.0335	1.0410
12.6915	1.0403	1.0370	1.0408	1.0351	1.0410	1.0311	1.0321	1.0408
12.7169	1.0395	1.0369	1.0402	1.0336	1.0397	1.0304	1.0305	1.0401
12.7423	1.0381	1.0365	1.0392	1.0320	1.0382	1.0297	1.0298	1.0392
12.7677	1.0373	1.0364	1.0388	1.0312	1.0376	1.0295	1.0301	1.0387
12.7931	1.0356	1.0348	1.0374	1.0299	1.0358	1.0283	1.0295	1.0380
12.8185	1.0333	1.0320	1.0351	1.0282	1.0333	1.0266	1.0279	1.0369
12.8439	1.0312	1.0290	1.0328	1.0265	1.0310	1.0251	1.0262	1.0354
12.8693	1.0295	1.0263	1.0311	1.0251	1.0288	1.0234	1.0244	1.0333
12.8948	1.0283	1.0247	1.0292	1.0238	1.0266	1.0213	1.0226	1.0314
12.9202	1.0270	1.0242	1.0284	1.0227	1.0245	1.0196	1.0213	1.0302
12.9456	1.0252	1.0237	1.0274	1.0210	1.0228	1.0181	1.0201	1.0286
12.9710	1.0235	1.0231	1.0260	1.0193	1.0214	1.0166	1.0191	1.0264
12.9964	1.0217	1.0222	1.0244	1.0184	1.0205	1.0149	1.0176	1.0243
13.0218	1.0199	1.0212	1.0224	1.0179	1.0197	1.0135	1.0164	1.0220
13.0472	1.0178	1.0198	1.0203	1.0172	1.0187	1.0123	1.0150	1.0195
13.0726	1.0156	1.0178	1.0183	1.0159	1.0170	1.0106	1.0129	1.0169
13.0980	1.0136	1.0159	1.0159	1.0148	1.0153	1.0088	1.0109	1.0144
13.1234	1.0118	1.0138	1.0135	1.0133	1.0141	1.0070	1.0089	1.012
13.1488	1.0101	1.0118	1.0118	1.0120	1.0131	1.0052	1.0069	1.01(
13.1742	1.0083	1.0092	1.0099	1.0110	1.0118	1.0030	1.0044	1.0090
13.1997	1.0065	1.0066	1.0078	1.0100	1.0106	1.0008	1.0019	1.0070
13.2251	1.0046	1.0041	1.0054	1.0091	1.0089	0.9988	1.0001	1.0050
13.2505	1.0027	1.0017	1.0031	1.0080	1.0070	0.9968	0.9988	1.0034
13.2759	1.0010	0.9996	1.0010	1.0068	1.0053	0.9948	0.9976	1.0023
13.3013	0.9984	0.9962	0.9977	1.0044	1.0023	0.9918	0.9954	1.0003
13.3267	0.9960	0.9931	0.9946	1.0018	0.9994	0.9892	0.9932	0.9978
13.3521	0.9937	0.9909	0.9923	0.9991	0.9970	0.9871	0.9915	0.9949
13.3775	0.9920	0.9899	0.9908	0.9963	0.9954	0.9849	0.9897	0.9927
13.4029	0.9907	0.9890	0.9891	0.9946	0.9935	0.9826	0.9876	0.9912
13.4283	0.9896	0.9882	0.9879	0.9922	0.9914	0.9808	0.9856	0.9900
13.4537	0.9883	0.9877	0.9872	0.9899	0.9894	0.9792	0.9839	0.9888
13.4791	0.9874	0.9871	0.9867	0.9884	0.9880	0.9778	0.9827	0.9878
13.5046	0.9871	0.9870	0.9860	0.9875	0.9869	0.9765	0.9815	0.9871
13.5300	0.9866	0.9867	0.9848	0.9864	0.9858	0.9755	0.9801	0.9862
13.5554	0.9859	0.9863	0.9843	0.9852	0.9854	0.9750	0.9793	0.9854
13.5808	0.9853	0.9857	0.9840	0.9844	0.9855	0.9745	0.9785	0.9847
13.6062	0.9854	0.9853	0.9840	0.9843	0.9862	0.9747	0.9782	0.9841
13.6316	0.9857	0.9851	0.9845	0.9844	0.9871	0.9753	0.9777	0.9838
13.6570	0.9860	0.9853	0.9855	0.9850	0.9881	0.9762	0.9779	0.9837
13.6824	0.9868	0.9856	0.9867	0.9861	0.9895	0.9773	0.9784	0.9841
13.7078	0.9884	0.9861	0.9883	0.9874	0.9890	0.9786	0.9791	0.9853
13.7332	0.9901	0.9869	0.9895	0.9888	0.9898	0.9801	0.9797	0.9867

13.7586	0.9918	0.9880	0.9910	0.9901	0.9915	0.9815	0.9800	0.9882
13.7840	0.9930	0.9893	0.9923	0.9915	0.9933	0.9830	0.9804	0.9894
13.8095	0.9942	0.9907	0.9938	0.9936	0.9949	0.9847	0.9810	0.9906
13.8349	0.9958	0.9928	0.9955	0.9959	0.9966	0.9863	0.9815	0.9920
13.8603	0.9973	0.9948	0.9971	0.9976	0.9980	0.9880	0.9824	0.9938
13.8857	0.9986	0.9962	0.9982	0.9994	0.9989	0.9897	0.9831	0.9956
13.9111	0.9997	0.9977	0.9995	1.0009	0.9997	0.9915	0.9836	0.9978
13.9365	1.0005	0.9994	1.0011	1.0017	1.0003	0.9936	0.9845	1.0000
13.9619	1.0011	1.0016	1.0027	1.0021	1.0016	0.9949	0.9861	1.0021
13.9873	1.0013	1.0029	1.0032	1.0027	1.0030	0.9954	0.9877	1.0037
14.0127	1.0009	1.0037	1.0029	1.0030	1.0036	0.9954	0.9891	1.0047
14.0381	1.0002	1.0041	1.0025	1.0034	1.0039	0.9955	0.9903	1.0054
14.0635	0.9996	1.0046	1.0029	1.0038	1.0048	0.9959	0.9917	1.0064
14.0889	0.9990	1.0051	1.0034	1.0038	1.0059	0.9960	0.9927	1.0064
14.1144	0.9983	1.0052	1.0036	1.0032	1.0059	0.9955	0.9934	1.0059
14.1398	0.9978	1.0052	1.0034	1.0027	1.0053	0.9947	0.9937	1.0052
14.1652	0.9972	1.0048	1.0029	1.0019	1.0042	0.9934	0.9939	1.0041
14.1906	0.9969	1.0037	1.0020	1.0012	1.0029	0.9921	0.9935	1.0032
14.2160	0.9963	1.0021	1.0009	0.9999	1.0017	0.9904	0.9929	1.0025
14.2414	0.9954	1.0005	0.9997	0.9986	1.0008	0.9885	0.9922	1.0011
14.2668	0.9945	0.9984	0.9982	0.9972	0.9993	0.9862	0.9912	0.9990
14.2922	0.9942	0.9964	0.9969	0.9961	0.9973	0.9844	0.9900	0.9969
14.3176	0.9944	0.9946	0.9960	0.9956	0.9951	0.9828	0.9883	0.9952
14.3430	0.9942	0.9931	0.9953	0.9947	0.9931	0.9815	0.9868	0.9937
4.3684	0.9932	0.9914	0.9941	0.9933	0.9911	0.9807	0.9860	0.9921
4.3938	0.9917	0.9903	0.9926	0.9915	0.9889	0.9801	0.9847	0.9900
14.4193	0.9907	0.9897	0.9917	0.9895	0.9875	0.9799	0.9833	0.9887
14.4447	0.9901	0.9889	0.9905	0.9877	0.9863	0.9795	0.9824	0.9875
14.4701	0.9897	0.9884	0.9891	0.9868	0.9858	0.9790	0.9788	0.9870
14.4955	0.9891	0.9877	0.9878	0.9871	0.9850	0.9789	0.9738	0.9866
14.5209	0.9885	0.9877	0.9867	0.9877	0.9845	0.9792	0.9722	0.9866
14.5463	0.9879	0.9887	0.9866	0.9883	0.9846	0.9803	0.9737	0.9872
14.5717	0.9879	0.9899	0.9873	0.9888	0.9854	0.9821	0.9788	0.9879
14.5971	0.9885	0.9911	0.9879	0.9891	0.9866	0.9836	0.9913	0.9884
14.6225	0.9902	0.9927	0.9882	0.9900	0.9881	0.9837	1.0025	0.9895
14.6479	0.9925	0.9947	0.9892	0.9915	0.9903	0.9796	1.0123	0.9909
14.6733	0.9947	0.9970	0.9910	0.9932	0.9930	0.9742	1.0210	0.9925
14.6987	0.9971	0.9991	0.9926	0.9951	0.9956	0.9783	1.0288	0.9948
14.7242	0.9997	1.0013	0.9947	0.9977	0.9984	0.9918	1.0358	0.9974
14.7496	1.0029	1.0034	0.9974	1.0007	1.0010	1.0051	1.0413	0.9997
14.7750	1.0062	1.0049	1.0000	1.0035	1.0038	1.0168	1.0448	1.0020
14.8004	1.0098	1.0065	1.0034	1.0063	1.0068	1.0272	1.0466	1.0046
14.8258	1.0127	1.0081	1.0070	1.0089	1.0098	1.0358	1.0465	1.0071
14.8512	1.0152	1.0098	1.0105	1.0114	1.0128	1.0429	1.0453	1.0095
14.8766	1.0175	1.0112	1.0139	1.0134	1.0156	1.0483	1.0426	1.0117
14.9020	1.0197	1.0124	1.0170	1.0148	1.0179	1.0518	1.0374	1.0138
14.9274	1.0218	1.0131	1.0203	1.0163	1.0203	1.0537	1.0307	1.0160
14.9528	1.0235	1.0138	1.0233	1.0182	1.0225	1.0540	1.0222	1.0184
14.9782	1.0246	1.0142	1.0260	1.0200	1.0244	1.0528	1.0119	1.0205

Table A-13: Numerical values of SF for Liquid Al-10%Si alloy at various melt temperatures.

Q ($Å^{-1}$)	S(Q) 885K	S(Q) 907K	S(Q) 929K	S(Q) 973K	S(Q) 995K	S(Q) 1017K	S(Q) 1039K
0.6479	0.0194	0.0205	0.0206	0.0202	0.0255	0.0282	0.0289
0.6733	0.0176	0.0199	0.0221	0.0295	0.0252	0.0274	0.0287
0.6987	0.0206	0.0219	0.0213	0.0295	0.0266	0.0294	0.0299
0.7242	0.0251	0.0281	0.0220	0.0301	0.0298	0.0317	0.0314
0.7496	0.0273	0.0229	0.0241	0.0320	0.0334	0.0336	0.0321
0.7750	0.0299	0.0250	0.0264	0.0360	0.0364	0.0343	0.0334
0.8004	0.0302	0.0284	0.0267	0.0377	0.0356	0.0369	0.0362
0.8258	0.0314	0.0306	0.0299	0.0365	0.0347	0.0382	0.0369
0.8512	0.0313	0.0320	0.0298	0.0394	0.0370	0.0396	0.0386
0.8766	0.0327	0.0334	0.0339	0.0418	0.0412	0.0419	0.0404
0.9020	0.0354	0.0370	0.0372	0.0442	0.0434	0.0424	0.0421
0.9274	0.0384	0.0390	0.0426	0.0462	0.0442	0.0434	0.0432
0.9528	0.0397	0.0424	0.0423	0.0472	0.0445	0.0445	0.0443
0.9782	0.0425	0.0436	0.0429	0.0468	0.0468	0.0457	0.0439
1.0036	0.0478	0.0460	0.0479	0.0511	0.0518	0.0521	0.0501
1.0290	0.0522	0.0487	0.0512	0.0529	0.0556	0.0538	0.0548
1.0544	0.0552	0.0533	0.0562	0.0566	0.0577	0.0557	0.0573
1.0799	0.0582	0.0604	0.0605	0.0567	0.0584	0.0587	0.0600
1.1053	0.0621	0.0587	0.0650	0.0632	0.0621	0.0619	0.0603
1.1307	0.0674	0.0721	0.0687	0.0672	0.0666	0.0667	0.0671
1.1561	0.0721	0.0735	0.0725	0.0703	0.0682	0.0721	0.0720
1.1815	0.0783	0.0771	0.0760	0.0724	0.0720	0.0731	0.0738
1.2069	0.0814	0.0833	0.0826	0.0765	0.0780	0.0775	0.0787
1.2323	0.0881	0.0900	0.0893	0.0821	0.0836	0.0827	0.0813
1.2577	0.0942	0.0972	0.0956	0.0887	0.0871	0.0868	0.0867
1.2831	0.1010	0.1033	0.1022	0.0904	0.0905	0.0933	0.0931
1.3085	0.1080	0.1095	0.1095	0.0952	0.0956	0.0977	0.0954
1.3339	0.1154	0.1161	0.1167	0.0997	0.1002	0.1017	0.1042
1.3593	0.1237	0.1226	0.1242	0.1051	0.1049	0.1060	0.1101
1.3849	0.1308	0.1300	0.1314	0.1117	0.1121	0.1131	0.1155
1.4102	0.1369	0.1380	0.1414	0.1186	0.1190	0.1192	0.1215
1.4356	0.1446	0.1469	0.1506	0.1256	0.1250	0.1258	0.1284
1.4610	0.1527	0.1550	0.1564	0.1316	0.1307	0.1328	0.1344
1.4864	0.1575	0.1607	0.1618	0.1357	0.1365	0.1381	0.1401
1.5118	0.1624	0.1653	0.1680	0.1403	0.1419	0.1438	0.1440
1.5372	0.1691	0.1704	0.1730	0.1452	0.1481	0.1494	0.1522
1.5626	0.1749	0.1754	0.1781	0.1502	0.1546	0.1554	0.1588
1.5880	0.1787	0.1798	0.1831	0.1550	0.1601	0.1632	0.1651
1.6134	0.1819	0.1841	0.1862	0.1612	0.1652	0.1665	0.1712
1.6388	0.1856	0.1879	0.1884	0.1676	0.1690	0.1725	0.1768
1.6642	0.1893	0.1910	0.1925	0.1735	0.1744	0.1790	0.1851
1.6897	0.1940	0.1966	0.1978	0.1807	0.1813	0.1865	0.1918
1.7151	0.1990	0.2044	0.2045	0.1896	0.1901	0.1942	0.2014
1.7405	0.2043	0.2118	0.2122	0.1980	0.1989	0.2025	0.2109
1.7659	0.2109	0.2187	0.2202	0.2073	0.2075	0.2117	0.2197
1.7913	0.2190	0.2264	0.2279	0.2174	0.2181	0.2220	0.2291
1.8167	0.2277	0.2344	0.2364	0.2294	0.2307	0.2344	0.2418
1.8421	0.2367	0.2439	0.2470	0.2409	0.2436	0.2475	0.2547
1.8929	0.2629	0.2690	0.2739	0.2680	0.2730	0.2788	0.2870

Q ($Å^{-1}$)	S(Q) 885K	S(Q) 907K	S(Q) 929K	S(Q) 973K	S(Q) 995K	S(Q) 1017K	S(Q) 1039K
1.9133	0.2793	0.2867	0.2919	0.2879	0.2936	0.2968	0.3070
1.9437	0.2963	0.3039	0.3084	0.3067	0.3059	0.3078	0.3220
1.9692	0.3128	0.3214	0.3273	0.3276	0.3326	0.3404	0.3701
1.9946	0.3324	0.3397	0.3464	0.3486	0.3568	0.3660	0.3910
2.0200	0.3586	0.3682	0.3702	0.3742	0.3796	0.3868	0.4136
2.0454	0.3868	0.3898	0.3972	0.4030	0.4090	0.4165	0.4459
2.0708	0.4146	0.4187	0.4271	0.4362	0.4432	0.4506	0.4829
2.0962	0.4441	0.4525	0.4607	0.4681	0.4760	0.4869	0.5193
2.1216	0.4806	0.4825	0.4887	0.4967	0.5053	0.5171	0.5514
2.1470	0.5128	0.5180	0.5234	0.5305	0.5421	0.5511	0.5814
2.1724	0.5409	0.5456	0.5475	0.5529	0.5625	0.5707	0.5997
2.1978	0.5655	0.5685	0.5676	0.5707	0.5776	0.5840	0.6087
2.2232	0.5782	0.5802	0.5800	0.5812	0.5852	0.5900	0.6100
2.2486	0.5880	0.5906	0.5904	0.5904	0.5940	0.5980	0.6100
2.2740	0.5901	0.5917	0.5902	0.5900	0.5933	0.5970	0.6100
2.2994	0.5897	0.5902	0.5900	0.5874	0.5901	0.5940	0.6100
2.3248	0.5878	0.5886	0.5864	0.5849	0.5870	0.5910	0.6100
2.3502	0.5847	0.5853	0.5830	0.5824	0.5840	0.5880	0.6100
2.3756	0.5814	0.5820	0.5797	0.5799	0.5810	0.5850	0.6100
2.4010	0.5784	0.5788	0.5765	0.5774	0.5780	0.5820	0.6100
2.4264	0.5756	0.5757	0.5734	0.5749	0.5750	0.5790	0.6100
2.4518	0.5729	0.5727	0.5704	0.5724	0.5720	0.5760	0.6100
2.4772	0.5703	0.5698	0.5675	0.5699	0.5690	0.5730	0.6100
2.5026	0.5678	0.5670	0.5647	0.5674	0.5660	0.5700	0.6100
2.5280	0.5654	0.5643	0.5620	0.5649	0.5630	0.5670	0.6100
2.5534	0.5631	0.5617	0.5594	0.5624	0.5600	0.5640	0.6100
2.5788	0.5609	0.5592	0.5569	0.5599	0.5570	0.5610	0.6100
2.6042	0.5588	0.5568	0.5545	0.5574	0.5540	0.5580	0.6100
2.6296	0.5568	0.5545	0.5522	0.5549	0.5510	0.5550	0.6100
2.6550	0.5549	0.5523	0.5500	0.5524	0.5480	0.5520	0.6100
2.6804	0.5531	0.5502	0.5479	0.5499	0.5450	0.5490	0.6100
2.7058	0.5514	0.5482	0.5459	0.5474	0.5420	0.5460	0.6100
2.7312	0.5498	0.5463	0.5440	0.5449	0.5390	0.5430	0.6100
2.7566	0.5483	0.5445	0.5422	0.5424	0.5360	0.5400	0.6100
2.7820	0.5469	0.5428	0.5405	0.5399	0.5330	0.5370	0.6100
2.8074	0.5456	0.5412	0.5389	0.5374	0.5300	0.5340	0.6100
2.8328	0.5444	0.5397	0.5374	0.5349	0.5270	0.5310	0.6100
2.8582	0.5433	0.5383	0.5360	0.5324	0.5240	0.5280	0.6100
2.8836	0.5423	0.5370	0.5347	0.5299	0.5210	0.5250	0.6100
2.9090	0.5414	0.5358	0.5335	0.5274	0.5180	0.5220	0.6100
2.9344	0.5406	0.5347	0.5324	0.5249	0.5150	0.5190	0.6100
2.9598	0.5399	0.5337	0.5314	0.5224	0.5120	0.5160	0.6100
2.9852	0.5393	0.5328	0.5305	0.5199	0.5090	0.5130	0.6100
3.0106	0.5388	0.5320	0.5297	0.5174	0.5060	0.5100	0.6100
3.0360	0.5384	0.5313	0.5290	0.5149	0.5030	0.5070	0.6100
3.0614	0.5381	0.5307	0.5284	0.5124	0.5000	0.5040	0.6100
3.0868	0.5379	0.5302	0.5279	0.5099	0.4970	0.5010	0.6100
3.1122	0.5378	0.5298	0.5275	0.5074	0.4940	0.4980	0.6100
3.1376	0.5378	0.5295	0.5272	0.5049	0.4910	0.4950	0.6100
3.1630	0.5379	0.5293	0.5270	0.5024	0.4880	0.4920	0.6100
3.1884	0.5381	0.5292	0.5269	0.4999	0.4850	0.4890	0.6100
3.2138	0.5384	0.5292	0.5269	0.4974	0.4820	0.4860	0.6100
3.2392	0.5388	0.5293	0.5270	0.4949	0.4790	0.4830	0.6100
3.2646	0.5393	0.5295	0.5272	0.4924	0.4760	0.4800	0.6100
3.2900	0.5399	0.5298	0.5275	0.4899	0.4730	0.4770	0.6100
3.3154	0.5406	0.5302	0.5279	0.4874	0.4700	0.4740	0.6100
3.3408	0.5414	0.5307	0.5284	0.4849	0.4670	0.4710	0.6100
3.3662	0.5423	0.5313	0.5290	0.4824	0.4640	0.4680	0.6100
3.3916	0.5433	0.5320	0.5297	0.4799	0.4610	0.4650	0.6100
3.4170	0.5444	0.5328	0.5305	0.4774	0.4580	0.4620	0.6100
3.4424	0.5456	0.5337	0.5314	0.4749	0.4550	0.4590	0.6100
3.4678	0.5469	0.5347	0.5324	0.4724	0.4520	0.4560	0.6100
3.4932	0.5483	0.5358	0.5335	0.4699	0.4490	0.4530	0.6100
3.5186	0.5498	0.5370	0.5347	0.4674	0.4460	0.4500	0.6100
3.5440	0.5514	0.5383	0.5360	0.4649	0.4430	0.4470	0.6100
3.5694	0.5531	0.5397	0.5374	0.4624	0.4400	0.4440	0.6100
3.5948	0.5549	0.5412	0.5389	0.4599	0.4370	0.4410	0.6100
3.6202	0.5568	0.5428	0.5405	0.4574	0.4340	0.4380	0.6100
3.6456	0.5588	0.5445	0.5422	0.4549	0.4310	0.4350	0.6100
3.6710	0.5609	0.5463	0.5440	0.4524	0.4280	0.4320	0.6100
3.6964	0.5631	0.5482	0.5459	0.4499	0.4250	0.4290	0.6100
3.7218	0.5654	0.5502	0.5479	0.4474	0.4220	0.4260	0.6100
3.7472	0.5678	0.5523	0.5500	0.4449	0.4190	0.4230	0.6100
3.7726	0.5703	0.5545	0.5522	0.4424	0.4160	0.4200	0.6100
3.7980	0.5729	0.5568	0.5545	0.4399	0.4130	0.4170	0.6100
3.8234	0.5756	0.5592	0.5569	0.4374	0.4100	0.4140	0.6100
3.8488	0.5784	0.5617	0.5594	0.4349	0.4070	0.4110	0.6100
3.8742	0.5813	0.5643	0.5620	0.4324	0.4040	0.4080	0.6100
3.8996	0.5843	0.5670	0.5647	0.4299	0.4010	0.4050	0.6100
3.9250	0.5874	0.5698	0.5675	0.4274	0.3980	0.4020	0.6100
3.9504	0.5906	0.5727	0.5704	0.4249	0.3950	0.3990	0.6100
3.9758	0.5939	0.5757	0.5734	0.4224	0.3920	0.3960	0.6100
4.0012	0.5973	0.5788	0.5765	0.4199	0.3890	0.3930	0.6100
4.0266	0.6008	0.5820	0.5797	0.4174	0.3860	0.3900	0.6100
4.0520	0.6044	0.5853	0.5830	0.4149	0.3830	0.3870	0.6100
4.0774	0.6081	0.5886	0.5864	0.4124	0.3800	0.3840	0.6100
4.1028	0.6119	0.5920	0.5900	0.4099	0.3770	0.3810	0.6100
4.1282	0.6158	0.5955	0.5936	0.4074	0.3740	0.3780	0.6100
4.1536	0.6198	0.5991	0.5973	0.4049	0.3710	0.3750	0.6100
4.1790	0.6239	0.6028	0.6011	0.4024	0.3680	0.3720	0.6100
4.2044	0.6281	0.6066	0.6050	0.3999	0.3650	0.3690	0.6100
4.2298	0.6324	0.6105	0.6090	0.3974	0.3620	0.3660	0.6100
4.2552	0.6368	0.6145	0.6131	0.3949	0.3590	0.3630	0.6100
4.2806	0.6413	0.6186	0.6173	0.3924	0.3560	0.3600	0.6100
4.3060	0.6459	0.6228	0.6216	0.3899	0.3530	0.3570	0.6100
4.3314	0.6506	0.6271	0.6260	0.3874	0.3500	0.3540	0.6100
4.3568	0.6554	0.6315	0.6305	0.3849	0.3470	0.3510	0.6100
4.3822	0.6603	0.6360	0.6351	0.3824	0.3440	0.3480	0.6100
4.4076	0.6653	0.6406	0.6398	0.3799	0.3410	0.3450	0.6100
4.4330	0.6704	0.6453	0.6446	0.3774	0.3380	0.3420	0.6100
4.4584	0.6756	0.6501	0.6495	0.3749	0.3350	0.3390	0.6100
4.4838	0.6809	0.6550	0.6545	0.3724	0.3320	0.3360	0.6100
4.5092	0.6863	0.6600	0.6596	0.3699	0.3290	0.3330	0.6100
4.5346	0.6918	0.6651	0.6648	0.3674	0.3260	0.3300	0.6100
4.5600	0.6974	0.6703	0.6701	0.3649	0.3230	0.3270	0.6100
4.5854	0.7031	0.6756	0.6755	0.3624	0.3200	0.3240	0.6100
4.6108	0.7089	0.6810	0.6810	0.3599	0.3170	0.3210	0.6100
4.6362	0.7148	0.6865	0.6866	0.3574	0.3140	0.3180	0.6100
4.6616	0.7208	0.6921	0.6923	0.3549	0.3110	0.3150	0.6100
4.6870	0.7269	0.6978	0.6981	0.3524	0.3080	0.3120	0.6100
4.7124	0.7331	0.7036	0.7040	0.3499	0.3050	0.3090	0.6100
4.7378	0.7394	0.7095	0.7100	0.3474	0.3020	0.3060	0.6100
4.7632	0.7458	0.7155	0.7161	0.3449	0.2990	0.3030	0.6100
4.7886	0.7523	0.7216	0.7223	0.3424	0.2960	0.3000	0.6100
4.8140	0.7589	0.7278	0.7286	0.3399	0.2930	0.2970	0.6100
4.8394	0.7656	0.7341	0.7350	0.3374	0.2900	0.2940	0.6100
4.8648	0.7724	0.7405	0.7415	0.3349	0.2870	0.2910	0.6100
4.8902	0.7793	0.7470	0.7481	0.3324	0.2840	0.2880	0.6100
4.9156	0.7863	0.7536	0.7548	0.3299	0.2810	0.2850	0.6100
4.9410	0.7934	0.7603	0.7616	0.3274	0.2780	0.2820	0.6100
4.9664	0.8006	0.7671	0.7685	0.3249	0.2750	0.2790	0.6100
4.9918	0.8079	0.7740	0.7755	0.3224	0.2720	0.2760	0.6100
5.0172	0.8153	0.7810	0.7826	0.3199	0.2690	0.2730	0.6100
5.0426	0.8228	0.7881	0.7898	0.3174	0.2660	0.2700	0.6100
5.0680	0.8304	0.7953	0.7971	0.3149	0.2630	0.2670	0.6100
5.0934	0.8381	0.8026	0.8045	0.3124	0.2600	0.2640	0.6100
5.1188	0.8459	0.8100	0.8120	0.3099	0.2570	0.2610	0.6100
5.1442	0.8538	0.8175	0.8196	0.3074	0.2540	0.2580	0.6100
5.1696	0.8618	0.8251	0.8273	0.3049	0.2510	0.2550	0.6100
5.1950	0.8699	0.8328	0.8351	0.3024	0.2480	0.2520	0.6100
5.2204	0.8781	0.8406	0.8430	0.2999	0.2450	0.2490	0.6100
5.2458	0.8864	0.8485	0.8510	0.2974	0.2420	0.2460	0.6100
5.2712	0.8948	0.8565	0.8591	0.2949	0.2390	0.2430	0.6100
5.2966	0.9033	0.8646	0.8673	0.2924	0.2360	0.2400	0.6100
5.3220	0.9119	0.8728	0.8756	0.2899	0.2330	0.2370	0.6100
5.3474	0.9206	0.8811	0.8840	0.2874	0.2300	0.2340	0.6100
5.3728	0.9294	0.8895	0.8925	0.2849	0.2270	0.2310	0.6100
5.3982	0.9383	0.8980	0.9011	0.2824	0.2240	0.2280	0.6100
5.4236	0.9473	0.9066	0.9098	0.2799	0.2210	0.2250	0.6100
5.4490	0.9564	0.9153	0.9186	0.2774	0.2180	0.2220	0.6100
5.4744	0.9656	0.9241	0.9275	0.2749	0.2150	0.2190	0.6100
5.4998	0.9749	0.9330	0.9365	0.2724	0.2120	0.2160	0.6100
5.5252	0.9843	0.9420	0.9456	0.2699	0.2090	0.2130	0.6100
5.5506	0.9938	0.9511	0.9548	0.2674	0.2060	0.2100	0.6100
5.5760	1.0034	0.9603	0.9641	0.2649	0.2030	0.2070	0.6100
5.6014	1.0131	0.9696	0.9735	0.2624	0.2000	0.2040	0.6100
5.6268	1.0229	0.9790	0.9830	0.2599	0.1970	0.2010	0.6100
5.6522	1.0328	0.9885	0.9926	0.2574	0.1940	0.1980	0.6100
5.6776	1.0428	0.9981	1.0023	0.2549	0.1910	0.1950	0.6100
5.7030	1.0529	1.0078	1.0121	0.2524	0.1880	0.1920	0.6100
5.7284	1.0631	1.0176	1.0220	0.2499	0.1850	0.1890	0.6100
5.7538	1.0734	1.0275	1.0320	0.2474	0.1820	0.1860	0.6100
5.7792	1.0838	1.0375	1.0421	0.2449	0.1790	0.1830	0.6100
5.8046	1.0943	1.0476	1.0523	0.2424	0.1760	0.1800	0.6100
5.8300	1.1049	1.0578	1.0626	0.2399	0.1730	0.1770	0.6100
5.8554	1.1156	1.0681	1.0730	0.2374	0.1700	0.1740	0.6100
5.8808	1.1264	1.0785	1.0835	0.2349	0.1670	0.1710	0.6100
5.9062	1.1373	1.0890	1.0941	0.2324	0.1640	0.1680	0.6100
5.9316	1.1483	1.0996	1.1048	0.2299	0.1610	0.1650	0.6100
5.9570	1.1594	1.1103	1.1156	0.2274	0.1580	0.1620	0.6100
5.9824	1.1706	1.1211	1.1265	0.2249	0.1550	0.1590	0.6100
6.0078	1.1819	1.1320	1.1375	0.2224	0.1520	0.1560	0.6100
6.0332	1.1933	1.1430	1.1486	0.2199	0.1490	0.1530	0.6100
6.0586	1.2048	1.1541	1.1598	0.2174	0.1460	0.1500	0.6100
6.0840	1.2164	1.1653	1.1711	0.2149	0.1430	0.1470	0.6100
6.1094	1.2281	1.1766	1.1825	0.2124	0.1400	0.1440	0.6100
6.1348	1.2399	1.1880	1.1940	0.2099	0.1370	0.1410	0.6100
6.1602	1.2518	1.1995	1.2056	0.2074	0.1340	0.1380	0.6100
6.1856	1.2638	1.2111	1.2173	0.2049	0.1310	0.1350	0.6100
6.2110	1.2759	1.2228	1.2291	0.2024	0.1280	0.1320	0.6100
6.2364	1.2881	1.2346	1.2410	0.1999	0.1250	0.1290	0.6100
6.2618	1.3004	1.2465	1.2530	0.1974	0.1220	0.1260	0.6100
6.2872	1.3128	1.2585	1.2651	0.1949	0.1190	0.1230	0.6100
6.3126	1.3253	1.2706	1.2773	0.1924	0.1160	0.1200	0.6100
6.3380	1.3379	1.2828	1.2896	0.1899	0.1130	0.1170	0.6100
6.3634	1.3506	1.2951	1.3020	0.1874	0.1100	0.1140	0.6100
6.3888	1.3634	1.3075	1.3145	0.1849	0.1070	0.1110	0.6100
6.4142	1.3763	1.3200	1.3271	0.1824	0.1040	0.1080	0.6100
6.4396	1.3893	1.3326	1.3398	0.1799	0.1010	0.1050	0.6100
6.4650	1.4024	1.3453	1.3526	0.1774	0.0980	0.1020	0.6100
6.4904	1.4156	1.3581	1.3655	0.1749	0.0950	0.0990	0.6100
6.5158	1.4289	1.3710	1.3785	0.1724	0.0920	0.0960	0.6100
6.5412	1.4423	1.3840	1.3916	0.1699	0.0890	0.0930	0.6100
6.5666	1.4558	1.3971	1.4048	0.1674	0.0860	0.0900	0.6100
6.5920	1.4694	1.4103	1.4181	0.1649	0.0830	0.0870	0.6100
6.6174	1.4831	1.4236	1.4315	0.1624	0.0800	0.0840	0.6100
6.6428	1.4969	1.4370	1.4450	0.1599	0.0770	0.0810	0.6100
6.6682	1.5108	1.4505	1.4586	0.1574	0.0740	0.0780	0.6100
6.6936	1.5248	1.4641	1.4723	0.1549	0.0710	0.0750	0.6100
6.7190	1.5389	1.4778	1.4861	0.1524	0.0680	0.0720	0.6100
6.7444	1.5531	1.4916	1.5000	0.1499	0.0650	0.0690	0.6100
6.7698	1.5674	1.5055	1.5140	0.1474	0.0620	0.0660	0.6100
6.7952	1.5818	1.5195	1.5281	0.1449	0.0590	0.0630	0.6100
6.8206	1.5963	1.5336	1.5423	0.1424	0.0560	0.0600	0.6100
6.8460	1.6109	1.5478	1.5566	0.1399	0.0530	0.0570	0.6100
6.8714	1.6256	1.5621	1.5710	0.1374	0.0500	0.0540	0.6100
6.8968	1.6404	1.5765	1.5855	0.1349	0.0470	0.0510	0.6100
6.9222	1.6553	1.5910	1.6001	0.1324	0.0440	0.0480	0.6100
6.9476	1.6703	1.6056	1.6148	0.1299	0.0410	0.0450	0.6100
6.9730	1.6854	1.6203	1.6296	0.1274	0.0380	0.0420	0.6100
6.9984	1.7006	1.6351	1.6445	0.1249	0.0350	0.0390	0.6100
7.0238	1.7159	1.6500	1.6595	0.1224	0.0320	0.0360	0.6100
7.0492	1.7313	1.6650	1.6746	0.1199	0.0290	0.0330	0.6100
7.0746	1.7468	1.6801	1.6898	0.1174	0.0260	0.0300	0.6100
7.1000	1.7624	1.6953	1.7051	0.1149	0.0230	0.0270	0.6100
7.1254	1.7781	1.7106	1.7205	0.1124	0.0200	0.0240	0.6100
7.1508	1.7939	1.7260	1.7360	0.1099	0.0170	0.0210	0.6100
7.1762	1.8098	1.7415	1.7516	0.1074	0.0140	0.0180	0.6100
7.2016	1.8258	1.7571	1.7673	0.1049	0.0110	0.0150	0.6100
7.2270	1.8419	1.7728	1.7831	0.1024	0.0080	0.0120	0.6100
7.2524	1.8581	1.7886	1.7990	0.0999	0.0050	0.0090	0.6100
7.2778	1.8744	1.8045	1.8150	0.0974	0.0020	0.0060	0.6100
7.3032	1.8908	1.8205	1.8311	0.0949	0.0000	0.0030	0.6100
7.3286	1.9073	1.8366	1.8473	0.0924	0.0000	0.0000	0.6100
7.3540	1.9239	1.8528	1.8636	0.0899	0.0000	0.0000	0.6100
7.3794	1.9406	1.8691	1.8800	0.0874	0.0000	0.0000	0.6100
7.4048	1.9574	1.8855	1.8965	0.0849	0.0000	0.0000	0.6100
7.4302	1.9743	1.9020	1.9131	0.0824	0.0000	0.0000	0.6100
7.4556	1.9913	1.9186	1.9298	0.0799	0.0000	0.0000	0.6100
7.4810	2.0084	1.9353	1.9466	0.0774	0.0000	0.0000	0.6100
7.5064	2.0256	1.9521	1.9635	0.0749	0.0000	0.0000	0.6100
7.5318	2.0429	1.9690	1.9805	0.

Q ($Å^{-1}$)	S(Q) 885K	S(Q) 907K	S(Q) 929K	S(Q) 973K	S(Q) 995K	S(Q) 1017K	S(Q) 1039K
3.1888	1.0634	1.0696	1.0724	1.0666	1.0679	1.0692	1.0893
3.2142	1.0281	1.0311	1.0352	1.0304	1.0319	1.0327	1.0509
3.2396	0.9916	0.9924	0.9954	0.9916	0.9923	0.9989	1.0135
3.2650	0.9574	0.9591	0.9605	0.9544	0.9566	0.9651	0.9794
3.2904	0.9249	0.9298	0.9290	0.9227	0.9250	0.9327	0.9484
3.3158	0.8927	0.8962	0.8979	0.8913	0.8966	0.9004	0.9177
3.3412	0.8617	0.8636	0.8669	0.8615	0.8648	0.8700	0.8863
3.3666	0.8307	0.8307	0.8350	0.8302	0.8335	0.8401	0.8547
3.3920	0.8015	0.8031	0.8052	0.8009	0.8053	0.8113	0.8257
3.4174	0.7729	0.7775	0.7792	0.7739	0.7793	0.7850	0.7994
3.4428	0.7476	0.7549	0.7586	0.7520	0.7576	0.7632	0.7761
3.4682	0.7275	0.7341	0.7394	0.7333	0.7386	0.7443	0.7579
3.4937	0.7104	0.7153	0.7214	0.7165	0.7215	0.7266	0.7419
3.5191	0.6972	0.6994	0.7077	0.7028	0.7081	0.7119	0.7271
3.5445	0.6825	0.6864	0.6941	0.6893	0.6979	0.6982	0.7128
3.5699	0.6708	0.6784	0.6834	0.6784	0.6859	0.6882	0.7017
3.5953	0.6611	0.6687	0.6742	0.6701	0.6764	0.6800	0.6929
3.6207	0.6526	0.6584	0.6650	0.6630	0.6674	0.6741	0.6860
3.6461	0.6481	0.6516	0.6609	0.6592	0.6622	0.6697	0.6815
3.6715	0.6466	0.6491	0.6574	0.6564	0.6622	0.6653	0.6781
3.6969	0.6457	0.6464	0.6576	0.6561	0.6624	0.6636	0.6757
3.7223	0.6443	0.6461	0.6573	0.6574	0.6609	0.6669	0.6780
.7477	0.6462	0.6485	0.6555	0.6586	0.6627	0.6698	0.6813
.7731	0.6479	0.6517	0.6571	0.6596	0.6628	0.6689	0.6824
3.7986	0.6517	0.6553	0.6623	0.6615	0.6659	0.6710	0.6864
3.8240	0.6547	0.6600	0.6680	0.6652	0.6683	0.6770	0.6969
3.8494	0.6606	0.6667	0.6736	0.6707	0.6756	0.6822	0.6979
3.8748	0.6687	0.6750	0.6791	0.6771	0.6845	0.6884	0.7010
3.9002	0.6793	0.6824	0.6869	0.6833	0.6898	0.6951	0.7066
3.9256	0.6890	0.6904	0.6982	0.6919	0.6989	0.7022	0.7140
3.9510	0.6977	0.7003	0.7076	0.7036	0.7091	0.7107	0.7228
3.9764	0.7096	0.7124	0.7195	0.7160	0.7181	0.7219	0.7339
4.0018	0.7220	0.7257	0.7309	0.7303	0.7296	0.7330	0.7458
4.0272	0.7368	0.7386	0.7434	0.7524	0.7443	0.7456	0.7593
4.0526	0.7514	0.7516	0.7566	0.7683	0.7588	0.7588	0.7752
4.0780	0.7652	0.7698	0.7708	0.7761	0.7735	0.7741	0.7891
4.1035	0.7811	0.7871	0.7873	0.7837	0.7869	0.7888	0.8017
4.1289	0.8000	0.8043	0.8054	0.7977	0.8018	0.8036	0.8149
4.1543	0.8179	0.8203	0.8232	0.8147	0.8182	0.8202	0.8280
4.1797	0.8373	0.8398	0.8421	0.8320	0.8376	0.8381	0.8445
4.2051	0.8581	0.8619	0.8612	0.8498	0.8563	0.8570	0.8637
4.2305	0.8771	0.8794	0.8791	0.8661	0.8716	0.8752	0.8799
4.2559	0.8995	0.8989	0.9017	0.8859	0.8881	0.8908	0.8990
4.2813	0.9210	0.9206	0.9225	0.9074	0.9082	0.9104	0.9194
4.3067	0.9411	0.9425	0.9409	0.9293	0.9306	0.9318	0.9377
4.3321	0.9614	0.9630	0.9624	0.9522	0.9525	0.9511	0.9581
4.3575	0.9825	0.9825	0.9849	0.9719	0.9705	0.9695	0.9764
4.3829	1.0064	1.0041	1.0072	0.9946	0.9905	0.9915	0.9972
4.4084	1.0315	1.0290	1.0289	1.0150	1.0136	1.0166	1.0214
4.4338	1.0552	1.0519	1.0503	1.0350	1.0354	1.0404	1.0460
4.4846	1.0994	1.0945	1.0904	1.0708	1.0726	1.0733	1.0775

Q ($Å^{-1}$)	S(Q) 885K	S(Q) 907K	S(Q) 929K	S(Q) 973K	S(Q) 995K	S(Q) 1017K	S(Q) 1039K
4.5100	1.1200	1.1163	1.1122	1.0891	1.0909	1.0912	1.0923
4.5354	1.1392	1.1387	1.1343	1.1088	1.1063	1.1078	1.1092
4.5608	1.1582	1.1563	1.1517	1.1249	1.1281	1.1221	1.1256
4.5862	1.1767	1.1737	1.1682	1.1422	1.1452	1.1400	1.1432
4.6116	1.1952	1.1912	1.1848	1.1572	1.1582	1.1560	1.1579
4.6370	1.2113	1.2085	1.2009	1.1705	1.1728	1.1719	1.1707
4.6624	1.2253	1.2209	1.2158	1.1857	1.1859	1.1858	1.1840
4.6878	1.2356	1.2269	1.2252	1.1986	1.1922	1.1930	1.1944
4.7133	1.2491	1.2365	1.2400	1.2131	1.2051	1.2018	1.2046
4.7387	1.2527	1.2454	1.2476	1.2239	1.2177	1.2098	1.2126
4.7641	1.2570	1.2514	1.2523	1.2306	1.2253	1.2157	1.2181
4.7895	1.2619	1.2545	1.2552	1.2324	1.2274	1.2220	1.2228
4.8149	1.2632	1.2553	1.2535	1.2349	1.2283	1.2245	1.2241
4.8403	1.2625	1.2600	1.2540	1.2366	1.2322	1.2257	1.2242
4.8657	1.2590	1.2603	1.2524	1.2292	1.2256	1.2225	1.2222
4.8911	1.2584	1.2574	1.2522	1.2254	1.2235	1.2213	1.2233
4.9165	1.2571	1.2551	1.2521	1.2244	1.2231	1.2208	1.2243
4.9419	1.2567	1.2524	1.2517	1.2235	1.2234	1.2210	1.2255
4.9673	1.2526	1.2482	1.2468	1.2208	1.2182	1.2169	1.2213
4.9927	1.2471	1.2434	1.2420	1.2144	1.2124	1.2115	1.2160
5.0182	1.2386	1.2386	1.2363	1.2075	1.2096	1.2050	1.2109
5.0436	1.2304	1.2305	1.2259	1.2013	1.2003	1.1973	1.2010
5.0690	1.2238	1.2205	1.2181	1.1948	1.1909	1.1902	1.1921
5.0944	1.2148	1.2099	1.2099	1.1873	1.1820	1.1816	1.1838
5.1198	1.2063	1.2002	1.2021	1.1755	1.1731	1.1703	1.1762
5.1452	1.1961	1.1926	1.1932	1.1681	1.1658	1.1618	1.1701
5.1706	1.1857	1.1856	1.1847	1.1593	1.1570	1.1531	1.1625
5.1960	1.1704	1.1719	1.1703	1.1472	1.1440	1.1425	1.1525
5.2214	1.1618	1.1592	1.1573	1.1346	1.1360	1.1347	1.1447
5.2468	1.1526	1.1489	1.1457	1.1244	1.1266	1.1252	1.1343
5.2722	1.1402	1.1370	1.1360	1.1151	1.1164	1.1115	1.1206
5.2976	1.1253	1.1245	1.1240	1.1012	1.1043	1.0976	1.1097
5.3231	1.1106	1.1112	1.1112	1.0869	1.0901	1.0871	1.0992
5.3485	1.0965	1.0968	1.0963	1.0752	1.0758	1.0769	1.0875
5.3739	1.0826	1.0831	1.0811	1.0603	1.0619	1.0650	1.0732
5.3993	1.0698	1.0691	1.0688	1.0499	1.0506	1.0532	1.0614
5.4247	1.0586	1.0556	1.0554	1.0374	1.0403	1.0404	1.0507
5.4501	1.0483	1.0454	1.0445	1.0276	1.0300	1.0285	1.0410
5.4755	1.0318	1.0312	1.0304	1.0147	1.0162	1.0147	1.0273
5.5009	1.0194	1.0192	1.0173	1.0048	1.0031	1.0047	1.0157
5.5263	1.0075	1.0073	1.0043	0.9938	0.9949	0.9955	1.0033
5.5517	0.9895	0.9919	0.9886	0.9786	0.9839	0.9850	0.9917
5.5771	0.9781	0.9807	0.9785	0.9674	0.9683	0.9751	0.9819
5.6025	0.9660	0.9705	0.9679	0.9557	0.9539	0.9618	0.9724
5.6280	0.9544	0.9614	0.9549	0.9462	0.9482	0.9509	0.9642
5.6534	0.9459	0.9460	0.9426	0.9379	0.9390	0.9404	0.9521
5.6788	0.9347	0.9348	0.9338	0.9303	0.9296	0.9318	0.9419
5.7042	0.9217	0.9227	0.9251	0.9215	0.9201	0.9236	0.9338
5.7296	0.9124	0.9127	0.9183	0.9124	0.9098	0.9153	0.9265
5.7550	0.9040	0.9054	0.9095	0.9021	0.8997	0.9051	0.9183
5.8058	0.8870	0.8913	0.8876	0.8835	0.8809	0.8895	0.8995

Q ($Å^{-1}$)	S(Q) 885K	S(Q) 907K	S(Q) 929K	S(Q) 973K	S(Q) 995K	S(Q) 1017K	S(Q) 1039K
5.8312	0.8811	0.8833	0.8805	0.8790	0.8781	0.8820	0.8944
5.8566	0.8750	0.8779	0.8766	0.8747	0.8747	0.8763	0.8884
5.8820	0.8663	0.8709	0.8702	0.8668	0.8656	0.8709	0.8812
5.9074	0.8600	0.8640	0.8629	0.8622	0.8615	0.8634	0.8766
5.9329	0.8550	0.8577	0.8571	0.8646	0.8593	0.8568	0.8725
5.9583	0.8490	0.8520	0.8534	0.8660	0.8544	0.8541	0.8704
5.9837	0.8435	0.8468	0.8509	0.8591	0.8517	0.8522	0.8659
6.0091	0.8405	0.8426	0.8455	0.8450	0.8467	0.8466	0.8567
6.0345	0.8405	0.8423	0.8453	0.8434	0.8453	0.8458	0.8553
6.0599	0.8401	0.8416	0.8448	0.8415	0.8436	0.8449	0.8533
6.0853	0.8397	0.8406	0.8440	0.8400	0.8416	0.8439	0.8514
6.1107	0.8390	0.8397	0.8432	0.8388	0.8396	0.8431	0.8497
6.1361	0.8381	0.8393	0.8422	0.8385	0.8377	0.8424	0.8486
6.1615	0.8377	0.8393	0.8414	0.8393	0.8370	0.8423	0.8485
6.1869	0.8381	0.8403	0.8413	0.8407	0.8375	0.8427	0.8495
6.2123	0.8385	0.8415	0.8418	0.8420	0.8388	0.8435	0.8507
6.2378	0.8394	0.8432	0.8430	0.8436	0.8411	0.8451	0.8526
6.2632	0.8414	0.8460	0.8457	0.8456	0.8439	0.8473	0.8553
6.2886	0.8445	0.8495	0.8500	0.8481	0.8473	0.8501	0.8585
6.3140	0.8485	0.8530	0.8547	0.8510	0.8516	0.8535	0.8619
6.3394	0.8525	0.8564	0.8594	0.8540	0.8560	0.8574	0.8652
6.3648	0.8569	0.8601	0.8642	0.8579	0.8604	0.8615	0.8691
6.3902	0.8610	0.8643	0.8687	0.8619	0.8645	0.8656	0.8732
6.4156	0.8657	0.8691	0.8730	0.8662	0.8685	0.8697	0.8773
6.4410	0.8718	0.8745	0.8772	0.8705	0.8726	0.8737	0.8813
6.4664	0.8783	0.8807	0.8819	0.8748	0.8770	0.8781	0.8853
6.4918	0.6844	0.8869	0.8873	0.8793	0.8817	0.8829	0.8893
6.5172	0.8906	0.8934	0.8932	0.8844	0.8872	0.8882	0.8938
6.5427	0.8971	0.9000	0.8993	0.8902	0.8930	0.8934	0.8990
6.5681	0.9042	0.9061	0.9058	0.8962	0.8985	0.8983	0.9039
6.5935	0.9111	0.9120	0.9124	0.9026	0.9049	0.9034	0.9090
6.6189	0.9174	0.9184	0.9190	0.9095	0.9119	0.9092	0.9145
6.6443	0.9238	0.9252	0.9255	0.9167	0.9193	0.9154	0.9206
6.6697	0.9303	0.9320	0.9317	0.9237	0.9260	0.9210	0.9268
6.6951	0.9380	0.9388	0.9379	0.9300	0.9322	0.9269	0.9328
6.7205	0.9456	0.9459	0.9439	0.9358	0.9386	0.9327	0.9387
6.7459	0.9526	0.9530	0.9500	0.9413	0.9466	0.9390	0.9443
6.7713	0.9592	0.9594	0.9565	0.9462	0.9540	0.9452	0.9498
6.7967	0.9658	0.9650	0.9624	0.9513	0.9608	0.9511	0.9553
6.8221	0.9719	0.9700	0.9679	0.9566	0.9664	0.9563	0.9608
6.8476	0.9778	0.9746	0.9733	0.9615	0.9706	0.9608	0.9657
6.8730	0.9840	0.9798	0.9794	0.9666	0.9751	0.9657	0.9705
6.8984	0.9899	0.9854	0.9852	0.9720	0.9798	0.9714	0.9752
6.9238	0.9956	0.9912	0.9905	0.9784	0.9835	0.9774	0.9807
6.9492	1.0014	0.9967	0.9955	0.9853	0.9863	0.9828	0.9867
6.9746	1.0073	1.0019	1.0008	0.9914	0.9893	0.9880	0.9927
7.0000	1.0125	1.0071	1.0056	0.9970	0.9939	0.9927	0.9985
7.0254	1.0171	1.0117	1.0099	1.0021	0.9996	0.9976	1.0035
7.0508	1.0213	1.0149	1.0137	1.0060	1.0039	1.0021	1.0077
7.0762	1.0249	1.0177	1.0167	1.0094	1.0068	1.0057	1.0115
7.1270	1.0303	1.0233	1.0222	1.0153	1.0108	1.0106	1.0169

Q ($Å^{-1}$)	S(Q) 885K	S(Q) 907K	S(Q) 929K	S(Q) 973K	S(Q) 995K	S(Q) 1017K	S(Q) 1039K
7.1525	1.0329	1.0260	1.0246	1.0170	1.0136	1.0127	1.0186
7.1779	1.0348	1.0285	1.0261	1.0181	1.0160	1.0147	1.0195
7.2033	1.0355	1.0303	1.0270	1.0193	1.0174	1.0165	1.0203
7.2287	1.0361	1.0314	1.0282	1.0201	1.0181	1.0181	1.0213
7.2541	1.0361	1.0318	1.0296	1.0204	1.0189	1.0189	1.0221
7.2795	1.0351	1.0316	1.0301	1.0208	1.0195	1.0194	1.0227
7.3049	1.0343	1.0309	1.0308	1.0212	1.0201	1.0205	1.0235
7.3303	1.0334	1.0299	1.0319	1.0213	1.0199	1.0219	1.0244
7.3557	1.0326	1.0297	1.0328	1.0220	1.0196	1.0227	1.0253
7.3811	1.0319	1.0301	1.0340	1.0231	1.0194	1.0234	1.0262
7.4065	1.0316	1.0308	1.0352	1.0238	1.0200	1.0243	1.0271
7.4319	1.0316	1.0310	1.0357	1.0242	1.0213	1.0249	1.0276
7.4574	1.0320	1.0313	1.0356	1.0241	1.0222	1.0253	1.0275
7.4828	1.0324	1.0312	1.0351	1.0231	1.0228	1.0253	1.0268
7.5082	1.0326	1.0312	1.0346	1.0223	1.0228	1.0244	1.0258
7.5336	1.0317	1.0307	1.0335	1.0211	1.0227	1.0222	1.0248
7.5590	1.0304	1.0297	1.0323	1.0194	1.0218	1.0192	1.0241
7.5844	1.0295	1.0288	1.0316	1.0178	1.0201	1.0166	1.0235
7.6098	1.0284	1.0276	1.0309	1.0168	1.0177	1.0147	1.0225
7.6352	1.0271	1.0261	1.0291	1.0163	1.0151	1.0132	1.0215
7.6606	1.0253	1.0249	1.0273	1.0149	1.0122	1.0124	1.0203
7.6860	1.0230	1.0237	1.0252	1.0132	1.0092	1.0120	1.0186
7.7114	1.0199	1.0215	1.0228	1.0111	1.0069	1.0111	1.0164
7.7368	1.0168	1.0192	1.0203	1.0085	1.0052	1.0099	1.0136
7.7623	1.0141	1.0170	1.0180	1.0062	1.0042	1.0083	1.0107
7.7877	1.0111	1.0142	1.0154	1.0038	1.0027	1.0055	1.0077
7.8131	1.0075	1.0111	1.0124	1.0008	1.0009	1.0015	1.0053
7.8385	1.0039	1.0079	1.0094	0.9975	0.9986	0.9968	1.0030
7.8639	1.0009	1.0045	1.0067	0.9946	0.9963	0.9928	1.0009
7.8893	0.9984	1.0011	1.0044	0.9917	0.9927	0.9897	0.9992
7.9147	0.9959	0.9977	1.0012	0.9886	0.9894	0.9866	0.9976
7.9401	0.9927	0.9944	0.9982	0.9851	0.9854	0.9836	0.9954
7.9655	0.9888	0.9916	0.9948	0.9821	0.9815	0.9813	0.9928
7.9909	0.9847	0.9890	0.9918	0.9792	0.9792	0.9791	0.9900
8.0163	0.9810	0.9866	0.9896	0.9764	0.9777	0.9769	0.9872
8.0417	0.9772	0.9845	0.9877	0.9741	0.9765	0.9747	0.9843
8.0672	0.9740	0.9821	0.9855	0.9718	0.9749	0.9719	0.9811
8.0926	0.9715	0.9796	0.9829	0.9693	0.9731	0.9687	0.9779
8.1180	0.9692	0.9774	0.9796	0.9668	0.9706	0.9657	0.9746
8.1434	0.9669	0.9752	0.9763	0.9639	0.9673	0.9631	0.9713
8.1688	0.9655	0.9735	0.9736	0.9613	0.9637	0.9612	0.9684
8.1942	0.9649	0.9708	0.9713	0.9587	0.9612	0.9596	0.9660
8.2196	0.9639	0.9676	0.9695	0.9553	0.9577	0.9584	0.9634
8.2450	0.9626	0.9642	0.9675	0.9512	0.9542	0.9579	0.9613
8.2704	0.9611	0.9614	0.9659	0.9478	0.9516	0.9576	0.9595
8.2958	0.9592	0.9588	0.9647	0.9445	0.9493	0.9567	0.9580
8.3212	0.9567	0.9565	0.9634	0.9411	0.9483	0.9550	0.9566
8.3466	0.9546	0.9547	0.9621	0.9403	0.9487	0.9527	0.9553
8.3721	0.9531	0.9534	0.9604	0.9425	0.9486	0.9511	0.9542
8.3975	0.9507	0.9525	0.9576	0.9454	0.9478	0.9501	0.9529
8.4483	0.9464	0.9507	0.9522	0.9489	0.9480	0.9477	0.9506

Q ($Å^{-1}$)	S(Q) 885K	S(Q) 907K	S(Q) 929K	S(Q) 973K	S(Q) 995K	S(Q) 1017K	S(Q) 1039K
8.4737	0.9457	0.9489	0.9517	0.9503	0.9484	0.9465	0.9500
8.4991	0.9442	0.9472	0.9521	0.9525	0.9471	0.9452	0.9496
8.5245	0.9422	0.9453	0.9519	0.9535	0.9455	0.9437	0.9491
8.5499	0.9408	0.9438	0.9512	0.9539	0.9435	0.9429	0.9488
8.5753	0.9407	0.9433	0.9509	0.9539	0.9421	0.9420	0.9487
8.6007	0.9408	0.9437	0.9507	0.9573	0.9410	0.9407	0.9485
8.6261	0.9411	0.9455	0.9508	0.9639	0.9396	0.9401	0.9483
8.6515	0.9427	0.9479	0.9511	0.9699	0.9384	0.9410	0.9487
8.6770	0.9448	0.9504	0.9512	0.9720	0.9382	0.9424	0.9494
8.7024	0.9468	0.9523	0.9509	0.9696	0.9389	0.9433	0.9497
8.7278	0.9493	0.9536	0.9517	0.9650	0.9402	0.9444	0.9501
8.7532	0.9510	0.9540	0.9534	0.9604	0.9415	0.9449	0.9502
8.7786	0.9523	0.9545	0.9555	0.9560	0.9429	0.9454	0.9508
8.8040	0.9531	0.9549	0.9563	0.9495	0.9445	0.9466	0.9514
8.8294	0.9543	0.9559	0.9569	0.9434	0.9458	0.9486	0.9525
8.8548	0.9566	0.9580	0.9582	0.9425	0.9473	0.9511	0.9539
8.8802	0.9589	0.9606	0.9594	0.9456	0.9488	0.9532	0.9554
8.9056	0.9615	0.9633	0.9607	0.9493	0.9502	0.9550	0.9568
8.9310	0.9647	0.9654	0.9624	0.9520	0.9522	0.9563	0.9581
8.9565	0.9679	0.9674	0.9644	0.9548	0.9540	0.9583	0.9598
8.9819	0.9710	0.9696	0.9667	0.9571	0.9563	0.9604	0.9615
9.0073	0.9742	0.9728	0.9706	0.9602	0.9596	0.9621	0.9638
9.0327	0.9774	0.9758	0.9750	0.9635	0.9636	0.9643	0.9663
9.0581	0.9811	0.9788	0.9783	0.9660	0.9676	0.9669	0.9686
9.0835	0.9843	0.9814	0.9809	0.9690	0.9713	0.9695	0.9710
9.1089	0.9877	0.9847	0.9835	0.9718	0.9755	0.9719	0.9736
9.1343	0.9912	0.9885	0.9866	0.9742	0.9799	0.9740	0.9765
9.1597	0.9940	0.9924	0.9889	0.9766	0.9832	0.9755	0.9793
9.1851	0.9966	0.9962	0.9915	0.9794	0.9848	0.9773	0.9816
9.2105	0.9981	0.9992	0.9956	0.9815	0.9851	0.9785	0.9834
9.2359	0.9988	1.0020	1.0000	0.9831	0.9846	0.9802	0.9855
9.2614	1.0005	1.0048	1.0049	0.9852	0.9845	0.9824	0.9876
9.2868	1.0021	1.0074	1.0097	0.9881	0.9850	0.9849	0.9904
9.3122	1.0036	1.0096	1.0123	0.9912	0.9865	0.9882	0.9934
9.3376	1.0053	1.0103	1.0130	0.9941	0.9887	0.9918	0.9954
9.3630	1.0078	1.0100	1.0136	0.9974	0.9918	0.9949	0.9972
9.3884	1.0111	1.0112	1.0145	1.0003	0.9965	0.9980	0.9999
9.4138	1.0148	1.0139	1.0150	1.0028	1.0010	1.0008	1.0025
9.4392	1.0177	1.0159	1.0146	1.0047	1.0042	1.0033	1.0047
9.4646	1.0200	1.0183	1.0145	1.0056	1.0054	1.0054	1.0059
9.4900	1.0219	1.0210	1.0154	1.0061	1.0062	1.0066	1.0070
9.5154	1.0229	1.0229	1.0163	1.0066	1.0067	1.0074	1.0076
9.5408	1.0230	1.0232	1.0171	1.0076	1.0065	1.0075	1.0073
9.5663	1.0220	1.0233	1.0174	1.0081	1.0060	1.0075	1.0072
9.5917	1.0213	1.0232	1.0175	1.0077	1.0056	1.0077	1.0073
9.6171	1.0213	1.0220	1.0187	1.0076	1.0058	1.0074	1.0078
9.6425	1.0219	1.0207	1.0205	1.0076	1.0063	1.0071	1.0090
9.6679	1.0223	1.0198	1.0219	1.0074	1.0075	1.0070	1.0105
9.6933	1.0235	1.0201	1.0230	1.0074	1.0098	1.0065	1.0118
9.7187	1.0246	1.0198	1.0243	1.0079	1.0128	1.0064	1.0125
9.7695	1.0279	1.0194	1.0250	1.0093	1.0166	1.0085	1.0131

Q ($Å^{-1}$)	S(Q) 885K	S(Q) 907K	S(Q) 929K	S(Q) 973K	S(Q) 995K	S(Q) 1017K	S(Q) 1039K
9.7949	1.0279	1.0187	1.0236	1.0097	1.0164	1.0097	1.0129
9.8203	1.0271	1.0178	1.0210	1.0095	1.0150	1.0098	1.0121
9.8457	1.0260	1.0180	1.0183	1.0091	1.0137	1.0094	1.0115
9.8712	1.0246	1.0184	1.0166	1.0084	1.0124	1.0092	1.0116
9.8966	1.0232	1.0188	1.0160	1.0079	1.0113	1.0089	1.0122
9.9220	1.0214	1.0189	1.0151	1.0068	1.0110	1.0087	1.0128
9.9474	1.0192	1.0192	1.0143	1.0063	1.0107	1.0084	1.0125
9.9728	1.0177	1.0196	1.0148	1.0075	1.0119	1.0076	1.0123
9.9982	1.0165	1.0194	1.0163	1.0091	1.0126	1.0073	1.0122
10.0236	1.0161	1.0194	1.0186	1.0104	1.0138	1.0078	1.0128
10.0490	1.0153	1.0198	1.0207	1.0112	1.0142	1.0080	1.0128
10.0744	1.0141	1.0184	1.0204	1.0110	1.0132	1.0075	1.0124
10.0998	1.0121	1.0164	1.0183	1.0101	1.0118	1.0059	1.0113
10.1252	1.0097	1.0142	1.0153	1.0091	1.0109	1.0043	1.0103
10.1506	1.0078	1.0116	1.0125	1.0074	1.0088	1.0033	1.0090
10.1761	1.0057	1.0085	1.0095	1.0058	1.0072	1.0027	1.0076
10.2015	1.0044	1.0056	1.0068	1.0041	1.0061	1.0019	1.0063
10.2269	1.0031	1.0033	1.0037	1.0030	1.0038	1.0003	1.0046
10.2523	1.0024	1.0024	1.0013	1.0022	1.0017	0.9988	1.0040
10.2777	1.0024	1.0027	1.0010	1.0009	0.9999	0.9977	1.0046
10.3031	1.0034	1.0041	1.0021	1.0001	0.9997	0.9969	1.0060
10.3285	1.0044	1.0055	1.0025	0.9998	1.0000	0.9957	1.0063
10.3539	1.0059	1.0064	1.0023	0.9996	1.0016	0.9950	1.0062
10.3793	1.0066	1.0082	1.0018	1.0000	1.0032	0.9946	1.0052
10.4047	1.0069	1.0101	1.0015	1.0003	1.0050	0.9952	1.0043
10.4301	1.0072	1.0118	1.0024	1.0009	1.0063	0.9968	1.0036
10.4555	1.0068	1.0115	1.0032	1.0028	1.0073	0.9991	1.0029
10.4810	1.0065	1.0110	1.0036	1.0037	1.0080	1.0006	1.0024
10.5064	1.0055	1.0109	1.0034	1.0034	1.0089	1.0010	1.0019
10.5318	1.0042	1.0104	1.0041	1.0026	1.0090	1.0019	1.0023
10.5572	1.0036	1.0083	1.0056	1.0015	1.0083	1.0019	1.0032
10.5826	1.0038	1.0056	1.0064	1.0009	1.0077	1.0014	1.0042
10.6080	1.0041	1.0025	1.0060	1.0009	1.0080	1.0001	1.0044
10.6334	1.0049	1.0009	1.0053	1.0023	1.0090	0.9989	1.0043
10.6588	1.0053	1.0010	1.0041	1.0038	1.0093	0.9978	1.0040
10.6842	1.0055	1.0020	1.0029	1.0043	1.0090	0.9975	1.0041
10.7096	1.0053	1.0032	1.0029	1.0050	1.0081	0.9980	1.0048
10.7350	1.0044	1.0029	1.0026	1.0048	1.0068	0.9987	1.0045
10.7604	1.0028	1.0021	1.0022	1.0026	1.0063	0.9986	1.0036
10.7859	1.0005	1.0005	1.0009	0.9998	1.0076	0.9993	1.0032
10.8113	0.9979	0.9980	1.0002	0.9975	1.0080	0.9998	1.0033
10.8367	0.9951	0.9961	0.9997	0.9953	1.0064	1.0004	1.0032
10.8621	0.9930	0.9949	0.9995	0.9933	1.0049	1.0007	1.0026
10.8875	0.9920	0.9934	0.9997	0.9929	1.0047	0.9996	1.0012
10.9129	0.9929	0.9929	1.0008	0.9936	1.0057	0.9992	1.0003
10.9383	0.9941	0.9940	1.0010	0.9938	1.0057	1.0001	1.0000
10.9637	0.9950	0.9972	1.0007	0.9946	1.0045	1.0022	1.0003
10.9891	0.9953	1.0009	1.0022	0.9962	1.0026	1.0048	1.0008
11.0145	0.9957	1.0032	1.0051	0.9975	1.0014	1.0063	1.0008
11.0399	0.9968	1.0038	1.0055	0.9983	1.0011	1.0055	1.0010
11.0908	0.9961	0.9989	1.0027	0.9999	1.0012	1.0025	1.0020

Q (Å^{-1})	S(Q) 885K	S(Q) 907K	S(Q) 929K	S(Q) 973K	S(Q) 995K	S(Q) 1017K	S(Q) 1039K
11.1162	0.9958	0.9980	1.0029	1.0006	1.0013	1.0003	1.0016
11.1416	0.9963	0.9966	1.0028	0.9994	1.0022	0.9970	1.0002
11.1670	0.9972	0.9934	1.0028	0.9974	1.0023	0.9928	0.9986
11.1924	0.9980	0.9911	1.0031	0.9952	1.0019	0.9899	0.9973
11.2178	0.9967	0.9912	1.0024	0.9929	0.9994	0.9885	0.9970
11.2432	0.9946	0.9927	1.0021	0.9914	0.9956	0.9884	0.9966
11.2686	0.9928	0.9938	1.0033	0.9903	0.9926	0.9886	0.9958
11.2940	0.9924	0.9947	1.0037	0.9886	0.9900	0.9877	0.9950
11.3194	0.9936	0.9946	1.0018	0.9876	0.9877	0.9865	0.9945
11.3448	0.9950	0.9942	1.0006	0.9879	0.9871	0.9862	0.9941
11.3703	0.9961	0.9935	1.0012	0.9897	0.9873	0.9865	0.9940
11.3957	0.9990	0.9947	1.0024	0.9930	0.9905	0.9879	0.9947
11.4211	1.0017	0.9951	1.0033	0.9966	0.9940	0.9895	0.9958
11.4465	1.0020	0.9949	1.0035	0.9999	0.9969	0.9904	0.9972
11.4719	1.0013	0.9956	1.0030	1.0019	0.9990	0.9904	0.9987
11.4973	1.0002	0.9965	1.0016	1.0021	1.0003	0.9902	0.9995
11.5227	0.9978	0.9975	0.9998	1.0007	1.0013	0.9908	0.9985
11.5481	0.9965	0.9997	0.9980	0.9985	1.0043	0.9914	0.9987
11.5735	0.9969	1.0022	0.9954	0.9965	1.0060	0.9919	0.9950
11.5989	0.9985	1.0042	0.9919	0.9961	1.0072	0.9924	0.9942
11.6243	1.0004	1.0077	0.9910	0.9965	1.0088	0.9932	0.9948
11.6497	1.0014	1.0103	0.9918	0.9973	1.0093	0.9953	0.9965
11.6752	1.0021	1.0122	0.9937	0.9989	1.0100	0.9974	0.9987
11.7006	1.0022	1.0127	0.9976	1.0010	1.0105	0.9992	1.0008
11.7260	1.0019	1.0128	1.0017	1.0030	1.0114	0.9998	1.0026
11.7514	1.0028	1.0118	1.0044	1.0031	1.0116	0.9998	1.0037
11.7768	1.0040	1.0104	1.0077	1.0019	1.0113	0.9996	1.0038
11.8022	1.0049	1.0095	1.0095	0.9997	1.0107	0.9997	1.0026
11.8276	1.0084	1.0102	1.0100	1.0000	1.0100	1.0005	1.0015
11.8530	1.0110	1.0103	1.0103	1.0014	1.0081	0.9997	1.0001
11.8784	1.0129	1.0110	1.0106	1.0034	1.0077	0.9990	0.9993
11.9038	1.0162	1.0132	1.0130	1.0060	1.0087	1.0001	1.0000
11.9292	1.0195	1.0148	1.0155	1.0076	1.0090	1.0022	1.0016
11.9546	1.0221	1.0170	1.0174	1.0092	1.0092	1.0045	1.0038
11.9801	1.0241	1.0190	1.0205	1.0107	1.0098	1.0074	1.0066
12.0055	1.0264	1.0215	1.0236	1.0125	1.0126	1.0098	1.0100
12.0309	1.0268	1.0233	1.0261	1.0136	1.0171	1.0115	1.0130
12.0563	1.0257	1.0228	1.0291	1.0136	1.0211	1.0121	1.0157
12.0817	1.0248	1.0221	1.0298	1.0133	1.0232	1.0119	1.0175
12.1071	1.0254	1.0224	1.0301	1.0148	1.0239	1.0114	1.0192
12.1325	1.0237	1.0213	1.0316	1.0154	1.0219	1.0095	1.0188
12.1579	1.0230	1.0210	1.0332	1.0157	1.0211	1.0084	1.0172
12.1833	1.0257	1.0224	1.0341	1.0177	1.0231	1.0085	1.0163
12.2087	1.0287	1.0231	1.0343	1.0189	1.0249	1.0079	1.0158
12.2341	1.0303	1.0238	1.0323	1.0194	1.0262	1.0079	1.0165
12.2595	1.0304	1.0236	1.0297	1.0191	1.0268	1.0092	1.0177
12.2850	1.0311	1.0246	1.0279	1.0191	1.0275	1.0106	1.0197
12.3104	1.0305	1.0258	1.0257	1.0188	1.0295	1.0115	1.0206
12.3358	1.0302	1.0247	1.0230	1.0181	1.0328	1.0124	1.0207
12.3612	1.0299	1.0242	1.0215	1.0178	1.0334	1.0136	1.0205
12.4120	1.0287	1.0274	1.0265	1.0177	1.0316	1.0144	1.0221

Q (Å^{-1})	S(Q) 885K	S(Q) 907K	S(Q) 929K	S(Q) 973K	S(Q) 995K	S(Q) 1017K	S(Q) 1039K
12.4374	1.0290	1.0309	1.0294	1.0180	1.0320	1.0156	1.0226
12.4628	1.0311	1.0364	1.0313	1.0190	1.0330	1.0172	1.0237
12.4882	1.0337	1.0406	1.0338	1.0200	1.0333	1.0185	1.0256
12.5136	1.0345	1.0418	1.0347	1.0195	1.0317	1.0198	1.0276
12.5390	1.0349	1.0413	1.0364	1.0190	1.0286	1.0218	1.0300
12.5644	1.0356	1.0410	1.0390	1.0208	1.0256	1.0229	1.0322
12.5899	1.0351	1.0400	1.0398	1.0224	1.0245	1.0236	1.0322
12.6153	1.0345	1.0366	1.0388	1.0237	1.0245	1.0242	1.0312
12.6407	1.0333	1.0337	1.0389	1.0257	1.0242	1.0244	1.0302
12.6661	1.0312	1.0307	1.0400	1.0285	1.0261	1.0231	1.0289
12.6915	1.0299	1.0276	1.0395	1.0315	1.0301	1.0211	1.0275
12.7169	1.0296	1.0251	1.0374	1.0323	1.0347	1.0233	1.0246
12.7423	1.0304	1.0244	1.0345	1.0326	1.0365	1.0300	1.0212
12.7677	1.0304	1.0226	1.0308	1.0309	1.0351	1.0358	1.0178
12.7931	1.0287	1.0204	1.0267	1.0269	1.0321	1.0400	1.0161
12.8185	1.0258	1.0199	1.0244	1.0226	1.0297	1.0421	1.0167
12.8439	1.0224	1.0195	1.0239	1.0201	1.0266	1.0413	1.0177
12.8693	1.0182	1.0202	1.0233	1.0166	1.0217	1.0380	1.0182
12.8948	1.0159	1.0228	1.0236	1.0131	1.0182	1.0342	1.0200
12.9202	1.0095	1.0218	1.0185	1.0084	1.0141	1.0257	1.0195
12.9456	1.0016	1.0178	1.0106	1.0056	1.0108	1.0141	1.0167
12.9710	0.9974	1.0137	1.0046	1.0055	1.0078	1.0037	1.0136
12.9964	0.9965	1.0111	1.0010	1.0061	1.0056	1.0011	1.0094
13.0218	0.9977	1.0086	0.9994	1.0074	1.0033	1.0016	1.0044
13.0472	0.9988	1.0066	0.9985	1.0088	1.0017	1.0001	1.0010
13.0726	0.9999	1.0056	0.9982	1.0096	1.0012	0.9979	0.9994
13.0980	1.0009	1.0045	0.9986	1.0093	1.0031	0.9963	0.9989
13.1234	1.0048	1.0038	1.0019	1.0099	1.0059	0.9968	0.9999
13.1488	1.0097	1.0044	1.0048	1.0096	1.0071	0.9981	1.0013
13.1742	1.0135	1.0063	1.0063	1.0081	1.0079	0.9998	1.0030
13.1997	1.0085	1.0010	0.9992	1.0021	1.0052	0.9956	0.9997
13.2251	1.0036	0.9957	0.9930	0.9973	1.0032	0.9901	0.9960
13.2505	1.0004	0.9914	0.9896	0.9940	1.0010	0.9870	0.9920
13.2759	0.9984	0.9887	0.9877	0.9909	0.9981	0.9859	0.9878
13.3013	0.9954	0.9870	0.9859	0.9878	0.9934	0.9843	0.9834
13.3267	0.9911	0.9868	0.9838	0.9863	0.9868	0.9821	0.9804
13.3521	0.9866	0.9858	0.9815	0.9849	0.9803	0.9806	0.9779
13.3775	0.9835	0.9847	0.9810	0.9830	0.9759	0.9805	0.9763
13.4029	0.9818	0.9833	0.9824	0.9812	0.9730	0.9819	0.9755
13.4283	0.9804	0.9816	0.9827	0.9793	0.9701	0.9825	0.9750
13.4537	0.9800	0.9811	0.9823	0.9777	0.9693	0.9830	0.9766
13.4791	0.9798	0.9798	0.9823	0.9748	0.9713	0.9824	0.9784
13.5046	0.9793	0.9784	0.9833	0.9733	0.9754	0.9815	0.9815
13.5300	0.9766	0.9764	0.9811	0.9718	0.9781	0.9803	0.9832
13.5554	0.9745	0.9746	0.9768	0.9714	0.9779	0.9786	0.9844
13.5808	0.9714	0.9724	0.9717	0.9717	0.9771	0.9759	0.9839
13.6062	0.9680	0.9711	0.9675	0.9732	0.9751	0.9739	0.9824
13.6316	0.9639	0.9700	0.9646	0.9733	0.9721	0.9720	0.9802
13.6570	0.9621	0.9697	0.9653	0.9740	0.9695	0.9702	0.9778
13.6824	0.9624	0.9683	0.9704	0.9754	0.9708	0.9703	0.9747
13.7078	0.9645	0.9668	0.9754	0.9777	0.9722	0.9722	0.9727

Q ($Å^{-1}$)	S(Q) 885K	S(Q) 902K	S(Q) 929K	S(Q) 973K	S(Q) 995K	S(Q) 1017K	S(Q) 1039K
13.7332	0.9681	0.9655	0.9773	0.9790	0.9739	0.9749	0.9736
13.7586	0.9719	0.9656	0.9780	0.9793	0.9773	0.9782	0.9767
13.7840	0.9740	0.9655	0.9774	0.9799	0.9812	0.9809	0.9805
13.8095	0.9761	0.9668	0.9746	0.9798	0.9818	0.9824	0.9825
13.8349	0.9796	0.9684	0.9719	0.9807	0.9827	0.9834	0.9838
13.8603	0.9808	0.9691	0.9694	0.9823	0.9848	0.9828	0.9844
13.8857	0.9816	0.9721	0.9692	0.9845	0.9843	0.9832	0.9857
13.9111	0.9821	0.9773	0.9703	0.9863	0.9813	0.9831	0.9879
13.9365	0.9840	0.9832	0.9743	0.9902	0.9780	0.9842	0.9899
13.9619	0.9876	0.9894	0.9809	0.9958	0.9764	0.9867	0.9914
13.9873	0.9896	0.9941	0.9846	1.0006	0.9736	0.9896	0.9932

Table A-14: Numerical values of SF for Liquid Al-12.5%Si alloy melt.

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 1065 K
0.6479	0.0279	0.0289	0.0304	0.0293	0.0312	0.0318	0.0316	0.0307	0.0304
0.6733	0.0309	0.0310	0.0318	0.0305	0.0329	0.0331	0.0333	0.0329	0.0334
0.6987	0.0325	0.0314	0.0327	0.0332	0.0325	0.0329	0.0341	0.0329	0.0347
0.7241	0.0335	0.0327	0.0333	0.0340	0.0333	0.0335	0.0346	0.0340	0.0346
0.7495	0.0342	0.0358	0.0356	0.0354	0.0366	0.0363	0.0369	0.0362	0.0375
0.7750	0.0362	0.0378	0.0380	0.0378	0.0389	0.0389	0.0391	0.0387	0.0400
0.8004	0.0385	0.0388	0.0390	0.0394	0.0403	0.0416	0.0415	0.0406	0.0409
0.8258	0.0397	0.0404	0.0402	0.0398	0.0414	0.0435	0.0432	0.0415	0.0416
0.8512	0.0409	0.0414	0.0414	0.0402	0.0427	0.0437	0.0442	0.0425	0.0427
0.8766	0.0427	0.0441	0.0443	0.0438	0.0459	0.0458	0.0468	0.0459	0.0450
0.9020	0.0444	0.0468	0.0458	0.0468	0.0482	0.0479	0.0489	0.0489	0.0470
0.9274	0.0462	0.0484	0.0466	0.0488	0.0489	0.0498	0.0501	0.0510	0.0482
0.9528	0.0480	0.0490	0.0489	0.0502	0.0505	0.0519	0.0514	0.0520	0.0502
0.9782	0.0490	0.0502	0.0509	0.0518	0.0523	0.0533	0.0531	0.0529	0.0519
1.0036	0.0505	0.0525	0.0525	0.0542	0.0553	0.0553	0.0552	0.0554	0.0537
1.0290	0.0528	0.0547	0.0548	0.0563	0.0574	0.0576	0.0575	0.0579	0.0559
1.0544	0.0558	0.0571	0.0575	0.0582	0.0598	0.0606	0.0603	0.0607	0.0584
1.0799	0.0592	0.0589	0.0600	0.0611	0.0630	0.0632	0.0629	0.0635	0.0609
1.1053	0.0619	0.0610	0.0628	0.0640	0.0658	0.0653	0.0657	0.0663	0.0637
1.1307	0.0644	0.0638	0.0656	0.0668	0.0683	0.0685	0.0682	0.0686	0.0670
1.1561	0.0669	0.0673	0.0683	0.0693	0.0708	0.0722	0.0717	0.0714	0.0699
1.1815	0.0695	0.0706	0.0713	0.0719	0.0735	0.0757	0.0755	0.0751	0.0723
1.2069	0.0730	0.0744	0.0751	0.0760	0.0768	0.0790	0.0800	0.0792	0.0759
1.2323	0.0776	0.0786	0.0799	0.0808	0.0816	0.0827	0.0853	0.0843	0.0801
1.2577	0.0822	0.0821	0.0837	0.0850	0.0872	0.0874	0.0893	0.0888	0.0838
1.2831	0.0860	0.0861	0.0877	0.0894	0.0923	0.0923	0.0934	0.0938	0.0877
1.3085	0.0900	0.0911	0.0933	0.0943	0.0976	0.0973	0.0992	0.0995	0.0924
1.3339	0.0943	0.0960	0.0987	0.0988	0.1026	0.1027	0.1055	0.1050	0.0975
1.3593	0.0991	0.1000	0.1040	0.1035	0.1066	0.1088	0.1108	0.1098	0.1033
1.3848	0.1045	0.1055	0.1092	0.1091	0.1116	0.1154	0.1156	0.1150	0.1090
1.4102	0.1097	0.1111	0.1143	0.1155	0.1171	0.1212	0.1210	0.1227	0.1140
1.4356	0.1149	0.1162	0.1197	0.1216	0.1232	0.1262	0.1267	0.1294	0.1191
1.4610	0.1206	0.1214	0.1253	0.1275	0.1295	0.1315	0.1330	0.1354	0.1257
1.4864	0.1254	0.1265	0.1307	0.1329	0.1344	0.1367	0.1385	0.1405	0.1317
1.5118	0.1299	0.1313	0.1357	0.1377	0.1394	0.1419	0.1437	0.1458	0.1369
1.5372	0.1346	0.1364	0.1406	0.1426	0.1445	0.1476	0.1494	0.1515	0.1425
1.5626	0.1399	0.1422	0.1453	0.1488	0.1496	0.1531	0.1558	0.1578	0.1490
1.5880	0.1441	0.1468	0.1495	0.1527	0.1548	0.1582	0.1606	0.1631	0.1547
1.6134	0.1487	0.1516	0.1538	0.1576	0.1603	0.1634	0.1659	0.1687	0.1605
1.6388	0.1552	0.1567	0.1596	0.1638	0.1663	0.1694	0.1724	0.1752	0.1674
1.6642	0.1626	0.1625	0.1663	0.1703	0.1732	0.1766	0.1793	0.1823	0.1757
1.7151	0.1741	0.1757	0.1796	0.1844	0.1881	0.1914	0.1950	0.1975	0.1939

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 1065 K
1.7405	0.1804	0.1836	0.1869	0.1920	0.1959	0.1997	0.2028	0.2059	0.2025
1.7659	0.1880	0.1923	0.1954	0.2007	0.2041	0.2087	0.2127	0.2150	0.2127
1.7913	0.1980	0.2019	0.2060	0.2115	0.2153	0.2188	0.2228	0.2261	0.2256
1.8167	0.2088	0.2126	0.2177	0.2233	0.2272	0.2304	0.2344	0.2394	0.2404
1.8421	0.2201	0.2243	0.2303	0.2348	0.2399	0.2429	0.2479	0.2533	0.2547
1.8675	0.2331	0.2373	0.2441	0.2472	0.2530	0.2573	0.2625	0.2688	0.2708
1.8929	0.2474	0.2518	0.2578	0.2630	0.2681	0.2738	0.2783	0.2837	0.2885
1.9183	0.2624	0.2666	0.2729	0.2798	0.2836	0.2908	0.2946	0.3014	0.3082
1.9437	0.2794	0.2836	0.2903	0.2973	0.3026	0.3095	0.3139	0.3217	0.3302
1.9691	0.2985	0.3031	0.3097	0.3162	0.3237	0.3301	0.3341	0.3436	0.3563
1.9946	0.3201	0.3244	0.3317	0.3386	0.3467	0.3538	0.3582	0.3674	0.3847
2.0200	0.3441	0.3488	0.3566	0.3645	0.3724	0.3799	0.3855	0.3937	0.4112
2.0454	0.3704	0.3755	0.3835	0.3922	0.4002	0.4081	0.4143	0.4224	0.4389
2.0708	0.4009	0.4057	0.4141	0.4242	0.4313	0.4399	0.4486	0.4555	0.4732
2.0962	0.4337	0.4375	0.4479	0.4598	0.4669	0.4748	0.4840	0.4915	0.5132
2.1216	0.4694	0.4751	0.4848	0.4976	0.5054	0.5138	0.5217	0.5300	0.5538
2.1470	0.5109	0.5173	0.5266	0.5382	0.5463	0.5557	0.5655	0.5722	0.5955
2.1724	0.5574	0.5636	0.5752	0.5856	0.5932	0.6048	0.6152	0.6224	0.6444
2.1978	0.6059	0.6126	0.6259	0.6361	0.6437	0.6544	0.6666	0.6758	
2.2232	0.6603	0.6677	0.6814	0.6919	0.7013	0.7122	0.7228	0.73	
2.2486	0.7218	0.7302	0.7425	0.7546	0.7642	0.7768	0.7852	0.7	
2.2740	0.7906	0.7982	0.8106	0.8234	0.8333	0.8441	0.8547	0.86	
2.2995	0.8656	0.8726	0.8842	0.8974	0.9052	0.9177	0.9301	0.9399	
2.3249	0.9492	0.9577	0.9674	0.9804	0.9918	1.0005	1.0124	1.0204	1.0385
2.3503	1.0413	1.0480	1.0584	1.0703	1.0817	1.0893	1.0993	1.1070	1.1221
2.3757	1.1384	1.1439	1.1535	1.1641	1.1737	1.1800	1.1885	1.1964	1.2078
2.4011	1.2442	1.2473	1.2580	1.2653	1.2724	1.2786	1.2858	1.2913	1.3022
2.4265	1.3569	1.3578	1.3653	1.3728	1.3770	1.3797	1.3856	1.3891	1.3954
2.4519	1.4719	1.4715	1.4746	1.4807	1.4829	1.4839	1.4875	1.4881	1.4882
2.4773	1.5908	1.5880	1.5845	1.5891	1.5890	1.5872	1.5888	1.5866	1.5806
2.5027	1.7065	1.6988	1.6936	1.6933	1.6906	1.6862	1.6833	1.6790	1.6671
2.5281	1.8178	1.8053	1.7948	1.7917	1.7866	1.7792	1.7702	1.7632	1.7455
2.5535	1.9220	1.9048	1.8906	1.8846	1.8736	1.8626	1.8516	1.8423	1.8188
2.5789	2.0108	1.9893	1.9728	1.9636	1.9467	1.9316	1.9189	1.9079	1.8804
2.6044	2.0858	2.0590	2.0395	2.0260	2.0064	1.9896	1.9749	1.9590	1.9287
2.6298	2.1412	2.1101	2.0872	2.0690	2.0488	2.0322	2.0122	1.9936	1.9598
2.6552	2.1706	2.1370	2.1137	2.0897	2.0704	2.0544	2.0301	2.0111	1.9718
2.6806	2.1810	2.1456	2.1224	2.0969	2.0782	2.0577	2.0355	2.0156	1.9734
2.7060	2.1743	2.1372	2.1124	2.0901	2.0681	2.0479	2.0267	2.0077	1.9656
2.7314	2.1456	2.1091	2.0837	2.0634	2.0427	2.0233	2.0037	1.9853	1.9437
2.7568	2.1023	2.0691	2.0439	2.0259	2.0049	1.9870	1.9692	1.9533	1.9105
2.8076	1.9836	1.9580	1.9370	1.9228	1.9063	1.8917	1.8766	1.8604	1.8270

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 1065 K
2.8330	1.913 8	1 891 1	1 871 4	1.859 9	1.845 5	1.833 1	1.818 7	1.805 8	1.776 6
2.8584	1 840 6	1.821 2	1.804 0	1.794 0	1.782 9	1.771 6	1.758 2	1.749 9	1.725 1
2 8839	1.766 2	1.750 1	1.736 1	1.727 7	1.717 8	1.709 3	1.697 1	1.691 8	1.668 5
2.9093	1.697 5	1.681 5	1.670 5	1.664 8	1.654 9	1.650 3	1.640 2	1.635 1	1.616 2
2.9347	1.628 6	1.614 4	1.605 1	1.602 6	1.594 4	1.591 5	1.582 6	1.579 0	1.563 9
2.9601	1.559 3	1.548 9	1.540 8	1.540 5	1.535 1	1.532 5	1.525 3	1.522 9	1.511 0
2.9855	1.492 2	1.484 6	1.478 7	1.478 9	1.475 3	1.472 7	1.468 9	1.466 7	1.457 0
3.0109	1.430 2	1.423 4	1.420 5	1.420 3	1.417 3	1.415 5	1.414 4	1.414 2	1.406 6
3.0363	1.371 0	2.363 9	1.364 4	1.363 9	1.362 9	1.361 1	1.362 0	1 362 6	1.359 2
3.0617	1.317 7	1.311 3	1.313 2	1.312 4	1.313 6	1.313 2	1.313 6	1.314 6	1.315 1
3.0871	1.266 2	1.260 8	1.262 9	1.264 1	1.265 7	1.267 2	1.267 5	1.268 4	1.272 6
3.1125	1.219 0	1.214 3	1.217 1	1.219 4	1.221 9	1.223 3	1.224 8	1.225 6	1.236 3
3.1379	1.173 3	1.171 0	1.173 7	1.176 5	1.178 6	1.180 6	1.182 9	1.183 8	1.201 8
3.1633	1.130 9	1.130 3	1.131 6	1.136 2	1.138 0	1.140 0	1.142 8	1.145 4	1.164 7
3.1888	1.090 8	1.089 5	1.089 9	1.097 0	1.098 1	1.100 5	1.104 1	1.107 0	1.122 9
3.2142	1.052 9	1.051 5	1.051 4	1.059 9	1.061 2	1.062 3	1.067 2	1.069 8	1 084 2
3.2396	1.015 7	1.013 5	1.016 4	1.022 9	1.025 5	1 026 2	1.031 3	1.034 2	1.049 0
3.2650	0 980 6	0.977 7	0.982 9	0.986 5	0.989 8	0.992 3	0.996 4	0.999 3	1.013 8
3.2904	0.947 9	0.946 8	0 950 2	0.953 7	0.957 0	0.961 4	0.964 8	0.966 8	0.978 7
9158	0.915 6	0.915 8	0.917 7	0.922 3	0.926 1	0 929 1	0.933 5	0.935 8	0.945 9
1412	0 883 1	0.883 7	0.887 1	0.892 6	0.895 5	0.897 3	0.901 4	0.904 3	0.915 3
3666	0.851 8	0.853 0	0.856 0	0.863 0	0.864 5	0.867 1	0.870 8	0.874 2	0.884 8
3.3920	0 822 3	0.824 2	0.825 8	0.833 2	0.835 3	0 839 9	0.842 3	0.845 6	0.855 5
3.4174	0.794 9	0.795 9	0.798 4	0 804 9	0 807 1	0.812 6	0.814 9	0.818 8	0.828 2
3.4428	0.769 2	0.770 9	0.774 1	0.780 1	0.783 3	0.788 0	0.790 6	0.793 8	0.804 4
3.4682	0.746 3	0.748 2	0.752 5	0.757 9	0.762 2	0.767 6	0.769 3	0.772 2	0.784 8
3.4937	0.725 7	0.727 2	0.731 0	0.738 8	0 742 5	0.747 5	0.750 1	0.753 7	0.765 3
3 5191	0.707 7	0.708 8	0.713 1	0 722 0	0.725 1	0.731 0	0.733 8	0.738 0	0.748 5
3.5445	0.693 1	0.692 7	0.698 3	0.705 9	0.709 7	0.715 6	0.719 3	0.722 8	0.733 4
3.5699	0.679 4	0.679 7	0.685 5	0.691 9	0.696 9	0.703 1	0.706 4	0.710 3	0.721 7
3.5953	0.668 3	0.669 3	0.674 9	0.680 4	0.686 1	0.692 8	0.696 5	0.701 6	0.712 2
3.6207	0.659 3	0.661 4	0.666 9	0.672 3	0.676 5	0.684 5	0.687 8	0.693 0	0.703 8
3.6461	0 651 8	0.656 3	0.660 0	0.665 8	0.670 0	0.678 2	0.680 6	0.686 4	0.696 7
3.6715	0.647 5	0.651 2	0.656 8	0.661 2	0.666 4	0.673 4	0.676 7	0 682 5	0.691 0
3.6969	0.642 8	0.645 7	0.652 1	0.656 8	0 662 1	0.668 3	0.672 1	0.679 5	0.685 7
3.7223	0 640 8	0.644 0	0.648 4	0.654 8	0.660 1	0.667 1	0 671 8	0 677 6	0 685 1
3.7477	0.641 4	0.644 5	0.649 5	0.655 3	0.660 7	0.666 3	0 671 9	0.677 2	0.686 9
3.7731	0.642 2	0.644 5	0.651 7	0.657 2	0.661 3	0.666 8	0.673 1	0.678 5	0.689 4
3.7986	0.643 4	0.646 3	0.652 4	0.659 5	0.662 9	0.669 1	0.675 0	0.680 4	0.692 8
3 8240	0.647 8	0.649 9	0.656 0	0.661 8	0.665 7	0.672 6	0.678 1	0.683 6	0.695 5
3 8494	0.653 6	0.654 5	0 659 8	0.665 7	0.670 7	0.675 7	0.681 7	0 687 6	0.697 6
3.8748	0.659 8	0 661 7	0 665 3	0.671 6	0.677 1	0.681 2	0 688 0	0.692 7	0.701 6
3.9002	0.665 7	0.668 3	0.672 3	0 678 7	0.683 5	0.688 0	0.694 2	0.697 6	0.707 2
3.9510	0 684 4	0.685 8	0.690 4	0.696 1	0.700 9	0.706 0	0.710 3	0.714 6	0.725 6

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 106 K
3.9764	0.693 7	0.694 4	0.700 0	0.706 0	0.710 9	0.715 1	0.719 6	0.724 3	0.73 3
4.0018	0.705 2	0.705 8	0.710 4	0.717 0	0.722 2	0.725 6	0.730 9	0.734 9	0.74 0
4.0272	0.718 9	0.719 0	0.722 9	0.729 3	0.733 4	0.736 8	0.742 0	0.746 3	0.76 1
4.0526	0.732 1	0.731 3	0.734 8	0.741 3	0.745 2	0.748 4	0.753 1	0.756 4	0.77 6
4.0780	0.745 8	0.745 5	0.748 9	0.754 0	0.760 3	0.762 4	0.766 5	0.770 7	0.78 5
4.1035	0.760 1	0.760 8	0.764 6	0.769 5	0.774 0	0.776 3	0.781 4	0.784 6	0.79 1
4.1289	0.776 3	0.776 9	0.780 8	0.786 0	0.788 9	0.791 6	0.797 2	0.800 3	0.81 0
4.1543	0.793 2	0.794 2	0.797 3	0.803 2	0.805 8	0.808 6	0.811 7	0.816 4	0.82 1
4.1797	0.812 1	0 811 9	0.814 6	0.820 4	0 822 7	0.825 4	0.826 8	0 832 0	0.83 8
4.2051	0.832 9	0.830 5	0.833 0	0.839 1	0.840 7	0 844 5	0.843 9	0.848 0	0.85 1
4.2305	0.850 6	0.847 2	0.849 7	0.856 0	0.857 0	0.860 6	0.860 0	0.862 1	0.86 1
4.2559	0.870 5	0.867 7	0.870 0	0.874 4	0.876 8	0 878 2	0.878 8	0.880 7	0 88 9
4.2813	0.892 6	0 889 5	0.892 1	0.893 9	0 898 1	0 897 7	0 896 7	0 901 0	0 90 3
4.3067	0.913 1	0.909 1	0.913 1	0 912 6	0 916 8	0.917 1	0 917 1	0 918 5	0 91 0
4.3321	0.934 6	0.929 5	0.932 3	0.932 7	0.935 8	0.936 2	0.935 1	0 936 4	0 93 3
4.3575	0.956 0	0.949 5	0.951 4	0.953 3	0.954 7	0.954 6	0 952 9	0.954 2	0.95 0
4.3829	0.977 1	0.970 7	0.973 3	0.974 2	0 976 1	0.973 3	0.973 6	0.972 4	0.97 8
4.4084	0 998 0	0.993 6	0.994 7	0.994 0	0 995 1	0.992 5	0 992 3	0 992 6	1 00 2
4.4338	1 018 9	1.014 3	1.015 3	1.013 6	1.014 2	1.012 2	1.011 6	1 013 8	1 02 3
4.4592	1.041 0	1.035 7	1.034 0	1.033 5	1.034 3	1 032 1	1.030 7	1 034 7	1 05 8
4.4846	1.062 1	1.055 6	1.052 2	1.051 7	1.052 9	1.051 0	1.047 4	1.050 6	1 06 8
4.5100	1.082 6	1.075 4	1.071 8	1.071 1	1.070 4	1.068 9	1.064 9	1.066 6	1 07 5
4 5354	1.101 2	1.093 4	1.090 4	1.089 1	1 086 5	1.085 3	1.081 5	1.080 3	1 08 7
4.5608	1.118 3	1.109 5	1.107 3	1.105 7	1.100 6	1.101 2	1 095 1	1.093 1	1.09 8
4.5862	1.135 4	1.127 3	1.125 1	1.121 4	1 118 8	1.116 8	1.110 3	1 108 5	1.10 3
4 6116	1.150 9	1.143 1	1.139 3	1.135 9	1.133 7	1.129 9	1.124 6	1.122 8	1.11 6
4.6370	1.164 8	1.157 1	1.152 2	1.149 1	1 146 1	1.141 0	1.138 5	1 135 2	1 12 7
4.6624	1.179 5	1.172 2	1 166 6	1.161 8	1 158 4	1.153 5	1.151 4	1.148 5	1.13 4
4.6878	1.188 2	1.180 8	1.174 1	1.170 9	1.167 1	1.163 6	1.158 6	1.156 5	1 14 6
4.7133	1.198 9	1.190 8	1.184 9	1.183 4	1 178 3	1.174 5	1.168 5	1.166 9	1.15 2
4.7387	1.206 7	1.199 5	1.193 5	1 191 7	1.187 0	1.181 4	1.176 3	1 174 2	1.15 3
4.7641	1.212 9	1.205 7	1.197 6	1 197 2	1.190 3	1.186 0	1.181 6	1.178 3	1.16 0
4.7895	1.220 1	1.210 7	1.203 3	1.201 8	1.194 8	1.190 2	1.187 3	1.183 1	1.17 3
4.8149	1.223 2	1.212 9	1.206 6	1.204 8	1.198 0	1.194 7	1.190 9	1.187 7	1.17 9
4 8403	1.225 8	1 214 5	1.208 9	1.205 9	1.201 8	1.198 8	1.193 9	1.190 5	1 17 5
4.8657	1.225 2	1.212 6	1.208 2	1.205 9	1.202 0	1 198 2	1.192 8	1.188 9	1 17 7
4 8911	1.225 9	1.213 8	1.210 3	1.207 0	1 203 4	1.198 6	1.194 2	1.189 1	1.17 8
4.9165	1.225 3	1.216 0	1.210 9	1 208 2	1.203 2	1.199 6	1.195 2	1.191 8	1.18 1
4.9419	1.224 1	1.217 6	1.210 8	1.207 2	1.202 7	1.200 1	1.196 7	1.193 4	1.18 9
4.9673	1.220 5	1.212 9	1.205 6	1.202 8	1.199 8	1.198 0	1.194 2	1.191 3	1.18 4
4.9927	1.216 6	1.207 5	1.199 8	1.199 3	1.195 3	1.195 5	1.190 9	1 187 8	1.18 5
5.0182	1.212 2	1.202 9	1.197 1	1.196 7	1.189 4	1.192 1	1.185 3	1.184 2	1.18 9
5.0436	1.206 5	1.194 8	1.193 3	1.191 3	1.185 6	1.186 1	1.180 8	1.179 9	1.18 1
5.0944	1.192 7	1.187 1	1.182 5	1.181 6	1.178 5	1.173 4	1.173 0	1.170 0	1.18 2

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 1065 K
5.1198	1.184 4	1.177 7	1 173 9	1.172 7	1.171 3	1.167 0	1.164 8	1.162 8	1.154 1
5.1452	1.177 3	1.169 7	1 166 0	1 166 5	1 164 7	1.161 3	1.158 8	1 157 6	1 148 5
5.1706	1 168 4	1.160 1	1.157 9	1.158 4	1.155 9	1.153 0	1 150 9	1 149 8	1 139 4
5.1960	1.157 0	1.149 6	1.148 1	1.148 2	1 145 2	1.142 8	1 140 3	1 139 5	1.130 3
5.2214	1.147 3	1.140 3	1.139 4	1 138 0	1.136 3	1 133 4	1.131 4	1 131 6	1.123 6
5.2468	1.137 7	1.130 6	1.129 8	1.129 0	1.127 3	1 124 8	1 122 2	1 123 4	1.114 7
5.2722	1.126 0	1.119 6	1 119 1	1.117 7	1.115 1	1 113 9	1 112 9	1.112 1	1 104 1
5.2976	1.114 0	1.107 5	1.107 9	1.107 0	1.104 3	1.103 5	1.103 5	1.101 7	1 094 7
5.3231	1.104 4	1.096 2	1 094 7	1.096 3	1 095 2	1 092 7	1 094 8	1.091 9	1.083 7
5.3485	1.094 9	1 086 4	1 085 8	1 087 7	1.087 0	1.082 7	1.086 2	1.082 6	1 075 4
5.3739	1 081 1	1.074 7	1.073 1	1 074 5	1 074 4	1.071 0	1 073 4	1 070 3	1 066 2
5.3993	1 069 0	1.064 6	1.063 9	1 062 9	1.063 7	1 062 4	1 061 1	1 062 2	1 059 7
5.4247	1.057 8	1.053 6	1 053 6	1.051 1	1.052 3	1 052 5	1.051 3	1.051 8	1 050 9
5.4501	1.045 9	1 038 9	1 041 6	1.039 7	1 040 5	1 042 0	1.041 1	1 040 1	1.040 9
5.4755	1.033 4	1.025 3	1 028 0	1.027 8	1.027 1	1.029 5	1 030 6	1.029 6	1.028 5
5.5009	1.021 9	1.014 4	1.017 1	1.017 8	1.017 5	1 017 8	1 019 6	1.019 9	1 019 6
5.5263	1 009 2	1 003 9	1 005 5	1.007 3	1.006 6	1.007 4	1 009 7	1 009 3	1.010 4
5.5517	0.996 8	0.992 4	0.993 1	0.994 8	0.994 9	0 996 8	0 997 5	0.999 4	1 000 0
5.5771	0 985 4	0.980 4	0.981 8	0.983 7	0 984 1	0 986 3	0.986 1	0 989 5	0.988 8
5.6025	0.973 9	0.969 5	0.971 9	0 973 4	0 973 6	0 975 4	0.976 6	0.979 6	0.979 8
5.6280	0.963 2	0 960 8	0.962 2	0.963 5	0 963 0	0 966 7	0.968 1	0.969 7	0.972 1
5.6534	0.952 6	0 949 7	0.950 1	0.950 3	0 951 1	0.954 0	0 957 3	0.957 7	0.961 2
5.6788	0 944 1	0.940 1	0.940 1	0 941 1	0 943 8	0.945 8	0.949 2	0 948 7	0.952 1
5.7042	0.931 9	0.930 0	0.930 4	0 932 0	0.934 2	0.936 5	0.938 9	0 938 6	0.942 5
5.7296	0 921 1	0.920 3	0.920 9	0.922 6	0.923 6	0.927 9	0.928 9	0.929 8	0.933 5
5.7550	0 912 2	0 911 2	0 912 7	0.915 3	0.914 9	0.918 7	0 921 8	0.922 2	0.926 9
5.7804	0.903 6	0.902 1	0.904 0	0.907 5	0.905 2	0.909 8	0.913 7	0.913 8	0 918 7
5.8058	0 895 3	0 894 7	0.896 7	0 900 1	0.898 3	0.903 2	0.907 0	0.906 0	0.911 2
5.8312	0.887 1	0.885 7	0 888 1	0.891 9	0.891 6	0 895 5	0.898 9	0.898 7	0.903 4
5.8566	0.880 6	0.878 6	0.880 1	0.884 9	0 884 7	0.887 0	0.892 1	0 892 1	0.897 4
5.8820	0.872 8	0.871 4	0 873 8	0 877 6	0.877 5	0.879 5	0 885 6	0.885 1	0.891 5
5.9074	0.865 9	0.865 8	0 869 1	0.869 6	0.872 0	0.873 2	0.879 0	0 880 0	0.884 4
5.9329	0.859 6	0.860 5	0 862 6	0.863 8	0.867 7	0.869 0	0.872 1	0.875 5	0 880 1
5.9583	0.852 9	0.853 2	0.856 1	0.859 3	0.862 9	0.864 7	0.867 2	0 869 2	0 877 3
5.9837	0 847 9	0.847 5	0.851 5	0.854 1	0 857 6	0.859 8	0 862 0	0.864 8	0.874 3
6.0091	0.843 4	0.842 8	0.844 5	0 849 4	0 852 3	0.854 0	0.856 1	0 860 5	0.869 9
6.0345	0.841 9	0.841 1	0 842 4	0.848 3	0.851 1	0 852 7	0.854 5	0.858 5	0.867 9
6.0599	0.840 2	0.839 2	0.840 4	0.846 7	0.849 8	0.851 2	0.852 6	0.856 1	0 865 3
6.0853	0.838 4	0.837 3	0.838 2	0.844 7	0.848 0	0.849 6	0.850 7	0.853 4	0 862 3
6.1107	0.836 7	0.835 3	0.836 2	0 842 7	0.845 9	0.847 8	0 848 9	0.850 8	0.859 4
6.1361	0.835 2	0.833 7	0.834 7	0.840 9	0.843 9	0.846 1	0 847 5	0.848 7	0.856 9
6.1615	0.834 5	0.832 9	0.834 2	0 839 9	0 842 4	0.844 9	0.846 8	0 847 7	0.855 4
6.1869	0 834 8	0.833 2	0.835 1	0.839 8	0.842 0	0.844 8	0.847 0	0 848 2	0.855 5
6.2378	0.837 0	0.835 4	0.838 2	0 841 8	0.842 5	0 846 0	0.848 4	0 851 3	0 858 1

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 1065 K
6.2632	0 838 8	0 837 2	0.840 3	0 843 6	0 843 7	0 847 5	0 849 7	0.853 3	0.860 4
6 2886	0 841 3	0.839 6	0 842 8	0 846 2	0 846 1	0 849 8	0.851 4	0.855 7	0 863 1
6.3140	0.844 3	0 842 4	0 845 8	0.849 1	0 849 4	0.852 8	0 853 7	0 858 4	0 865 6
6 3394	0 847 8	0 845 5	0.849 1	0 852 1	0.853 2	0 856 1	0.856 2	0.861 1	0.867 6
6 3648	0 851 6	0.848 9	0 852 4	0 855 2	0 856 9	0.859 6	0.859 2	0.863 7	0 869 1
6.3902	0 855 7	0.852 5	0 855 5	0.858 4	0 860 5	0 863 0	0 862 4	0 866 2	0.871 0
6.4156	0.860 1	0 856 7	0 858 8	0.862 2	0.864 1	0 866 4	0.866 0	0.869 0	0 873 2
6.4410	0.864 8	0.861 2	0 862 6	0.866 2	0 867 8	0.870 2	0.870 0	0.872 3	0.875 8
6 4664	0 869 8	0 866 2	0 867 1	0 870 5	0.871 8	0 874 4	0.874 2	0 876 1	0.878 8
6.4918	0 875 1	0.871 5	0.872 1	0 875 2	0.876 0	0.879 0	0 878 6	0.880 2	0.882 1
6.5172	0.880 9	0 877 2	0 877 9	0.880 6	0.880 8	0.883 8	0.883 5	0.884 8	0.886 0
6.5427	0 887 0	0 883 2	0 884 0	0 886 1	0.886 0	0.888 6	0.888 8	0 889 8	0.890 6
6 5681	0.893 1	0 889 3	0.889 7	0.891 7	0 891 5	0 893 4	0.893 7	0.895 0	0 895 7
6.5935	0 899 5	0.895 4	0.895 4	0 897 7	0.897 3	0.898 6	0.898 7	0 900 3	0 900 8
6.6189	0.906 0	0.901 5	0 901 3	0.903 7	0.903 5	0.903 9	0 903 9	0.905 7	0 905 6
6 6443	0 912 6	0 908 0	0.906 8	0.909 5	0.909 7	0.909 6	0.909 2	0 911 0	0.910 4
6.6697	0.919 7	0 914 9	0.912 5	0.915 2	0.916 1	0.915 6	0.914 6	0.916 6	0.915 7
6.6951	0 926 8	0.922 0	0.918 6	0.921 2	0.922 2	0 921 9	0.920 2	0.922 2	0.921 3
6.7205	0.933 5	0 928 8	0.925 1	0.926 9	0.927 6	0.927 9	0.925 8	0.927 8	
6.7459	0.940 2	0.935 3	0 932 3	0.932 6	0 932 8	0.933 9	0.931 6	0.93 3	
6.7713	0.946 9	0 941 4	0.939 4	0.938 3	0.938 0	0 939 5	0.937 3	0 9 8	
6.7967	0.953 7	0.947 3	0.946 4	0.944 4	0.943 6	0.944 8	0.943 3	0.9 1	
6.8221	0 960 0	0.952 9	0.952 7	0.950 4	0.948 8	0.949 6	0.948 8	0.949 4	
6 8476	0.965 6	0.958 4	0.958 2	0.956 1	0.953 8	0.954 3	0.953 6	0.954 2	0 9 7
6.8730	0.971 5	0 964 1	0.963 7	0 962 1	0.959 2	0.959 3	0 958 5	0.958 7	0.955 9
6 8984	0.977 4	0.970 1	0.969 1	0 967 7	0.964 9	0.964 3	0.963 8	0.963 1	0.960 0
6.9238	0.983 5	0.976 3	0.974 1	0.973 1	0 971 0	0.969 9	0.969 2	0.967 9	0.964 3
6.9492	0.990 0	0 982 5	0.979 3	0.978 5	0.977 3	0.975 9	0.974 4	0.973 2	0.969 3
6.9746	0.996 3	0.988 7	0.984 7	0 983 8	0.983 3	0.981 6	0.979 6	0 978 6	0.974 7
7.0000	1.002 0	0.994 3	0.990 0	0.988 8	0.988 3	0.986 5	0.984 7	0.983 8	0.980 3
7.0254	1.007 3	0.999 1	0.995 1	0.993 2	0.992 3	0.991 0	0.989 2	0 988 7	0.985 4
7.0508	1.011 9	1 003 1	0.999 2	0.996 9	0 996 9	0.995 2	0.993 1	0.992 7	0.990 0
7.0762	1 016 0	1.006 7	1.002 8	1.000 4	1.000 5	0.999 1	0.997 0	0.996 2	0.994 1
7.1016	1.018 8	1.009 5	1.005 5	1 003 6	1.003 3	1.002 4	1 000 1	0.999 1	0.996 9
7.1270	1.021 2	1.012 4	1 008 2	1.006 5	1 006 3	1.005 4	1.002 8	1.001 6	0.998 8
7.1525	1.023 5	1.015 2	1 011 2	1.009 7	1.009 2	1.008 3	1.005 4	1.003 9	1.000 9
7.1779	1.025 5	1.017 6	1.013 8	1.012 4	1.011 7	1.010 9	1.007 8	1.006 0	1.003 0
7.2033	1.027 2	1 019 7	1.015 9	1 014 9	1.014 3	1.013 3	1.010 0	1.008 1	1.005 2
7.2287	1.028 8	1 021 4	1.017 6	1.017 1	1.016 6	1.015 4	1.012 0	1.010 1	1.007 3
7.2541	1.029 8	1.022 9	1.019 1	1.018 9	1.018 4	1.017 0	1.014 0	1.012 0	1.009 3
7.2795	1.030 4	1.024 1	1.020 6	1.020 1	1.019 7	1.018 2	1.015 8	1.013 8	1.011 0
7.3049	1.030 9	1.025 1	1.021 8	1.021 1	1.020 6	1.019 3	1.017 1	1.015 5	1.012 8
7.3303	1.031 3	1.025 9	1.022 4	1.021 8	1.021 0	1.020 4	1.017 9	1.016 9	1.014 6
7 3811	1.033 0	1.027 4	1.023 4	1.023 4	1.022 5	1.022 4	1.019 8	1.018 8	1.017 2

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 1065 K
7.4065	1.0342	1.0281	1.0243	1.0243	1.0235	1.0229	1.0210	1.0201	1.0181
7.4319	1.0351	1.0286	1.0252	1.0252	1.0243	1.0231	1.0218	1.0214	1.0196
7.4574	1.0356	1.0287	1.0256	1.0256	1.0246	1.0229	1.0219	1.0222	1.0210
7.4828	1.0355	1.0284	1.0257	1.0257	1.0247	1.0223	1.0216	1.0223	1.0220
7.5082	1.0350	1.0278	1.0253	1.0254	1.0244	1.0218	1.0217	1.0216	1.0225
7.5336	1.0338	1.0267	1.0245	1.0246	1.0239	1.0215	1.0218	1.0207	1.0226
7.5590	1.0323	1.0252	1.0237	1.0235	1.0230	1.0211	1.0213	1.0199	1.0225
7.5844	1.0305	1.0234	1.0228	1.0224	1.0216	1.0209	1.0202	1.0189	1.0222
7.6098	1.0285	1.0215	1.0215	1.0211	1.0202	1.0206	1.0192	1.0177	1.0217
7.6352	1.0265	1.0198	1.0203	1.0195	1.0192	1.0200	1.0186	1.0164	1.0211
7.6606	1.0244	1.0179	1.0191	1.0179	1.0185	1.0193	1.0183	1.0153	1.0205
7.6860	1.0224	1.0161	1.0179	1.0164	1.0175	1.0179	1.0179	1.0147	1.0200
7.7114	1.0206	1.0142	1.0162	1.0146	1.0164	1.0157	1.0161	1.0140	1.0197
7.7368	1.0186	1.0121	1.0138	1.0130	1.0151	1.0133	1.0150	1.0127	1.0188
7.7623	1.0164	1.0101	1.0112	1.0116	1.0133	1.0109	1.0130	1.0110	1.0170
7.7877	1.0140	1.0081	1.0083	1.0101	1.0110	1.0085	1.0109	1.0091	1.0146
7.8131	1.0113	1.0058	1.0054	1.0081	1.0084	1.0061	1.0085	1.0070	1.0120
7.8385	1.0078	1.0030	1.0022	1.0054	1.0057	1.0036	1.0057	1.0048	1.0091
7.8639	1.0041	1.0000	0.9990	1.0024	1.0028	1.0014	1.0034	1.0024	1.0059
7.8893	1.0002	0.9971	0.9960	0.9990	0.9997	0.9992	1.0005	0.9998	1.0025
7.9147	0.9961	0.9941	0.9932	0.9955	0.9964	0.9966	0.9978	0.9971	0.9991
7.9401	0.9923	0.9908	0.9903	0.9921	0.9929	0.9941	0.9950	0.9944	0.9956
7.9655	0.9891	0.9876	0.9876	0.9889	0.9899	0.9917	0.9923	0.9924	0.9928
7.9909	0.9863	0.9841	0.9845	0.9858	0.9870	0.9889	0.9902	0.9902	0.9904
8.0163	0.9835	0.9806	0.9814	0.9829	0.9843	0.9858	0.9860	0.9874	0.9881
8.0417	0.9807	0.9772	0.9781	0.9803	0.9815	0.9826	0.9827	0.9847	0.9856
8.0672	0.9777	0.9739	0.9750	0.9778	0.9785	0.9794	0.9797	0.9817	0.9832
8.0926	0.9743	0.9709	0.9717	0.9749	0.9753	0.9762	0.9768	0.9785	0.9812
8.1180	0.9708	0.9680	0.9680	0.9714	0.9723	0.9730	0.9742	0.9752	0.9793
8.1434	0.9673	0.9652	0.9646	0.9679	0.9697	0.9699	0.9720	0.9719	0.9771
8.1688	0.9638	0.9627	0.9617	0.9644	0.9671	0.9670	0.9698	0.9687	0.9747
8.1942	0.9609	0.9606	0.9592	0.9612	0.9646	0.9643	0.9676	0.9660	0.9723
8.2196	0.9584	0.9586	0.9568	0.9591	0.9619	0.9621	0.9656	0.9640	0.9698
8.2450	0.9564	0.9564	0.9552	0.9569	0.9599	0.9604	0.9639	0.9628	0.9676
8.2704	0.9546	0.9541	0.9540	0.9548	0.9578	0.9588	0.9615	0.9620	0.9655
8.2958	0.9530	0.9522	0.9530	0.9528	0.9560	0.9569	0.9591	0.9612	0.9637
8.3212	0.9516	0.9504	0.9516	0.9514	0.9543	0.9555	0.9566	0.9604	0.9620
8.3466	0.9499	0.9482	0.9499	0.9499	0.9520	0.9539	0.9546	0.9591	0.9600
8.3721	0.9484	0.9463	0.9478	0.9482	0.9495	0.9524	0.9524	0.9571	0.9579
8.3975	0.9471	0.9444	0.9454	0.9466	0.9476	0.9500	0.9505	0.9548	0.9559
8.4229	0.9452	0.9422	0.9430	0.9453	0.9460	0.9488	0.9484	0.9521	0.9536
8.4483	0.9434	0.9398	0.9401	0.9437	0.9445	0.9466	0.9462	0.9494	0.9513
8.4737	0.9421	0.9378	0.9373	0.9422	0.9432	0.9445	0.9444	0.9469	0.9492
8.5245	0.9400	0.9350	0.9341	0.9391	0.9414	0.9422	0.9416	0.9437	0.9466

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 1065 K
8.5499	0.9396	0.9343	0.9338	0.9382	0.9407	0.9415	0.9408	0.9432	0.9461
8.5753	0.9401	0.9343	0.9343	0.9378	0.9405	0.9416	0.9410	0.9433	0.9466
8.6007	0.9411	0.9347	0.9349	0.9381	0.9402	0.9422	0.9420	0.9436	0.9472
8.6261	0.9419	0.9352	0.9353	0.9388	0.9396	0.9427	0.9427	0.9440	0.9479
8.6515	0.9424	0.9358	0.9360	0.9395	0.9394	0.9434	0.9433	0.9445	0.9488
8.6770	0.9424	0.9361	0.9368	0.9403	0.9396	0.9438	0.9441	0.9451	0.9489
8.7024	0.9422	0.9366	0.9374	0.9410	0.9400	0.9444	0.9447	0.9458	0.9487
8.7278	0.9426	0.9373	0.9380	0.9415	0.9408	0.9453	0.9451	0.9465	0.9485
8.7532	0.9435	0.9385	0.9390	0.9421	0.9419	0.9462	0.9454	0.9472	0.9486
8.7786	0.9444	0.9402	0.9404	0.9432	0.9433	0.9473	0.9465	0.9488	0.9495
8.8040	0.9455	0.9422	0.9420	0.9449	0.9445	0.9481	0.9465	0.9488	0.9505
8.8294	0.9472	0.9441	0.9441	0.9457	0.9458	0.9490	0.9477	0.9492	0.9516
8.8548	0.9496	0.9461	0.9463	0.9487	0.9475	0.9503	0.9489	0.9501	0.9530
8.8802	0.9518	0.9481	0.9476	0.9508	0.9490	0.9513	0.9500	0.9511	0.9541
8.9056	0.9538	0.9498	0.9486	0.9529	0.9505	0.9518	0.9508	0.9523	0.9552
8.9310	0.9557	0.9511	0.9497	0.9546	0.9525	0.9520	0.9520	0.9537	0.9564
8.9565	0.9579	0.9523	0.9512	0.9560	0.9543	0.9530	0.9534	0.9555	0.9572
8.9819	0.9605	0.9539	0.9532	0.9574	0.9555	0.9543	0.9554	0.9557	0.9578
9.0073	0.9635	0.9555	0.9552	0.9585	0.9567	0.9555	0.9571	0.9589	0.9586
9.0327	0.9665	0.9572	0.9575	0.9599	0.9576	0.9577	0.9594	0.9605	0.9598
9.0581	0.9694	0.9593	0.9602	0.9617	0.9586	0.9601	0.9623	0.9623	0.9613
9.0835	0.9720	0.9621	0.9630	0.9636	0.9597	0.9626	0.9652	0.9639	0.9630
9.1089	0.9746	0.9651	0.9658	0.9658	0.9614	0.9658	0.9678	0.9659	0.9644
9.1343	0.9776	0.9687	0.9688	0.9685	0.9641	0.9688	0.9703	0.9688	0.9672
9.1597	0.9803	0.9725	0.9709	0.9715	0.9670	0.9716	0.9723	0.9711	0.9697
9.1851	0.9828	0.9762	0.9730	0.9747	0.9703	0.9743	0.9735	0.9733	0.9725
9.2105	0.9853	0.9796	0.9754	0.9777	0.9737	0.9765	0.9765	0.9762	0.9753
9.2359	0.9882	0.9831	0.9785	0.9812	0.9775	0.9789	0.9784	0.9790	0.9782
9.2614	0.9913	0.9863	0.9816	0.9840	0.9808	0.9815	0.9806	0.9815	0.9807
9.2868	0.9941	0.9891	0.9841	0.9865	0.9835	0.9840	0.9830	0.9835	0.9829
9.3122	0.9969	0.9913	0.9865	0.9890	0.9862	0.9868	0.9857	0.9860	0.9849
9.3376	0.9992	0.9930	0.9887	0.9909	0.9886	0.9891	0.9884	0.9884	0.9865
9.3630	1.0017	0.9945	0.9910	0.9928	0.9906	0.9924	0.9907	0.9916	0.9883
9.3884	1.0045	0.9960	0.9934	0.9950	0.9931	0.9948	0.9929	0.9942	0.9905
9.4138	1.0071	0.9977	0.9962	0.9971	0.9959	0.9967	0.9949	0.9966	0.9928
9.4392	1.0089	0.9994	0.9996	0.9987	0.9979	0.9988	0.9966	0.9984	0.9954
9.4646	1.0100	1.0011	1.0023	1.0003	1.0004	1.0007	0.9994	1.0006	0.9978
9.4900	1.0108	1.0024	1.0040	1.0009	1.0004	1.0017	0.9995	0.9999	0.9995
9.5154	1.0120	1.0035	1.0055	1.0014	1.0013	1.0026	1.0007	1.0002	1.0010
9.5408	1.0131	1.0046	1.0063	1.0018	1.0012	1.0034	1.0014	1.0008	1.0015
9.5663	1.0138	1.0057	1.0061	1.0025	1.0011	1.0038	1.0019	1.0013	1.0010
9.5917	1.0142	1.0062	1.0052	1.0032	1.0008	1.0046	1.0018	1.0022	1.0008
9.6171	1.0146	1.0062	1.0047	1.0038	1.0006	1.0058	1.0021	1.0034	1.0009
9.6679	1.0177	1.0072	1.0064	1.0068	1.0035	1.0077	1.0032	1.0066	1.0026

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 1065 K
9.6933	1.018 8	1.008 2	1.008 1	1.008 5	1.005 4	1 008 4	1.004 5	1.008 1	1.003 8
9.7187	1.019 8	1.009 4	1.009 9	1.009 8	1.007 3	1.009 3	1.006 1	1.009 3	1.005 3
9.7441	1.020 3	1.010 3	1.010 7	1.010 7	1.008 9	1 009 6	1.007 4	1.009 3	1.006 2
9.7695	1.020 5	1.011 0	1.010 2	1.010 7	1.010 0	1 009 2	1 008 3	1.009 0	1.006 8
9.7949	1.020 6	1.011 7	1.009 5	1.010 4	1.010 6	1 009 1	1 009 2	1.009 3	1.007 8
9.8203	1.020 3	1.012 3	1.008 5	1 010 0	1.010 8	1.009 4	1.009 6	1.009 7	1.008 7
9.8457	1.019 5	1.012 7	1.007 5	1.009 5	1 010 9	1.009 3	1.009 7	1.009 4	1 009 5
9.8712	1.018 5	1.012 7	1.006 8	1.009 0	1.010 3	1.009 3	1.009 8	1.009 0	1.010 8
9.8966	1.018 0	1.012 2	1.006 4	1.008 9	1.009 4	1.010 0	1.010 2	1 008 8	1.012 0
9.9220	1.018 8	1.011 8	1.007 2	1.009 0	1.009 3	1.010 9	1.010 7	1 009 2	1 013 2
9.9474	1.019 6	1.011 8	1.008 5	1.009 7	1.009 5	1.011 4	1.011 5	1.009 7	1 014 0
9.9728	1.020 4	1.011 8	1.009 8	1.010 7	1 009 4	1.012 0	1.011 9	1.010 2	1.014 6
9.9982	1.020 7	1.011 5	1.010 5	1.011 6	1.008 6	1 011 8	1.011 6	1.010 4	1.014 4
10.023 6	1.020 6	1.011 3	1.010 3	1.012 4	1.008 9	1.011 3	1.011 3	1 010 6	1.013 9
10.049 0	1.020 6	1.011 0	1.009 7	1.012 8	1.010 6	1 011 3	1 011 2	1.011 7	1 013 7
10.074 4	1.020 4	1.010 6	1.009 5	1.012 0	1.011 6	1 011 0	1.010 8	1.012 3	1.013 4
10.099 8	1.019 8	1.010 2	1.009 1	1.011 2	1.012 0	1.010 4	1 010 4	1.012 3	1.012 7
10.125 2	1.018 9	1.010 2	1.008 5	1.010 0	1.012 0	1 009 6	1.010 5	1 011 8	1.011 7
10.150 6	1.018 0	1.009 9	1.007 1	1.008 4	1 010 9	1.008 4	1 010 6	1.010 8	1.010 7
10.176 1	1.017 1	1.008 8	1.005 6	1.006 8	1.009 4	1.007 7	1.009 8	1.009 4	1.009 6
10.201 5	1.016 7	1.007 6	1.005 1	1.005 7	1.008 1	1.007 5	1 008 9	1.008 1	1 009 0
10.226 9	1.015 6	1.006 8	1.004 9	1.005 4	1.006 3	1.007 4	1 008 4	1.007 3	1.008 8
10 252 3	1.014 1	1.005 8	1.004 2	1.005 2	1.003 9	1.007 2	1 007 5	1 006 7	1.009 2
10.277 7	1.012 8	1.005 5	1.002 8	1.004 9	1.001 8	1.006 7	1.007 0	1.006 6	1.009 7
10.303 1	1 012 0	1.005 9	1.001 7	1.004 8	1.001 8	1 006 4	1.006 8	1 007 6	1.009 4
10.328 5	1.011 4	1 005 6	1 001 4	1 004 5	1.002 5	1 006 0	1 006 4	1.008 5	1.008 7
10.353 9	1.011 0	1.005 6	1.001 5	1 004 0	1.002 0	1.005 8	1.006 5	1.008 6	1.008 3
10.379 3	1.010 7	1.005 9	1.001 5	1.004 0	1.002 2	1.005 9	1.007 3	1.009 1	1.008 9
10.404 7	1.010 5	1 006 2	1.001 4	1.003 7	1.003 0	1.006 3	1.008 3	1.009 7	1.010 0
10.430 1	1.010 1	1.005 7	1 001 4	1.003 7	1.003 9	1.006 8	1.009 0	1 009 7	1.011 6
10.455 5	1.009 8	1.004 4	1.001 9	1.004 1	1.004 4	1.007 6	1 009 2	1.009 1	1.012 7
10.481 0	1.009 7	1.003 2	1 002 6	1.005 1	1.004 2	1 007 8	1.009 2	1.008 7	1.013 8
10.506 4	1.009 2	1.002 2	1.003 4	1.005 6	1.003 6	1.007 0	1.009 4	1.008 1	1.015 1
10.531 8	1.009 2	1.001 2	1.003 0	1 005 1	1.003 2	1.005 6	1.009 8	1 007 0	1.015 5
10.557 2	1.009 8	1.000 5	1.002 4	1.005 0	1.003 2	1.004 8	1.009 9	1.006 7	1.014 8
10.582 6	1.010 4	0.999 9	1.002 4	1.004 8	1.002 8	1.004 2	1.009 1	1.007 0	1 012 8
10 608 0	1.010 8	0.999 2	1 002 9	1.004 0	1.001 6	1.003 2	1.007 8	1.006 6	1.010 3
10.633 4	1.011 2	0.999 2	1.003 3	1.003 4	1.001 0	1 002 7	1.006 5	1.006 1	1.008 4
10.658 8	1.011 6	0.999 4	1.003 2	1.002 7	1.000 9	1.002 6	1.005 6	1 006 5	1.007 4
10.684 2	1.011 5	0.999 4	1.002 8	1.002 1	1.000 9	1.002 4	1.004 6	1.007 0	1.007 1
10.709 6	1.011 3	0.999 3	1.002 3	1.001 8	1.001 0	1.002 1	1.003 4	1.007 3	1.007 3
10.735 0	1.010 7	0.999 2	1.001 7	1.001 7	1.000 0	1.001 1	1.002 3	1.007 2	1.007 1
10.760 4	1.009 9	0.999 2	1.001 4	1 001 4	0.998 9	0.999 7	1.000 7	1.006 4	1.006 9
10.811	1.007 6	0.997 6	0.998 6	0.998 6	0.997 3	0 996 5	0.998 5	1.002 5	1.005 1

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 1065 K
10 836 7	1.005 8	0.996 0	0.996 7	0.997 1	0.996 1	0.995 3	0.997 5	1.000 5	1.003 8
10.862 1	1 004 0	0.994 3	0 995 3	0.995 3	0.994 6	0.994 1	0 996 7	0.998 6	1.002 4
10.887 5	1.002 8	0.993 1	0.994 6	0.993 8	0.993 5	0.993 4	0.996 0	0 996 1	1.000 9
10.912 9	1.002 2	0.992 9	0.994 0	0.993 2	0 993 2	0.993 5	0.995 6	0.994 2	0.999 6
10.938 3	1.001 2	0.992 7	0.992 8	0 992 9	0.993 3	0.993 7	0.995 3	0.993 0	0.999 0
10.963 7	1.000 3	0.992 3	0.991 3	0.992 3	0.993 8	0.993 6	0.994 5	0.992 5	0.999 2
10.989 1	1.000 2	0.991 8	0.990 1	0 991 9	0.995 0	0.993 4	0.993 0	0 992 7	0 999 9
11.014 5	1.000 5	0.991 4	0 989 1	0.991 4	0.995 9	0 993 1	0.992 1	0.993 1	1 000 6
11.039 9	1 000 6	0.991 1	0.988 5	0.991 0	0.996 5	0.993 2	0.991 7	0.993 5	1.001 1
11.065 4	1.000 4	0.991 3	0.988 8	0.990 9	0.997 1	0.993 5	0 991 6	0.994 2	1 001 7
11.090 8	0.999 9	0.990 7	0.988 8	0.990 7	0.997 0	0 993 5	0.991 1	0.994 6	1.001 8
11.116 2	0.999 7	0.990 0	0.988 8	0.990 6	0.995 8	0.992 7	0.990 4	0.994 3	1.001 5
11.141 6	1.000 1	0.989 6	0 988 4	0.990 7	0.994 0	0.992 0	0.990 0	0 994 0	1.000 8
11.167 0	1.000 2	0.989 0	0.988 4	0.990 7	0.992 0	0.991 6	0 989 2	0.993 6	0.999 6
11.192 4	1.000 0	0 988 8	0.988 3	0.990 7	0.990 6	0 991 5	0.988 6	0.993 3	0.998 1
11.217 8	0.999 0	0 989 0	0.988 0	0.990 8	0.990 3	0.991 6	0.988 0	0.993 4	0.997 1
11.243 2	0.998 5	0 989 4	0.987 2	0.990 5	0.990 9	0.991 3	0.987 3	0.993 6	
11.268 6	0 998 7	0.990 1	0.987 2	0.990 3	0.992 0	0.990 7	0.987 5	0.993 6	
11.294 0	0.999 2	0.990 6	0.987 3	0.990 0	0.991 7	0.989 9	0.988 6	0.99 4	
11.319 4	0.999 5	0.991 4	0.988 2	0.989 8	0.991 5	0.989 9	0.989 5	0.99 5	
11.344 8	1.000 0	0.992 7	0.989 7	0.990 2	0.991 6	0.990 6	0.990 8	0.993 4	
11.370 3	1.000 8	0 993 7	0.991 0	0.990 3	0.991 6	0.991 4	0.991 8	0.993 0	0.998 4
11.395 7	1 001 5	0.994 8	0.992 1	0.991 0	0.991 8	0.992 0	0.992 2	0.992 4	0.999 1
11.421 1	1.001 7	0.995 4	0.992 3	0.992 0	0.992 2	0.992 8	0.992 5	0.992 3	0 999 3
11.446 5	1.000 9	0.994 9	0.992 3	0.992 4	0.992 2	0.993 5	0.991 6	0.991 7	0 998 6
11.471 9	1.000 2	0.995 0	0.992 1	0.992 5	0.992 6	0.994 1	0.990 9	0.991 3	0.997 8
11.497 3	0.999 9	0.995 3	0.991 7	0.992 6	0.993 2	0.994 3	0.990 4	0.990 9	0.997 3
11.522 7	1.000 3	0.995 2	0.991 6	0.992 3	0 993 9	0.993 4	0.989 5	0.990 2	0.996 9
11.548 1	1.000 5	0.994 5	0.992 2	0.991 9	0.994 5	0.992 2	0.989 0	0.990 2	0.996 5
11.573 5	1 000 8	0.993 3	0.993 0	0.991 3	0.994 3	0.990 6	0.988 5	0.990 2	0.995 9
11.598 9	1.001 6	0.992 3	0.994 0	0.991 2	0.993 9	0.990 2	0.988 6	0.991 3	0.996 2
11.624 3	1.002 7	0.992 0	0.994 7	0.990 8	0.993 3	0.990 2	0.989 3	0.991 9	0.996 4
11.649 7	1.003 9	0.992 6	0.994 7	0.990 6	0.994 0	0.990 6	0.991 1	0.992 5	0.997 1
11.675 2	1.005 7	0.993 2	0.994 2	0.991 3	0.995 9	0.991 3	0.992 8	0.993 3	0.997 6
11.700 6	1.007 9	0.994 4	0.994 1	0.993 7	0.998 0	0 993 2	0.994 9	0.995 1	0.998 4
11.726 0	1.009 1	0.995 1	0.994 4	0.995 9	0.999 2	0.995 0	0 995 9	0.996 8	0.999 1
11.751 4	1.010 2	0.996 0	0.995 2	0.997 4	1.000 0	0.996 5	0.996 8	0.998 0	1.000 2
11.776 8	1.010 9	0.997 2	0.996 3	0.998 2	1.000 3	0.997 2	0.996 9	0.998 2	1.001 4
11.802 2	1.011 2	0.997 4	0.997 2	0 998 1	1.000 1	0.997 2	0.996 3	0.998 1	1.001 8
11.827 6	1.011 0	0.997 3	0 997 8	0.997 8	1.000 0	0.997 4	0.996 5	0.998 4	1.001 4
11.853 0	1.010 6	0.997 1	0.998 0	0.998 0	0.999 6	0.997 3	0.997 0	0.998 4	1.000 4
11.878 4	1.010 7	0.997 7	0.998 6	0.998 4	0.999 0	0.997 5	0.997 4	0.999 6	1.000 0
11.903 8	1.010 8	0.998 7	0.999 4	0.998 3	0.999 0	0.998 0	0.997 2	0.999 7	0.999 0
11.954 6	1.014 2	1.000 7	1.000 3	1.001 0	1.000 3	0.999 9	1.000 8	0.999 7	0.998 2

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 1065 K
11.980 1	1.016 6	1.001 7	1.002 9	1.003 8	1.002 4	1.001 9	1.003 3	1.000 4	0.999 4
12.005 5	1.017 2	1.001 7	1.005 4	1.005 8	1.003 9	1.003 3	1.004 9	1.001 4	1.000 9
12.030 9	1.017 2	1.002 3	1.007 6	1.007 3	1.005 7	1.004 5	1.006 1	1.002 8	1.002 8
12.056 3	1.017 4	1.004 0	1.009 7	1.008 2	1.007 0	1.006 1	1.006 5	1.004 2	1.005 3
12.081 7	1.017 7	1.005 1	1.011 0	1.008 6	1.007 5	1.007 5	1.007 3	1.005 2	1.006 9
12.107 1	1.017 7	1.006 4	1.011 8	1.008 7	1.008 2	1.008 7	1.009 0	1.006 5	1.007 3
12.132 5	1.017 2	1.007 5	1.012 4	1.008 6	1.009 1	1.009 3	1.009 7	1.008 0	1.006 4
12.157 9	1.017 2	1.008 7	1.013 0	1.008 2	1.010 0	1.009 8	1.009 4	1.010 3	1.006 0
12.183 3	1.017 8	1.008 7	1.013 5	1.007 6	1.010 7	1.010 5	1.008 4	1.011 5	1.005 1
12.208 7	1.019 3	1.008 4	1.013 9	1.008 7	1.011 4	1.011 4	1.008 7	1.011 7	1.004 8
12.234 1	1.021 1	1.009 4	1.015 0	1.010 3	1.011 9	1.012 3	1.010 1	1.011 5	1.005 4
12.259 5	1.022 6	1.010 7	1.016 4	1.011 9	1.012 1	1.013 8	1.011 1	1.012 0	1.007 3
12.285 0	1.023 9	1.012 6	1.017 1	1.013 2	1.012 9	1.015 1	1.011 8	1.013 9	1.009 7
12.310 4	1.025 3	1.015 2	1.017 7	1.014 5	1.014 3	1.016 4	1.012 6	1.015 8	1.012 8
12.335 8	1.027 4	1.018 1	1.018 0	1.015 6	1.016 0	1.017 7	1.013 4	1.016 9	1.016 0
12.361 2	1.029 5	1.020 4	1.017 7	1.016 8	1.017 6	1.018 5	1.015 2	1.017 1	1.018 2
12.386 6	1.031 2	1.021 9	1.016 9	1.017 6	1.019 2	1.019 3	1.017 3	1.016 9	1.019 2
12	1.031 9	1.022 4	1.015 9	1.018 8	1.020 9	1.020 4	1.018 7	1.017 3	1.019 4
7	1.032 4	1.021 8	1.015 1	1.019 6	1.021 2	1.020 6	1.019 4	1.017 5	1.018 2
1	1.032 8	1.020 4	1.014 2	1.020 3	1.020 4	1.020 0	1.019 5	1.017 8	1.015 6
68	1.032 4	1.018 4	1.013 6	1.021 1	1.018 8	1.019 2	1.019 4	1.017 9	1.013 3
12 513 6	1.031 5	1.017 7	1.014 6	1.021 8	1.016 8	1.018 2	1.018 8	1.018 8	1.011 8
12.539 0	1.031 0	1.017 8	1.016 9	1.022 3	1 015 6	1.018 3	1.018 4	1.020 9	1.011 7
12.564 4	1.030 6	1.018 1	1.019 6	1.022 8	1.015 1	1 018 4	1.017 5	1.022 7	1.012 1
12.589 9	1.029 3	1.018 9	1.021 6	1.021 9	1.014 9	1.018 1	1.016 2	1.023 0	1.012 4
12.615 3	1.029 1	1.020 4	1.022 7	1.020 7	1.015 6	1.018 3	1.015 5	1.022 8	1.012 9
12.640 7	1.029 1	1.021 0	1.022 8	1.019 6	1.016 4	1.019 2	1.015 7	1.022 4	1.014 2
12.666 1	1.028 7	1.021 2	1.021 8	1.019 2	1.017 2	1.019 9	1 016 5	1.021 1	1.016 0
12.691 5	1.028 5	1.021 8	1.020 7	1.019 3	1.018 1	1.019 7	1.017 5	1.019 8	1.017 2
12.716 9	1.028 1	1.021 1	1.019 8	1.018 3	1.017 7	1.018 3	1.017 7	1.018 3	1.017 4
12.742 3	1.026 6	1.018 6	1.018 2	1.017 5	1.017 0	1.016 1	1.017 6	1.016 7	1.017 3
12.767 7	1.024 9	1.015 7	1 016 4	1.016 5	1.016 5	1.014 4	1.017 2	1.015 1	1.017 5
12.793 1	1.023 9	1.013 9	1.015 0	1.015 6	1.016 3	1.012 9	1.016 7	1.013 6	1.017 9
12.818 5	1.023 4	1.013 1	1.014 6	1.015 1	1.016 5	1.012 3	1.017 4	1.012 9	1.018 8
12.843 9	1.022 5	1.012 3	1.013 1	1.014 7	1.015 4	1.011 6	1.017 3	1.011 7	1.018 2
12.869 3	1.021 4	1.011 9	1.010 9	1.013 0	1.013 4	1.010 8	1.016 4	1.011 0	1.016 5
12.894 8	1.021 2	1.011 1	1.008 7	1.011 2	1.011 5	1.010 9	1.015 1	1.011 6	1.014 8
12.920 2	1.020 3	1.009 3	1.005 7	1.009 3	1.009 3	1.010 8	1.014 0	1.011 7	1.012 7
12.945 6	1.019 2	1.007 5	1.003 0	1.007 8	1.007 1	1.009 1	1.012 7	1.011 2	1.010 7
12.971 0	1.018 4	1.006 1	1 000 6	1.005 8	1.005 0	1.006 5	1.010 6	1.010 3	1.008 4
12.996 4	1.016 8	1.004 1	0.999 8	1.003 5	1.002 7	1.004 3	1.007 5	1.008 7	1 006 4
13.021 8	1.015 0	1.002 5	0 999 5	1.002 0	1.002 1	1.001 8	1.003 9	1.006 8	1.004 1
13.047 2	1.014 5	1.002 4	0.998 7	1.001 1	1.003 0	1.000 5	1.000 7	1.005 3	1.002 8
13.098 0	1.014 0	1.000 7	0.998 1	0.999 4	1 000 8	0.998 2	0.996 6	1.000 6	1.000 7

Q (Å^{-1})	S(Q) 867K	S(Q) 889K	S(Q) 911K	S(Q) 933K	S(Q) 956K	S(Q) 978K	S(Q) 1000 K	S(Q) 1022 K	S(Q) 1065 K
13.123 4	1.013 7	0.999 6	0.998 4	0.998 7	0.998 6	0.997 3	0.995 4	0.999 2	0.999 8
13.148 8	1.013 1	0.998 5	0.998 8	0.998 2	0.996 9	0.996 4	0.994 2	0.998 6	0.998 7
13.174 2	1.011 6	0.996 1	0.998 4	0.997 1	0.995 2	0.995 6	0.992 8	0.997 4	0.996 0
13.199 7	1.008 5	0.992 5	0.995 8	0.994 4	0.992 3	0.993 3	0.990 8	0.994 9	0.992 0
13.225 1	1.004 9	0.988 9	0.991 7	0.990 3	0.988 8	0.990 6	0.988 6	0.992 2	0.988 4
13.250 5	1.001 9	0.985 7	0.987 0	0.985 8	0.985 7	0.987 7	0.986 8	0 989 9	0.985 7
13.275 9	0.999 0	0.983 9	0.983 8	0.982 1	0.984 2	0.985 7	0.985 0	0.987 6	0.984 8
13.301 3	0.996 6	0.983 6	0.981 3	0.978 8	0.984 1	0.984 0	0.983 2	0.984 7	0 984 3
13.326 7	0.995 0	0.983 7	0.978 2	0.976 8	0.983 2	0.982 7	0.981 8	0.981 6	0.983 9
13.352 1	0.993 5	0.982 1	0.975 8	0.975 5	0.980 8	0.981 3	0.980 3	0.978 6	0.984 5
13.377 5	0.992 4	0.980 1	0.974 5	0.974 5	0.978 1	0.980 3	0.978 3	0.977 0	0.985 0
13.402 9	0.992 1	0.978 2	0.974 2	0.974 1	0.976 5	0.978 8	0.976 9	0.976 9	0 984 7
13.428 3	0.991 6	0.976 4	0.973 9	0.975 2	0.975 3	0.976 8	0.975 3	0.976 6	0.983 6
13.453 7	0.990 6	0.973 5	0.973 7	0.976 2	0.974 3	0.974 7	0.974 0	0.975 2	0.981 0
13.479 1	0.988 7	0.970 3	0.973 0	0.975 3	0.972 7	0.972 4	0 972 1	0.973 4	0.977 3
13.504 6	0.987 5	0.968 5	0.972 0	0.973 8	0.970 8	0.970 5	0.971 4	0.972 3	0.974 6
13.530 0	0.987 2	0.967 3	0.971 4	0.972 3	0.968 9	0.968 7	0.971 4	0.971 6	0.972 9
13.555 4	0.987 1	0.967 9	0.971 4	0.971 4	0.968 3	0.967 6	0.971 7	0.970 2	0.972 5
13.580 8	0.987 1	0.969 7	0.971 3	0.969 9	0.968 7	0.967 8	0.972 5	0.968 4	0.972 4
13.606 2	0.987 4	0.972 2	0.970 7	0.968 7	0.968 7	0.968 7	0.972 9	0.967 5	0.972 5
13.631 6	0.988 5	0.974 7	0.971 1	0.968 9	0.969 7	0.970 1	0.973 0	0.968 6	0.973 4
13.657 0	0.990 8	0.976 7	0.971 7	0.970 5	0.972 4	0.972 8	0.974 0	0.971 3	0.974 6
13.682 4	0.992 6	0.977 7	0.971 7	0.973 0	0.974 1	0.975 3	0.975 4	0.973 7	0.975 3
13.707 8	0.993 5	0.978 7	0.972 3	0 976 6	0.975 6	0.977 2	0.976 3	0.976 2	0 976 9
13.733 2	0.993 8	0.979 2	0.973 4	0.979 8	0.977 7	0.979 7	0 978 4	0.977 7	0.979 5
13.758 6	0.993 6	0.978 8	0.974 5	0.982 1	0.978 9	0.981 9	0.980 4	0.978 0	0.981 5
13.784 0	0.993 4	0.978 0	0.975 5	0.983 8	0.979 3	0.983 1	0 982 1	0.978 3	0.983 5
13.809 5	0.992 7	0.977 9	0.976 3	0.984 1	0.979 0	0.982 8	0.982 8	0.979 2	0.984 5
13.834 9	0.993 5	0.978 9	0.977 5	0.984 0	0.980 4	0.982 8	0.983 1	0.979 6	0.985 0
13.860 3	0.994 8	0 980 3	0.979 2	0.982 5	0.982 3	0.982 5	0.983 1	0.979 8	0.984 5
13.885 7	0.996 4	0.981 6	0.981 9	0.980 7	0.983 8	0.982 1	0.982 5	0.979 7	0.984 1
13.911 1	0.998 3	0.982 7	0.985 4	0.979 6	0.985 6	0.981 4	0.982 3	0.979 1	0.983 5
13.936 5	1.000 4	0.983 0	0.988 8	0.979 5	0.987 6	0.981 4	0.982 7	0.978 5	0.983 7
13.961 9	1.002 0	0.982 9	0.991 7	0.979 8	0.988 4	0.981 5	0.983 1	0.977 3	0.984 4
13.987 3	1.002 7	0.982 5	0.993 9	0.979 5	0.989 2	0.981 3	0.983 2	0.976 5	0.985 6

Table A-15: Viscosity values for Al-Si hypoeutectic alloys at various melt temperatures.

Alloy	Temperature (K)	Viscosity (mPa.s)	Alloy	Temperature (K)	Viscosity (mPa.s)
Al	938	2.41193	Al-3Si	920	2.12178
	963	2.38204		942	2.10874
	988	2.32308		964	2.03742
	1013	2.32063		1052	1.97722
	1038	2.28938	Al-7Si	898	1.90897
	1063	2.25917		920	1.85679
	1088	2.2582		942	1.83022
	1113	2.19168		964	1.80752
Al-12.5Si	867	1.69646		986	1.81058
	889	1.67959		1008	1.75142
	911	1.65479		1030	1.7154
	933	1.6296		1052	1.70663
	956	1.5997	Al-10Si	885	1.81276
	978	1.59236		907	1.80041
	1000	1.5305		929	1.7214
	1022	1.4861		973	1.61955
	1065	1.45403		995	1.59486
				1017	1.5822
				1039	1.54895

Table A-16: Viscosity values for Sr modified Al-Si hypoeutectic alloys at various melt temperatures

Alloy	Temperature (K)	Viscosity (mPa.s)	Alloy	Temperature (K)	Viscosity (mPa.s)
Al	938	2.41193	Al-3Si-04Sr	920	1.89668
	963	2.38204		942	1.8537
	988	2.32308		964	1.76325
	1013	2.32063		1052	1.68662
	1038	2.28938	Al-7Si-04Sr	898	1.68339
	1063	2.25917		920	1.66849
	1088	2.2582		942	1.67243
	1113	2.19168		964	1.61889
Al-12.5Si-04Sr	867	1.65096		986	1.62371
	889	1.62915		1008	1.59714
	911	1.61358		1030	1.61089
	933	1.60531		1052	1.54215
	956	1.56573	Al-10Si-04Sr	885	1.73271
	978	1.5433		907	1.77032
	1000	1.51197		929	1.66803
	1022	1.44839		973	1.62509
	1065	1.34947		995	1.62005
				1017	1.54931
				1039	1.53943

APPENDIX B DATA FOR PARTIAL PAIRDISTRIBUTION FUNCTIONS

Table B-1: The liquid structure information for partial pair correlations of Al-Al, Al-Si, Si-Si of Al-3%Si & Al-3%Si-0.04%Sr obtained from high energy diffraction experiments and RMC analysis (Sr in brackets represents the information for alloy with Strontium).

	g(r) First peak height, $g(r)_1$						g(r) First peak position, r_1(Å)					
Temp (K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
920	2.81	2.16	2.23	2.35	2.00	2.18	2.73	2.83	2.83	2.73	2.78	2.82
942	2.12	2.15	2.22	1.79	1.95	2.17	3.07	2.82	2.82	2.89	2.78	2.82
964	2.65	2.17	2.2	3.11	1.98	2.15	2.85	2.85	2.82	2.88	2.81	2.82
1052	2.43	2.07	2.11	2.41	1.92	2.09	2.73	2.81	2.82	2.58	2.77	2.82

	g(r) Second peak height, $g(r)_2$						g(r) Second peak position, r_2(Å)					
Temp (K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
920	1.19	1.18	1.185	1.33	1.156	1.178	5.37	5.15	5.08	4.59	5.08	5.08
942	1.51	1.18	1.183	1.16	1.171	1.177	4.51	5.05	5.09	4.58	5.05	5.08
964	1.43	1.2	1.18	1.15	1.159	1.175	5.24	5.17	5.09	4.78	5.37	5.08
1052	1.26	1.19	1.171	1.21	1.15	1.165	5.4	5.06	5.09	5.02	5.1	5.08

	Coordination number						Packing density					
Temp (K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
920	0.38	1.80	10.23	0.37	1.78	10.17	0.010	0.071	0.409	0.010	0.066	0.404
942	0.34	1.80	10.19	0.36	1.75	10.13	0.015	0.070	0.406	0.012	0.066	0.403
964	0.44	1.82	10.14	0.44	1.77	10.08	0.0123	0.071	0.405	0.012	0.068	0.401
1052	0.36	1.77	10.06	0.32	1.74	10.01	0.0108	0.068	0.403	0.009	0.065	0.400

Table B-2: The liquid structure information for partial pair correlations of Al-Al, Al-Si, Si-Si of Al-7%Si & Al-7%Si-0.04%Sr obtained from high energy diffraction experiments and RMC analysis (Sr in brackets represents the information for alloy with Strontium).

	g(r) First peak height, $g(r)_1$						g(r) First peak position, r_1(Å)					
Temp (K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
898	2.16	2.12	2.17	1.82	2.07	2.25	2.88	2.78	2.80	2.69	2.79	2.81
920	2.20	2.10	2.16	1.91	2.06	2.23	2.86	2.77	2.80	2.70	2.79	2.81
942	2.15	2.14	2.14	1.79	2.06	2.21	2.74	2.77	2.80	2.73	2.78	2.81
964	2.27	2.07	2.14	2.29	1.99	2.21	2.72	2.77	2.80	2.62	2.77	2.81
986	2.04	2.06	2.12	2.11	1.98	2.17	2.83	2.76	2.80	2.59	2.77	2.81
1008	2.23	2.06	2.09	2.18	1.93	2.15	2.78	2.76	2.78	2.58	2.75	2.81
1030	2.18	2.03	2.06	2.11	1.89	2.12	2.72	2.75	2.78	2.77	2.73	2.81
1052	2.08	2.00	2.06	2.12	1.99	2.18	2.69	2.74	2.77	2.59	2.76	2.80

	g(r) Second peak height, $g(r)_2$						g(r) Second peak position, r_2(Å)					
Temp (K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
898	1.16	1.17	1.18	1.20	1.18	1.18	4.93	5.10	5.13	5.09	5.08	5.01
920	1.22	1.20	1.17	1.18	1.18	1.17	5.11	5.14	5.13	5.02	5.08	5.09
942	1.23	1.19	1.17	1.20	1.17	1.18	5.05	5.10	5.12	4.91	5.08	5.08
964	1.20	1.14	1.17	1.09	1.17	1.16	5.33	5.10	5.12	5.05	5.08	5.09
986	1.36	1.18	1.16	1.33	1.17	1.15	5.07	5.08	5.12	5.01	5.09	5.11
1008	1.29	1.18	1.16	1.33	1.16	1.15	5.20	5.07	5.12	5.05	5.08	5.11
1030	1.16	1.18	1.16	1.27	1.16	1.17	5.19	5.10	5.12	5.13	5.09	5.03
1052	1.16	1.14	1.16	1.34	1.17	1.15	5.13	5.11	5.12	5.01	5.08	5.12

	Coordination number						Packing density					
Temp (K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
898	0.63	2.66	9.60	0.56	2.40	8.92	0.030	0.101	0.378	0.025	0.105	0.377
920	0.61	2.65	9.55	0.65	2.40	8.87	0.029	0.099	0.377	0.025	0.105	0.376
942	0.73	2.60	9.52	0.65	2.38	8.84	0.026	0.099	0.375	0.026	0.104	0.373
964	0.86	2.58	9.49	0.75	2.35	8.82	0.025	0.098	0.373	0.023	0.104	0.368
986	0.82	2.58	9.45	0.74	2.36	8.75	0.028	0.097	0.372	0.022	0.104	0.367
1008	0.71	2.52	9.40	0.72	2.32	8.72	0.027	0.097	0.368	0.021	0.103	0.359
1030	0.86	2.53	9.35	0.77	2.31	8.65	0.025	0.096	0.365	0.026	0.103	0.349
1052	0.60	2.51	9.31	0.73	2.34	8.70	0.024	0.095	0.364	0.021	0.103	0.361

Table B-3: The liquid structure information for partial pair correlations of Al-Al, Al-Si, Si-Si of Al-10%Si & Al-10%Si-0.04%Sr obtained from high energy diffraction experiments and RMC analysis (Sr in brackets represents the information for alloy with Strontium).

	g(r) First peak height, $g(r)_1$						g(r) First peak position, r_1(Å)					
Temp(K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
885	2.21	2.11	2.19	2.13	2.05	2.18	2.83	2.80	2.81	2.71	2.79	2.81
907	1.90	2.12	2.17	1.98	2.03	2.16	2.83	2.80	2.81	2.67	2.79	2.81
929	1.87	2.12	2.15	1.79	1.98	2.15	2.79	2.81	2.81	2.70	2.79	2.81
973	1.84	2.01	2.10	2.19	1.98	2.11	2.74	2.80	2.81	2.61	2.79	2.81
995	1.84	2.01	2.10	1.74	1.96	2.09	2.70	2.80	2.81	2.70	2.79	2.81
1017	1.79	1.99	2.09	1.85	1.96	2.06	2.75	2.80	2.81	2.68	2.78	2.81
1039	1.86	2.02	2.07	1.69	1.95	2.04	2.76	2.79	2.817	2.65	2.78	2.80

	g(r) Second peak height, $g(r)_2$						g(r) Second peak position, r_2(Å)					
Temp(K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
885	1.20	1.17	1.16	1.20	1.14	1.17	5.17	5.05	5.07	5.29	5.04	5.06
907	1.19	1.16	1.17	1.17	1.15	1.16	5.22	5.03	5.06	4.87	5.05	5.06
929	1.16	1.16	1.16	1.19	1.16	1.16	5.08	5.09	5.08	5.33	5.04	5.06
973	1.20	1.15	1.16	1.18	1.15	1.16	4.94	5.08	5.10	4.94	5.08	5.06
995	1.17	1.15	1.15	1.13	1.14	1.16	4.99	5.09	5.07	5.48	5.04	5.06
1017	1.16	1.17	1.15	1.16	1.15	1.15	4.98	5.08	5.08	5.02	5.04	5.06
1039	1.16	1.15	1.157	1.16	1.14	1.15	5.05	5.07	5.08	5.14	5.04	5.06

	Coordination number						Packing density					
Temp (K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
885	0.91	2.87	8.66	1.05	2.82	8.64	0.041	0.123	0.379	0.036	0.121	0.379
907	0.86	2.88	8.63	1.05	2.82	8.60	0.041	0.122	0.378	0.034	0.120	0.378
929	0.91	2.84	8.61	0.91	2.80	8.56	0.039	0.123	0.377	0.036	0.121	0.377
973	0.87	2.79	8.52	1.03	2.78	8.49	0.037	0.121	0.376	0.032	0.119	0.375
995	0.82	2.77	8.48	0.84	2.76	8.45	0.035	0.120	0.375	0.035	0.119	0.371
1017	0.89	2.77	8.43	0.77	2.74	8.41	0.037	0.120	0.374	0.034	0.117	0.370
1039	0.88	2.76	8.41	0.85	2.74	8.36	0.037	0.118	0.372	0.033	0.117	0.366

Table B-4: The liquid structure information for partial pair correlations of Al-Al, Al-Si, Si-Si of Al-12.5%Si & Al-12.5%Si-0.04%Sr obtained from high energy diffraction experiments and RMC analysis (Sr in brackets represents the information for alloy with Strontium).

	g(r) First peak height, $g(r)_1$						g(r) First peak position, r_1(Å)					
Temp K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
867	1.97	2.12	2.14	1.81	2.05	2.17	2.82	2.79	2.81	2.62	2.7	2.80
889	1.97	2.02	2.13	1.91	2.04	2.15	2.76	2.78	2.79	2.71	2.77	2.80
911	2.27	2.00	2.11	2.17	2.01	2.12	2.74	2.78	2.79	2.66	2.77	2.79
933	1.94	2.03	2.09	2.01	2.01	2.11	2.79	2.78	2.79	2.71	2.77	2.79
956	1.92	2.00	2.08	1.89	1.98	2.10	2.75	2.78	2.79	2.65	2.77	2.79
978	1.87	2.01	2.05	1.90	1.97	2.08	2.78	2.78	2.79	2.69	2.76	2.79
1000	1.85	1.98	2.04	1.99	1.95	2.10	2.77	2.78	2.79	2.66	2.76	2.79
1022	1.83	1.99	2.02	1.84	1.94	2.03	2.74	2.78	2.78	2.77	2.75	2.79
1065	1.80	1.93	1.98	1.95	1.92	1.98	2.76	2.78	2.78	2.62	2.74	2.78

	g(r) Second peak height, $g(r)_2$						g(r) Second peak position, r_2(Å)					
Temp (K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
867	1.15	1.15	1.17	1.15	1.14	1.16	5.07	5.06	5.03	4.96	5.07	5.07
889	1.11	1.15	1.16	1.14	1.15	1.16	5.06	5.05	5.02	4.99	5.07	5.06
911	1.17	1.15	1.16	1.18	1.15	1.15	5.05	5.04	5.02	5.24	5.07	5.05
933	1.16	1.15	1.16	1.14	1.14	1.15	4.92	5.04	5.02	4.83	5.06	5.04
956	1.14	1.14	1.15	1.09	1.14	1.15	5.14	5.03	5.02	5.06	5.05	5.04
978	1.14	1.14	1.15	1.13	1.14	1.14	5.11	5.02	5.01	5.06	5.04	5.03
1000	1.16	1.14	1.14	1.09	1.14	1.13	5.08	5.02	5.01	5.13	5.04	5.03
1022	1.15	1.14	1.14	1.14	1.13	1.13	5.10	5.02	5.01	5.07	5.03	5.03
1065	1.13	1.11	1.14	1.07	1.11	1.12	5.00	5.01	4.99	4.99	5.03	5.02

	Coordination number						Packing density					
Temp (K)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)	Si-Si	Al-Si	Al-Al	Si-Si(Sr)	Al-Si(Sr)	Al-Al(Sr)
867	1.15	3.16	8.53	1.13	3.10	8.39	0.05	0.134	0.367	0.041	0.132	0.366
889	1.15	3.15	8.49	1.1	3.09	8.35	0.04	0.132	0.366	0.044	0.131	0.365
911	1.21	3.13	8.46	1.18	3.08	8.31	0.04	0.132	0.365	0.043	0.130	0.364
933	1.15	3.11	8.43	1.14	3.07	8.28	0.04	0.131	0.364	0.045	0.129	0.363
956	1.13	3.12	8.39	1.11	3.04	8.21	0.04	0.130	0.363	0.042	0.129	0.362
978	1.16	3.10	8.35	1.14	3.05	8.22	0.04	0.130	0.361	0.044	0.128	0.361
1000	1.13	3.09	8.32	1.12	3.04	8.12	0.04	0.130	0.360	0.045	0.127	0.360
1022	1.13	3.08	8.29	1.11	3.00	8.06	0.04	0.129	0.359	0.048	0.126	0.358
1065	1.14	3.04	8.22	1.13	2.97	8.00	0.04	0.128	0.357	0.040	0.124	0.356

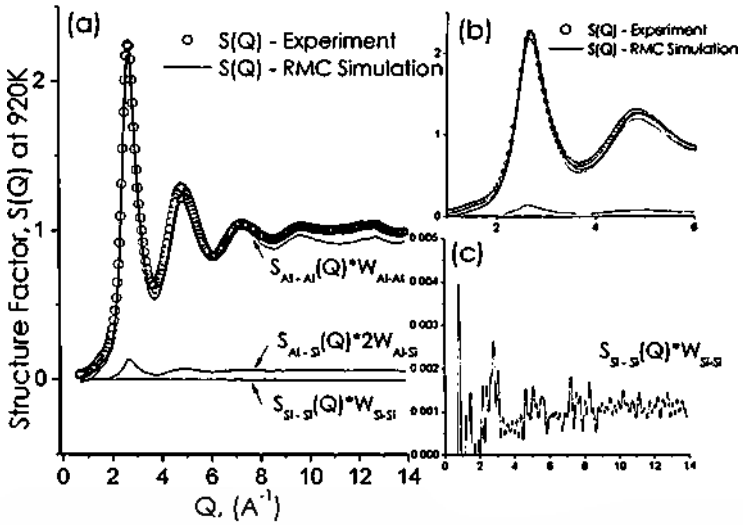


Figure B-1: **The variation of total and partial structure factors for Al-3wt%Si alloy at 920K. All three graphs have the same variables in the respective axes. (b) and (c) are magnified sections of (a) to show the first two peaks and the $S_{Si-Si}(Q)$, respectively.**

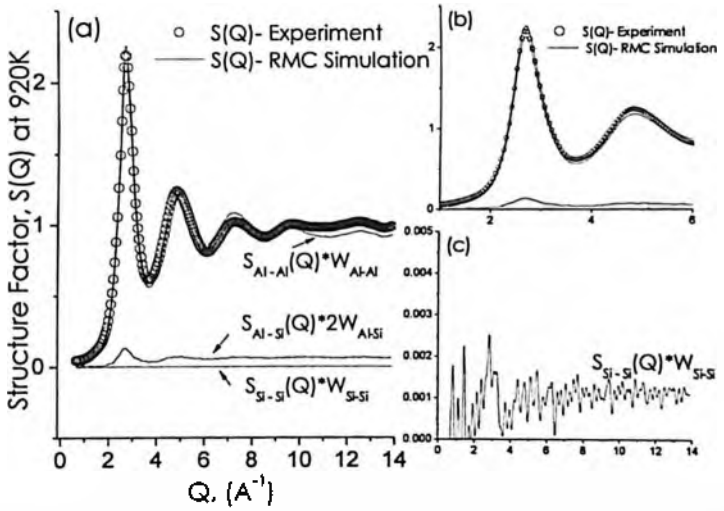


Figure B-2: **The variation of total and partial structure factors for Al-3wt%Si-0.04%Sr alloy at 920K. All three graphs have the same variables in the respective axes. (b) and (c) are magnified sections of (a) to show the first two peaks and the $S_{Si-Si}(Q)$, respectively.**

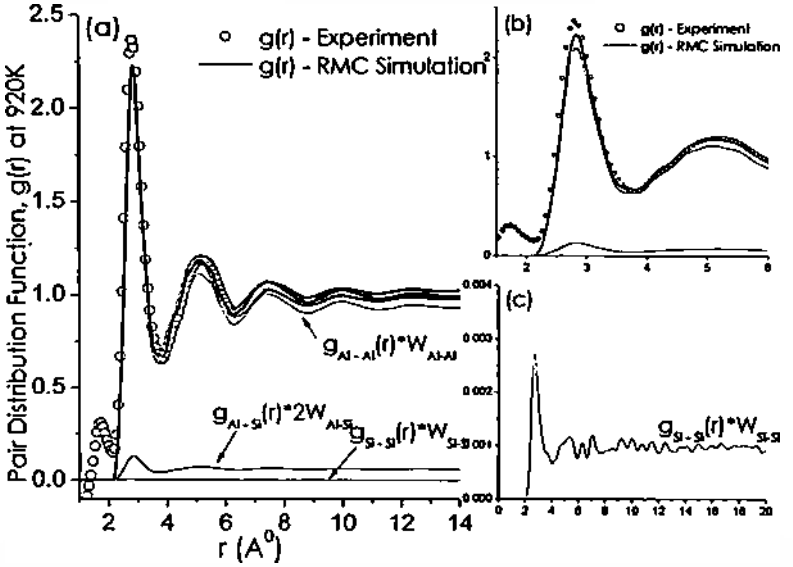


Figure B-3: **The variation of total and partial pair distribution functions with r, for Al-3wt%Si alloy at 920K. All three graphs have the same variables in the respective axes. (b) & (c) are magnified sections of (a) to show the first two peaks and the $g_{Si-Si}(r)$, respectively.**

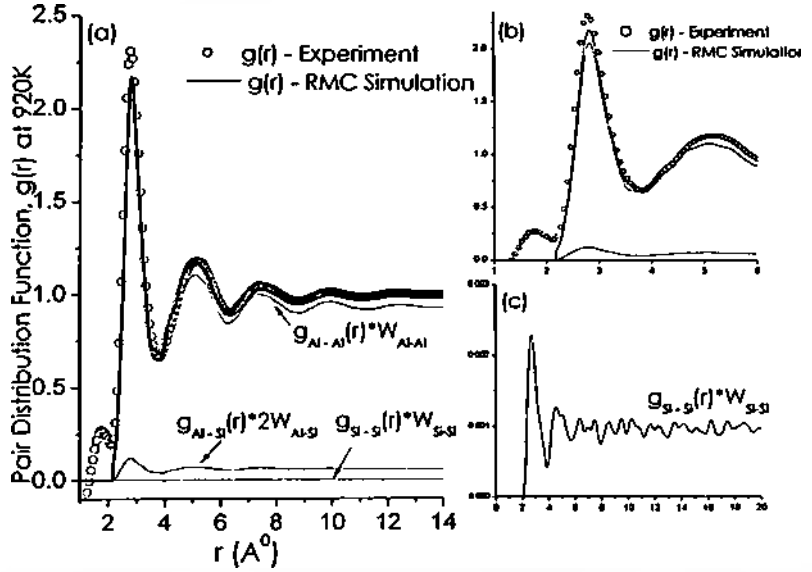


Figure B-4: **The variation of total and partial pair distribution functions with r, for Al-3wt%Si-0.04%Sr alloy at 942K. All three graphs have the same variables in the respective axes. (b) & (c) are magnified sections of (a) to show the first two peaks and the $g_{Si-Si}(r)$, respectively.**

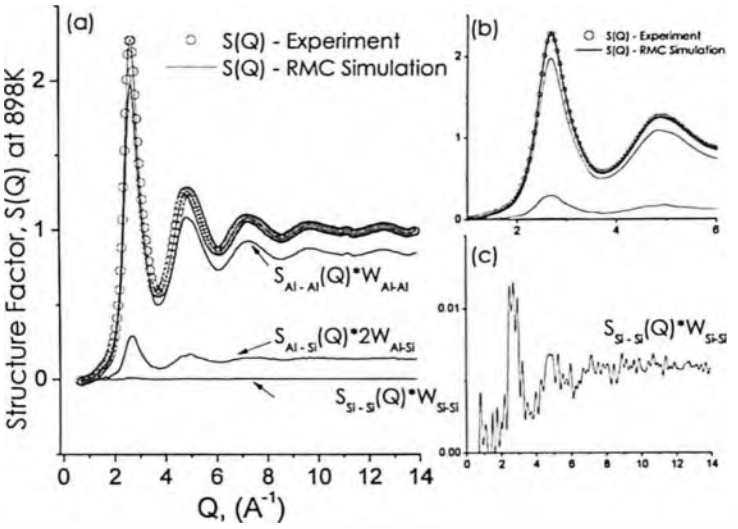


Figure B-5: **The variation of total and partial structure factors for Al-7wt%Si alloy at 898K. All three graphs have the same variables in the respective axes. (b) and (c) are magnified sections of (a) to show the first two peaks and the $S_{Si-Si}(Q)$, respectively.**

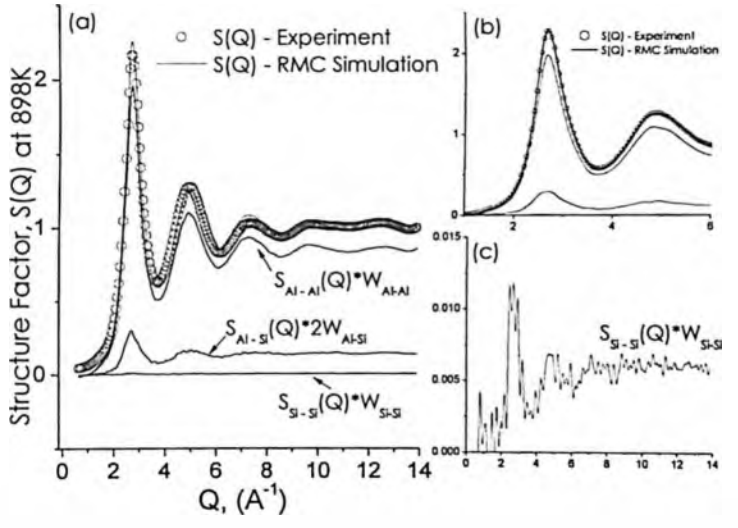


Figure B-6: **The variation of total and partial structure factors for Al-7wt%Si-0.04%Sr alloy at 898K. All three graphs have the same variables in the respective axes. (b) and (c) are magnified sections of (a) to show the first two peaks and the $S_{Si-Si}(Q)$, respectively.**

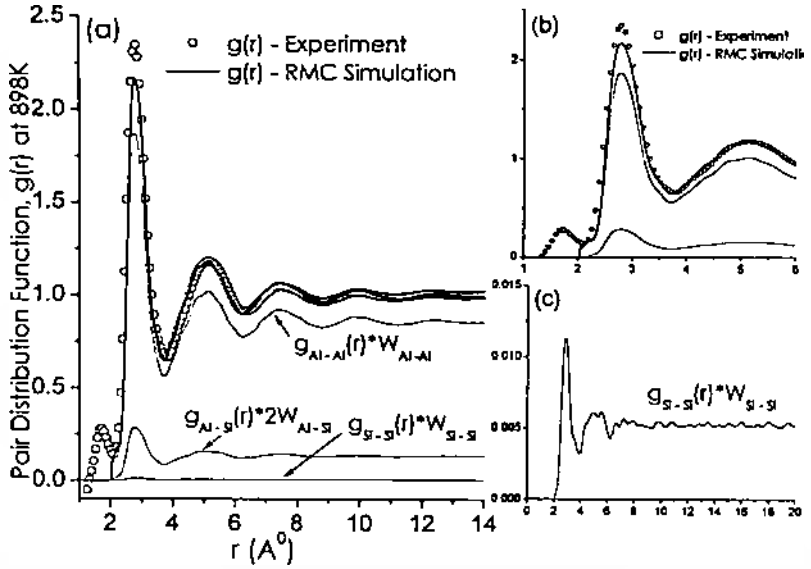


Figure B-7: **The variation of total and partial pair distribution functions with r, for Al-7wt%Si alloy at 898K. All three graphs have the same variables in the respective axes. (b) & (c) are magnified sections of (a) to show the first two peaks and the $g_{si-si}(r)$, respectively.**

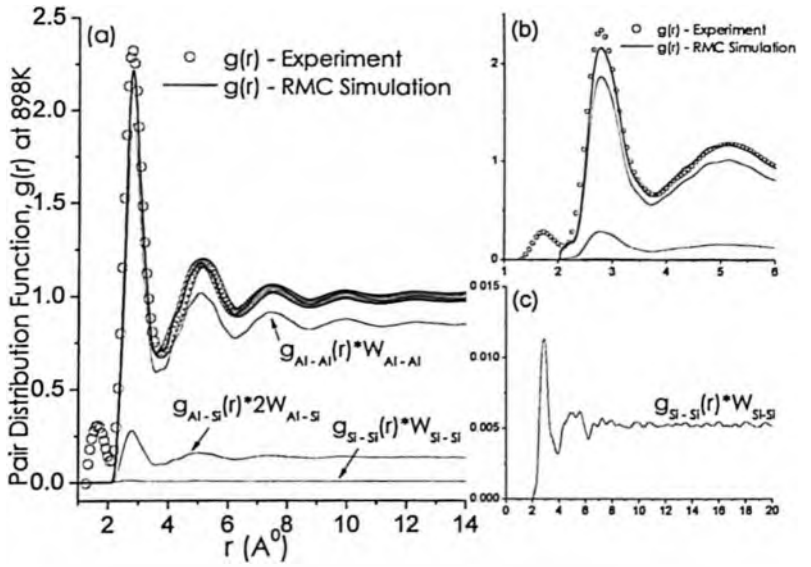


Figure B-8: **The variation of total and partial pair distribution functions with r, for Al-7wt%Si-0.04%Sr alloy at 867K. All three graphs have the same variables in the respective axes. (b) & (c) are magnified sections of (a) to show the first two peaks and the $g_{si-si}(r)$, respectively.**

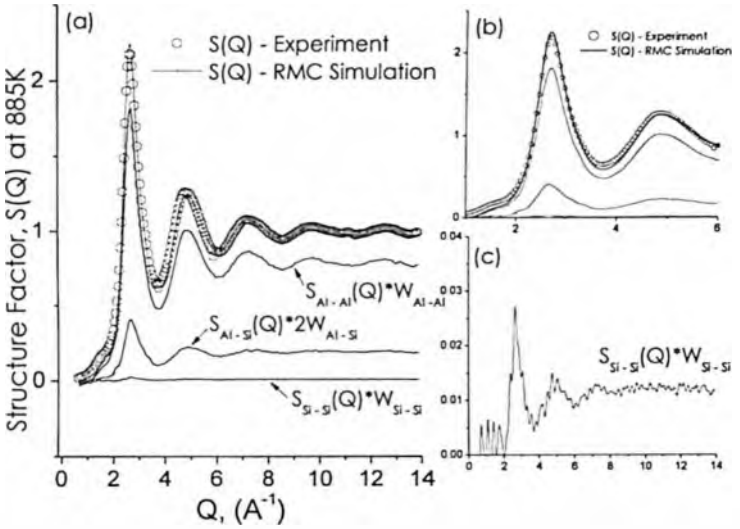


Figure B-9: **The variation of total and partial structure factors for Al-10wt%Si alloy at 885K. All three graphs have the same variables in the respective axes. (b) and (c) are magnified sections of (a) to show the first two peaks and the S $_{Si-Si}$(Q), respectively.**

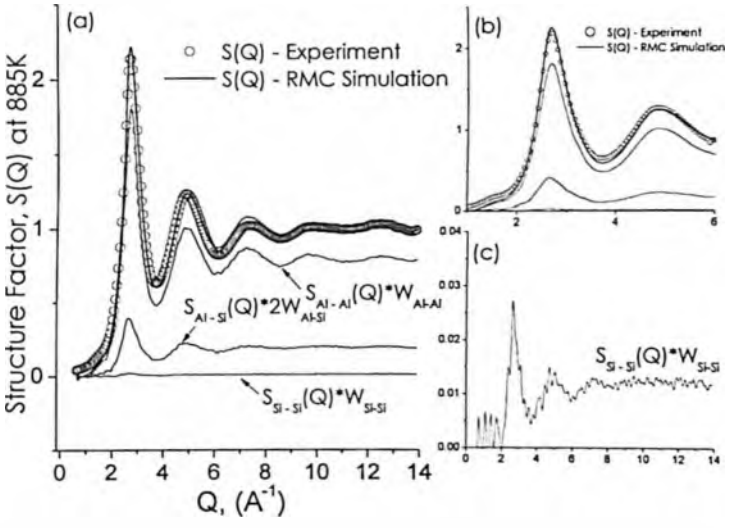


Figure B-10: **The variation of total and partial structure factors for Al-10wt%Si-0.04%Sr alloy at 885K. All three graphs have the same variables in the respective axes. (b) and (c) are magnified sections of (a) to show the first two peaks and the S $_{Si-Si}$(Q), respectively.**

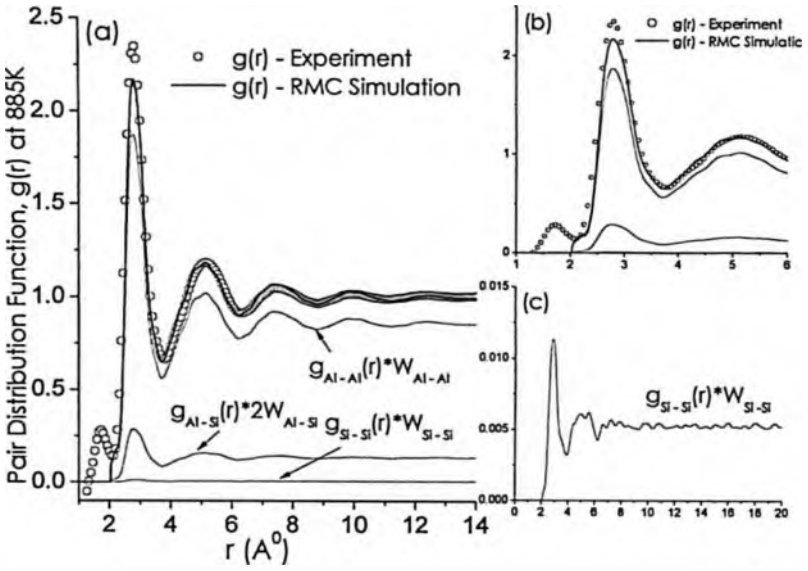


Figure B-11: **The variation of total and partial pair distribution functions with r, for Al-10wt%Si alloy at 885K. All three graphs have the same variables in the respective axes. (b) & (c) are magnified sections of (a) to show the first two peaks and the $g_{si-si}(r)$, respectively.**

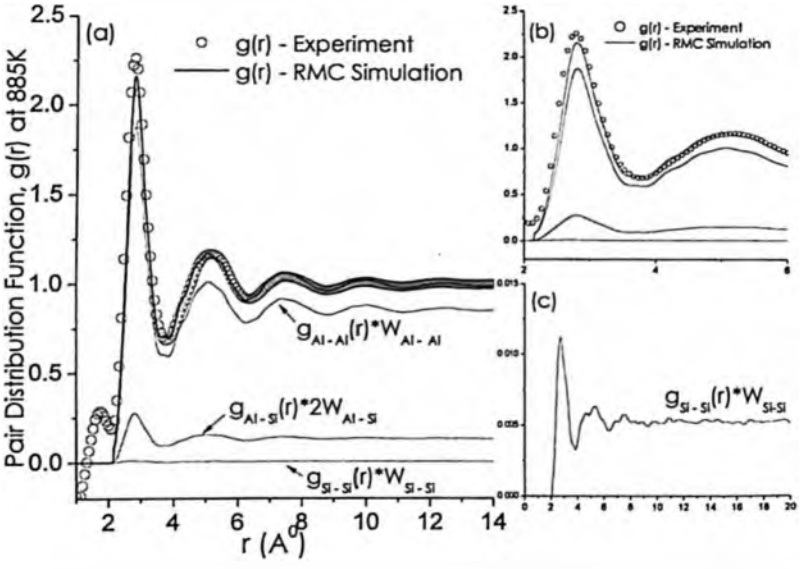


Figure B-12: **The variation of total and partial pair distribution functions with r, for Al-10wt%Si-0.04%Sr alloy at 885K. All three graphs have the same variables in the respective axes. (b) & (c) are magnified sections of (a) to show the first two peaks and the $g_{si-si}(r)$, respectively.**