INTRODUCING TEXTURE INTO ANISOTROPIC VBO TO MODEL THE
DEFORMATION OF ZIRCONIUM ALLOYS
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DEFORMATION OF ZIRCONIUM ALLOYS

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**TITLE:** Introducing texture into anisotropic VBO to model the deformation of Zirconium alloys

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Abstract

There is no unified phenomenological model available for Zr alloys that allows for the inclusion of a complete set of texture input parameters in order to describe the anisotropic behaviour during plastic deformation at different strain rates and thermal creep. This research shows how AVBO, an anisotropic version of VBO, can be enhanced by introducing single crystal based tensors to describe the material response to different Kearns factors, which uniquely describe the texture of a sample with two numbers only. It is demonstrated with the aid of published thermal creep test data that small tensile deformation behaviour of Zr-2.5Nb is consistent with predominant slip of Zr alloy crystals parallel to their single crystal α basal planes, supporting the strategy to model the behaviour of these HCP materials with a phenomenological constitutive model. It is demonstrated that the new version of AVBO, ATXVBO, predicts trends consistent with a slip mechanism parallel to the basal planes. Multi-objective optimization was employed successfully to determine the set of 67 constants. It is proven that the theory relies on a limited number of tests to perform optimization of all the unknown constants. Numerous validation and sensitivity evaluations were performed to test the optimized solutions despite the limited availability of plastic deformation test data with documented texture information. It is demonstrated that, in order to capture dynamic strain aging effects, different strategies will be required at different evaluation temperatures. It is also shown that although texture variation can be accommodated that different manufacturing routes each requires a unique optimized set of constants.
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List of Abbreviations, Symbols and Definitions

Some constants are defined in the text. Some of these symbols do not apply to the Appendices, where they are defined separately.

Abbreviations:

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<thead>
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<th>Definition</th>
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<tbody>
<tr>
<td>VBO</td>
<td>Viscoplastic theory Based on Overstress</td>
</tr>
<tr>
<td>AVBO</td>
<td>Anisotropic VBO</td>
</tr>
<tr>
<td>TVBO</td>
<td>Temperature dependent VBO</td>
</tr>
<tr>
<td>ATVBO</td>
<td>Temperature dependent AVBO</td>
</tr>
<tr>
<td>ATXVBO</td>
<td>Temperature and texture dependent AVBO for HCP materials</td>
</tr>
<tr>
<td>DSA</td>
<td>Dynamic Strain Aging</td>
</tr>
<tr>
<td>AET</td>
<td>Elastic Anisotropic Tensor Ratios</td>
</tr>
<tr>
<td>AIT</td>
<td>Inelastic Anisotropic Tensor Ratios employing Equation (A-55)</td>
</tr>
<tr>
<td>AIT, DSA</td>
<td>Inelastic Anisotropic Tensor Ratios employing Equation (A-53)</td>
</tr>
<tr>
<td>HCP</td>
<td>Hexagonally Close Packed</td>
</tr>
<tr>
<td>MOO</td>
<td>Multi-Objective Optimization</td>
</tr>
<tr>
<td>ODC</td>
<td>ODF Coefficients</td>
</tr>
<tr>
<td>ODE</td>
<td>Ordinary Differential Equation</td>
</tr>
<tr>
<td>ODF</td>
<td>Orientation Distribution Function</td>
</tr>
<tr>
<td>SLS</td>
<td>Standard Linear System</td>
</tr>
<tr>
<td>CW</td>
<td>Cold Work</td>
</tr>
</tbody>
</table>
Symbols\textsuperscript{1,2}:

\begin{align*}
A & \quad - \text{Isotropic stress} \\
A_f & \quad - \text{Final solution for } A_{c, A_{c}} \\
A_{c, A_{c}} & \quad - \text{Controls the speed at which the final solution } A_f \text{ is being approached} \\
A_o & \quad - \text{Constant in kinematic stress growth law of Majors} \\
B_0 & \quad - \text{Constant in kinematic stress growth law of Majors} \\
B^a, B^b, B^f & \quad - \text{Material polycrystal property tensors used with AVBO and ATXVBO, associated with the inelastic strain, equivalent stress and kinematic stress equations, respectively} \\
C, S & \quad - \text{Polycrystal stiffness and compliance tensor} \\
c^{sc}, s^{sc} & \quad - \text{Single crystal stiffness and compliance tensor} \\
d^{sc}, b^{sc} & \quad - \text{Equivalent generic single crystal inelastic stiffness and compliance tensor} \\
b^{sc}_e, b^{sc}_g, b^{sc}_f & \quad - \text{Equivalent single crystal inelastic material deformation tensors, associated with the inelastic strain, equivalent stress and kinematic stress equations (in crystal direction)} \\
d^{sc}_e, d^{sc}_g, d^{sc}_f & \quad - \text{Equivalent single crystal inelastic material deformation tensors, associated with the inelastic strain, equivalent stress and kinematic stress equations (in crystal direction)} \\
c & \quad - \text{Constant in equilibrium stress growth law of Majors (c approaches E)} \\
c^{sc(m)}_{ij} & \quad - \text{Single crystal stiffness tensor component coefficients} \\
d^{sc(m)}_{ij} & \quad - \text{Generic single crystal inelastic tensor component coefficients inelastic strain, equivalent stress and kinematic stress equations} \\
d^{sc(m)}_{ij}, d^{sc(m)}_{ij}, d^{sc(m)}_{ij} & \quad - \text{Single crystal inelastic tensor component coefficients}
\end{align*}

\textsuperscript{1} Some explanations of concepts use symbols only applicable to that discussion and are not listed here.

\textsuperscript{2} A bold symbol denotes a matrix or tensor.
E - Young’s modulus

Cᵣ, Cᵦ - Texture coefficients

E₁ E₂ - Spring stiffness in SLS

E₁, E₂, E₃, ν₁₃, ν₂₃, ν₂₁, G₂₃, G₃₁ and G₁₂ - Anisotropic elastic moduli, Poisson’s ratios and shear moduli

Eᵣ - Inelastic tangent modulus

e = εᵢⱼ - True strain

γᵢⱼ - Engineering shear strain (εᵢⱼ = ½γᵢⱼ)

ė - Deviatoric strain

f - Kinematic stress

fᵣ, fᵦ, fᵢ - Kearns factors in the radial (or thickness), transverse and longitudinal (or axial or rolling) directions

Fₚₗ - Fitness, plastic deformation

Fₖᵦ - Fitness, creep

G - Equilibrium stress

Γ - σᵣ - gᵣ or σ - g based effective overstress

Θ - gᵣ - fᵣ or g - f based effective stress

ɡᵣᵢ - g based effective stress

G¹⁺ - Constant in isotropic stress of Majors

H - Rate sensitivity coefficient used to capture DSA

Z - Dashpot constant in SLS

H - Deformation history modified accumulated inelastic strain

λ - λ = hp - η allows history dependent softening
\( \mathbf{I} \) - Identity tensor

\( k[\Gamma] \) - Viscosity function \((\bar{k}[\Gamma] = k[\Gamma]/E \text{ or } \bar{k}[\Gamma] = k[\Gamma]/E_1)\)

\( k_1 \text{ to } k_5 \) - Viscosity function constants

\( k_1^{(\cdot)} \text{ to } k_3^{(\cdot)} \)

\( \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3 \) - Representation directional matrices

\( \psi[\Gamma] \) - Shape function \((\bar{\psi}[\Gamma] = \psi[\Gamma]/E \text{ or } \bar{\psi}[\Gamma] = \psi[\Gamma]/E_1)\)

\( \psi_1 \text{ to } \psi_3 \) - Shape function constants

\( \psi_1^{(\cdot)} \text{ to } \psi_3^{(\cdot)} \)

\( \varphi[\Gamma] \) - Adjusted normalized shape function

\( \dot{\xi} \) - Combined inelastic strain rate

\( \nu \) - Poisson’s ratio

\( \mathbf{o}^d \) - Deviatoric overstress \(= \sigma^d - \mathbf{g}^d\)

\( \mathbf{o} \) - Overstress \(= \sigma - \mathbf{g}\)

\( P_1 \) - AVBO equivalent of \(E_t\) in VBO

\( P \) - Coefficient of anisotropy for uniaxial specimen tested in the transverse direction

\( \text{Accumulated effective inelastic strain,} \)

\( \dot{p} = \frac{2}{3} \mathbf{e}^{\text{in}} \cdot \mathbf{e}^{\text{in}} = \Gamma/E \bar{k}[\Gamma] \)

\( R \) - Coefficient of anisotropy for uniaxial specimen tested in the rolling (longitudinal) direction

\( RG_1 \text{ to } RG_3 \) - Constants in recovery function \(R[g_{\text{eff}}]\)

\( RA_1 \text{ to } RA_3 \) - Constants in softening function \(R_1[\eta]\)

\( \sigma \text{ and } \sigma^d \) - True stress and deviatoric stress tensors
T - Temperature

\( S, B^e, D^g \) and \( D^f \) - Generator coefficient functions of polycrystal material property matrices

\( W_{000}, W_{200}, W_{220}, W_{400}, W_{420}, W_{440} \) - Six ODCs required for HCP material ODF

\( W_2 \) - \( W_{200}, W_{220} \)

\( \tilde{m} \) - “Without”

Brackets:

[ ] Square brackets denote “a function of”

Function dependency on strain and its rate, stress and its rate, equilibrium stress and its rate, kinematic stress and its rate as well as isotropic stress and its rate is not indicated in brackets. The functional dependency is either shown for the variables of a function as shown, or, as a function of the basic variables of the function and its associated imbedded functions. For the latter case, the possible variables are \( T, f_R \) and \( f_T \).

\{ \} Curly brackets denote “the asymptote of”

Arrow brackets denote “the volume average of”, obtained for a tensor \( Z \) from

\[ \langle Z \rangle = \langle Z_{ij}[\alpha, \beta] \rangle = \frac{1}{V} \int_{0}^{\pi/2} \int_{0}^{2\pi} Z_{ij}(\alpha, \beta) \cdot l(\alpha, \beta) \sin \alpha \, d\beta \, d\alpha \]
Superscripts:

- \(d\) - Deviatoric
- \(el\) - Elastic
- \(in\) - Inelastic
- \(sc\) - Single crystal
- \(\epsilon, g, f\) - Distinguish between inelastic tensors \(D^\epsilon, D^g, D^f\).

- \(R, V, H\) - Reuss, Voigt and Hill polycrystal approximations
- \(\cdot\) - Rate
- \(-\) - Normalized by \(E\) or \(E_1\)
- \(\cdot\) - Transformed from single crystal to polycrystal directions

Subscripts:

- \(R, T, L\) - Directions:
  - For tube: \(R\)-Radial, \(T\)-Tangential, \(L\)-Longitudinal
  - For plate: \(R\)-Thickness, \(T\)-Transverse, \(L\)-Length (Rolling direction)

Key definitions:

- \(c\)-axes - HCP crystal basal plane normal
- Kearns factors - Widely accepted method to characterize texture of Zr-alloys. See Appendix C for its definition and principles of derivation.
- Optimization - Constants are determined by minimizing residuals between measured and predicted results
- Material preferred directions - Directions that coincide with the material symmetry planes (Sütçü M., 1992)
**Declaration of Academic Achievement**

A unified phenomenological theory ATXVBO has been established that can predict the deformation of HCP materials, including Zr alloys, that can account for texture variation. The anisotropic phenomenological model selected as basis for this work, AVBO, does not permit texture as input variable. A set of optimized constants would be required for every state of material texture, which is not practical, considering the specimen to specimen variation observed for Zr alloys. Only limited texture variation is accounted for in other anisotropic unified theories. The complete texture is introduced here as input parameter.

A method is available in literature to determine elastic polycrystal properties for HCP materials from single crystal properties and the Kearns factors, used to describe texture. This research postulates that the inelastic polycrystalline properties can be derived analogously to the elastic properties. As a result of this proposed theory, it is no longer required to determine polycrystalline properties by optimization for each texture state: It is only necessary to determine the single crystal properties which are then used in conjunction with the Kearns factors to obtain the polycrystal properties for any texture state.

This study also established by evaluation of published test data that the small tensile deformation of Zr-2.5Nb can be explained by slip parallel to the basal planes of the $\alpha$-Zr HCP material. That conclusion supports the use of a phenomenological constitutive equation that do not account for twinning. Twinning is associated with compressive strains of Zr alloys, and recommendations are made on addressing it with ATXVBO.
It is also demonstrated that texture is the most suitable input variable, confirming its correlation with the key manufacturing aspects associated with the fabrication of Zr-2.5Nb, namely ingot melting practice, grain size, extrusion temperature and extrusion ratio. It is also established that separate optimization of constants is required for each combination of these manufacturing aspects.
CHAPTER 1. INTRODUCTION

HCP materials like Zr are anisotropic, exhibiting orientation-sensitive elastic and inelastic deformation when loaded. Inelastic deformation occurs either when the material exceeds its elastic strength limits, or when it creeps while in an elastic or plastic stress state. Plastic deformation and creep can be modelled separately or with a unified model. Either self-consistent crystal-based or phenomenological unified models are employed, or, other models with traits of both. A further distinction in these models is whether the separation between elastic and plastic material states requires knowledge of the material’s yield surface or not.

Zr alloys are extensively used in the nuclear industry, where it is a major undertaking to obtain deformation results of in-reactor components with limited strain measurement capability. It is well documented how the properties and deformation of a Zr alloy are influenced by its composition and manufacturing.

It is desired to model a Zr alloy with a unified phenomenological model that reflects its distinct HCP crystallography with no knowledge required of its yield properties. It also has to reflect the temperature-sensitive behaviour of the material. The target application is the prediction of small deformation of material with limited, difficult-to-obtain, measurement data available for benchmarking. The ultimate goal is for the model to predict plastic deformation as well as both thermal and irradiation creep. However, this study only treats thermal creep of Zr-2.5Nb with recommendations on the incorporation of irradiation creep and growth.
Apart from not explicitly capturing the orientation dependence in its variables, AVBO is one phenomenological anisotropic model that would meet these requirements. AVBO is a derivative of VBO, an overstress based theory pioneered by Krempl (1995). This research incorporates the texture of an HCP material as input variable into AVBO. Temperature is also considered as an input variable. Both texture and temperature are not treated as time-variables. The derived variant, ATXVBO, is validated against suitable test results available in literature for Zr alloys.

The objectives are provided in Chapter 2. Chapter 3 provides an overview of the manufacturing and deformation of Zr alloys, with specific attention to the relations between its texture and its material characteristics and deformation. Chapter 4 provides an overview of the selected theory, showing how the calculation of elastic polycrystal material properties from single crystal properties and Kearns factors serves as inspiration to derive anisotropic polycrystal material properties, the main contribution of this research. Chapter 5 explains how the constants for ATXVBO are obtained through optimization with a genetic algorithm and Chapter 6 demonstrates how the values obtained with ATXVBO using the optimized constants are validated against other experimental datasets. Chapter 7 investigates the sensitivity of the model to manufacturing variables, justifying the selection of texture as single input variable as well as ATXVBO’s ability to predict Poisson contraction and loading in arbitrary directions. Chapter 8 summarizes the conclusions, list the assumptions with their validations and show how the objectives were met. Chapter 9 provides recommendations for further work.
The following unique contributions are made by this study:

1) Identify texture as a single entity that can be used to characterise the material anisotropy of Zr-2.5Nb in a phenomenological model. It is demonstrated that texture does not capture the effects of grain size, extrusion temperature, extrusion ratio and cold work amount and that each manufacturing route combination requires its own set of constants.

2) Introduce texture as input parameter into AVBO: A set of elastic and inelastic anisotropic polycrystal material properties are required for every texture state of a material with AVBO. One way is to average these properties for various samples with different textures. For Zr alloys the variations in texture are significant and it could lead to unacceptable variations in predictions. A unique set of constants would be required for every state of texture to address that inaccuracy. A method is available in literature to determine elastic polycrystal properties for HCP materials from single crystal properties and the Kearns factors, which are used to describe HCP material texture. This study postulates that the inelastic polycrystalline properties can be derived in a manner similar to that used to determine the elastic properties. As a result of this theory, it is no longer required to determine polycrystalline properties for each state of texture: It is only necessary to determine the single crystal properties defined in this study which are then used in conjunction with the Kearns factors to obtain all the polycrystal properties.

3) Demonstrate the feasibility of determining 67 ATXVBO constants with limited experimental data: It is proven and demonstrated through both theoretical and
validation avenues that the constants can be determined from only a few experimental datasets, an attractive attribute when data for benchmarking is limited.

4) Demonstrate the need to employ inelastic anisotropy ratios in AVBO to describe anisotropic behaviour of Zr-2.5Nb: Sütçü and Krempl (1990) introduced a simplifying assumption that the elastic anisotropy ratios can be applied instead of inelastic ratios for AVBO. It is demonstrated here that their assumption is not valid for Zr-2.5Nb material.

Benefits and potential applications of the model:

1) Optimization of constants need not be performed for every state of material texture. ATXVBO eliminates the need for multiple optimization runs or having to apply sample to sample texture variation uncertainty bands on predictions to account for texture variation if an averaging strategy were to be followed.

2) ATXVBO could be applied to any HCP material, although validation of applicability will be required.

3) The methodology developed to determine polycrystal properties from postulated inelastic single crystal tensors could be applied to other phenomenological models to introduce texture as input variable.

4) ATXVBO lends itself well to applications where variety in measurement opportunities is limited.

5) Provided that irradiation deformation can be successfully introduced, ATXVBO could be extended to predict in-reactor deformation.
CHAPTER 2. OBJECTIVES

1) Select an anisotropic unified model that does not rely on an assumed yield surface.

2) Establish if material anisotropy can be characterised by texture only for modeling at a given constant temperature.

3) Demonstrate that the small tensile deformation of Zr-2.5Nb can be described by predominant slip parallel to basal planes.

4) Introduce the capability to predict inelastic deformation at any constant temperature and non-evolving texture into small deformation AVBO.

5) The theory has to model plastic deformation and thermal creep mechanisms, but in a manner that will allow future modeling of irradiation effects.

6) Limit the number of constants required: It is inevitable that the introduction of texture and temperature as input parameters will require many constants.

7) Derive a strategy to obtain numeric values of the constants from limited experimental data. This approach may prove to be invaluable considering the limited amount of deformation data available for in-reactor components (if this method were to be expanded to include irradiation effects).

8) Investigate the ability of the model to successfully predict deformation if variation in chemical composition, grain size, extrusion temperature and extrusion ratio as well as the amount of cold work done on the material during its manufacturing is introduced.

Section 8.3 summarizes how the objectives have been met in this study.
CHAPTER 3.  TEXTURE AS INPUT PARAMETER FOR
PHENOMENOLOGICAL DEFORMATION PREDICTIONS OF Zr-2.5Nb

It needs to be established whether texture can be used as single input parameter to
describe the anisotropy of a Zr alloy. There are other manufacturing driven material
aspects to consider as well, and it is necessary to understand their relationships with
texture. Section 3.1 provides an overview of the steps in the manufacturing of Zr-2.5Nb
pressure tubes. Section 3.2 establishes how texture is described most often for these
alloys and in this study. Section 3.3 demonstrates the relationships between texture and
material properties. Section 3.4 shows that the experimental Zr alloy deformation data
considered in this study exhibit predominant slip parallel to the basal planes, in support of
the use of a phenomenological model that does not distinguish between slip and twinning
mechanisms.

3.1 Manufacturing of Zr-2.5Nb pressure tubes

The steps for manufacturing Zr-2.5Nb pressure tubes are summarized by Holt and
Aldridge (1985) and Li (2009):

1) Sponge Zr and master alloys are formed into ingots with a diameter of 590 mm by
double arc melting (Holt & Aldridge, 1985) or quadruple melting (Li W., 2009).

2) The ingots are press forged into polygons, 360 mm wide, at 1015°C.

3) The polygons are preheated to 800°C and rotary forged to round logs with a diameter
   of 210 mm.

4) The logs are machined to hollow billets.
5) The billets are heated to 952°C and cooled either by quenching or slow cooling from the \( \beta \)-phase (Holt & Aldridge, 1985). Quenching results in a fine microstructure.

6) The hollow billets are then extruded. Extrusion of Zr-2.5Nb is normally done in the \( \alpha+\beta \) phase, which extends from 597 - 897°C. It is typically performed at 815°C (Holt & Aldridge, 1985). Specimens prepared by Li (2009) for thermal creep experiments were extruded at either 650°C, 700°C, 815°C or 975°C. These tubes were also subjected to different extrusion ratios, 12:1 (fuel sheath material, identified as FS), 10:1 (typical) or 4:1.

7) Cold work is then performed, typically between 25 and 30% or even as high as 70% as for some of Li’s capsules.

8) The material is then stress relieved at 400°C for 24 hours.

The data of Li (2009) is evaluated in detail in Appendix G\(^3\) to define datasets for subsequent ATXVBO optimization and validation purposes. Texture is believed to be established during the extrusion phase and not during the subsequent cold drawing (Holt & Aldridge, 1985).

3.2 The use of Kearns factors to describe texture

Texture, the crystallographic orientation in a polycrystal, is most often described for Zr alloys with the Kearns factors \( f_R \), \( f_T \) and \( f_L \) that are defined in Section C.1 and presented pictorially in Figure 1. Texture is also described with Orientation Distribution Coefficients (ODCs). The ODCs are the coefficients of an Orientation Distribution...

\(^3\) The various samples are compared in Table G-8.
Function (ODF) that expresses the texture as a spherical harmonic expansion, also explained in Section C.1. An ODF converts the area representation of the texture obtained as a set of pole figures into a spatial representation of texture. Six ODCs, \( W_{000} \), \( W_{200} \), \( W_{400} \), \( W_{420} \) and \( W_{440} \), fully describe an HCP material’s texture. The definition of the Kearns factors represent the effective fraction of HCP basal plane normals (c-axes) that are oriented in the radial (\( f_R \)), transverse (\( f_T \)) and longitudinal (\( f_L \)) directions. Also, since \( f_R + f_T + f_L = 1 \), the texture is described by only two of the factors. The published texture of Zr alloys is most often provided as two Kearns factors as opposed to five ODCs, with \( W_{000} \) a constant. The relationships between them are provided in Equation (1) (Anderson, Thompson, & Cook, 1999), showing that the Kearns factors are related to the zero and second order ODCs, ignoring the higher order ODCs, \( W_{400} \), \( W_{420} \) and \( W_{440} \).

\[
\begin{align*}
W_{000} &= \frac{1}{4\pi^2 \sqrt{2}} \\
W_{200} &= \frac{\sqrt{10}}{16\pi^2} (3f_L - 1) \\
W_{220} &= \frac{\sqrt{15}}{16\pi^2} (f_R - f_T)
\end{align*}
\] (1)
Figure 1  Orientation of HCP crystals in tube and plate samples and illustration of Kearns factor values.
3.3 Justification for selecting texture as input variable

To capture material anisotropy, the material parameters considered to be used as input are to be established. If it can be shown that the key manufacturing aspects are correlated with texture, the theory could be simplified substantially by introduction of texture dependence only. Differences in texture are expected as a result of the amount of diameter and thickness reduction when tubes are extruded or plate is rolled (Tenckhoff, 1988). Texture variation is also expected from differences in material composition, the ingot melting practice, grain size, extrusion temperature and extrusion ratio (Holt & Aldridge, 1985). It is demonstrated below that sufficient correlation exists between texture and the other stated manufacturing aspects to introduce texture as the only representative input variable for Zr-2.5Nb, thus meeting Objective 2) in Chapter 2. The data supporting the arguments presented below are compiled in Appendix G.

3.3.1 Variation in texture

Significant variation is observed for tubes even when manufactured in the same manner. Figure 2\textsuperscript{4} shows the variation for tube material extruded at 812 - 815°C at a ratio of 10:1. Texture data reported by Christodoulou et al. (2000) and Li (2009) used for optimization (Section 5.2) as well as texture information from Holt and Aldridge (1985) and Bickel and Griffiths (2008) are compared to quantify texture variability.

\textsuperscript{4} Repetition of Figure G-1.
The texture ranges are obtained from the graphs that depict a number of trends associated with the in-reactor performance of Zr-2.5Nb material. Sample sizes as high as 87 were reported. Only values of $f_R$ were provided as it showed the best or strongest correlation with in-reactor elongation. E through AA denote different series of tubes.

The texture was provided for 25 regular tubes as well as a value for mini tubes and plate material. It is assumed that the texture reported for the plate and mini tubes are also average values for multiple specimens as reported for Tube D. AC and D in the legend denote the tubes.

Only texture data obtained for an extrusion temperature of 812°C were used in this comparison. The sample sizes are small.

The cylinders for the the creep capsules were cut from a number of mini tubes, either from the front or back. The texture of the front and back ends of the mini tubes were reported.

Figure 2. Comparison of texture values of samples with billets that were either $\beta$-quenched or slow-cooled in the $\beta$-phase and extruded at 812 - 815°C at a ratio of 10:1.
The largest reported texture values for the data are $f_R=0.445$, $f_T=0.64$ and $f_L=0.088$. The minimum values are $f_R=0.200$, $f_T=0.523$ and $f_L=0.040$. The biggest variation for a series or tubes extruded at the same conditions is $\Delta f_R = 0.245$ for the double-melted Series E tubes (Bickel & Griffiths, 2008) for a sample size of 59 tubes. $f_T$ and $f_L$ were not reported by them. The biggest variation $\Delta f_T$ and $\Delta f_L$ is 0.092 and 0.045, respectively. Both of these are for Tubes A to C (Christodoulou, Turner, Ho, Chow, & Resta Levi, 2000) with a sample size of only 3.

### 3.3.2 Correlations between texture and manufacturing aspects

Texture as well as grain size, grain shape, dislocation density, impurity concentrations and heat treatment affect the inelastic deformation of Zr alloys (Lucas & Pelloux, 1981) (Bickel & Griffiths, 2008). Holt and Aldridge (1985) observed correlations between texture and extrusion ratio as well as temperature: A higher extrusion ratio was found to results in a decreasing $f_R/f_T$ (i.e. increasing $f_T-f_R$) and decreasing $f_L$. A higher extrusion temperature resulted in a higher $f_L$. They observed that a change to the grain size did not affect $f_T$. They also found that the front end of the extruded tubes had a smaller value of $f_R/f_T$ than the back ends, the result of a temperature decrease as extrusion progresses.

The ingots of the specimens used by Holt and Aldridge were made from material produced from double melted ingots (Section 3.11) while the specimens used by Li (2009) included quadruple melted material and significant differences in impurity

---

$^5 f_T-f_R$ represents the variation of the c-axes in the radial-transverse plane for extruded tube. Irradiation creep and growth are correlated with $f_T-f_R$ (Holt, Christodoulou, & Causey, 2003).
content. It requires confirmation whether the observations regarding texture dependency observed by Holt and Aldridge summarized in the previous paragraph still hold for the quadruple melted and lower impurity material. The texture data from both Holt and Aldridge (1985) and Li (2009) are compared in Appendix G, where it is shown that the trends regarding texture sensitivity to material grain size, extrusion temperature and extrusion ratio also apply to the material produced later, but the texture values at similar material manufacturing conditions do differ.

### 3.3.3 Texture evolution and texture-temperature dependency

Ballinger, Lucas, & Pelloux (1984) showed that the texture of Zircaloy plate does not evolve significantly in small deformation tensile tests carried out in the rolling and transverse directions. They showed a noticeable reorientation of c-axes during compressive testing.

Texture evolution is not expected when the application of interest is internally pressurized tubes 1) subjected to tensile creep while in an elastic state as well as 2) subjected to tension/compression cycles while in the elastic range and 3) subjected to plastic deformation in a tensile state.

---

6 Table G-9
7 Section G.1 and Table G-1 to Table G-3
8 The trends with respect to texture observed by Holt and Aldridge are not found to hold true for the Li material that received 70% cold work: See Section G.1.5.
9 There are a few uncertainties with these results: The specimens used by Ballinger et al. were cut from 12.7 mm thick plate. They had observed significant through-thickness and through-width texture variation. Tensile specimens had a $4.76 \times 4.76$ mm cross section, while compression samples had a 6.35 mm diameter. It is not stated if all samples were cut from the plate at similar depth and/or width locations. Texture of each sample was not obtained before the testing and it was assumed that texture from one sample was representative of the texture of all tested samples before testing.
Ballinger et al. also observed a nonlinear evolution of the ratio of the strain components in the non-test directions (changes to strain ratio R) when a change of texture was not observed. They attributed that observation to different hardening characteristics of the material in tension and compression.

Since their observations on tensile behaviour did not show texture evolution in tension for tests up to at least 10% strain, a small deformation model should suffice in that strange range for tensile strains. The plastic deformation experimental data of Christodoulou et al. (2000) being used for optimizing constants (Figure G-18) extend to 5% strain. The creep test data of Li (2009) used in this research extends to about 10% (Figure G-24). Therefore, texture evolution is not expected to be a concern with the tensile test results applied here. If the application of interest involves compressive plastic strain, the possible implications of texture evolution may require further attention. The non-evolution of texture observed during small deformation tensile testing of Zircaloy leads to Assumption 4) in Section 8.2 regarding the selection of a small deformation model. It also leads to Assumption 5) that the texture does not evolve. The tests of Ballinger et al. showed strong repeatability of texture at 25°C and 350°C, leading to Assumption 6) that texture is independent of temperature.

3.3.4 Texture sensitivity observed in experimental deformation results of Zr-2.5Nb specimens

Plastic deformation and thermal creep results for Zr-2.5Nb were collected and evaluated for suitability for ATXVBO optimization in Section 5.2. Although ample plastic deformation data is available for HCP materials, prospective test results with
associated texture were found to be very limited. However, sufficient data for both plastic deformation and thermal creep deformation with texture at different temperatures were found to exist for Zr-2.5Nb to evaluate ATXVBO, although it is recommended in Chapter 9 that more tests be conducted. Some data for Zircaloy is also included in Chapter 7 for reference and validation purposes.

3.3.4.1 Plastic deformation of Zr-2.5Nb

Christodoulou et al. (2000) demonstrated the significance of anisotropy on the plastic deformation of Zr-2.5Nb for tensile and torsion test specimens for a variety of test temperatures\(^{10}\). Tensile test results for tube and plate specimens are shown in Figure 3\(^{11}\).
Figure 3. Engineering stress versus strain at different temperatures, textures and strain rates for Zr-2.5Nb tested in the axial and transverse directions (Christodoulou, Turner, Ho, Chow, & Resta Levi, 2000).
Although the texture was reported, it was not associated uniquely with each test specimen prepared from tube or plate material\textsuperscript{12}, thereby limiting the usability of this data for optimization of model constants. Also, it cannot be deducted from Christodoulou et al. (2000) if the material used to produce the test samples were prepared from billets that were $\beta$-quenched or slow-cooled. The extrusion ratio was not reported either. It is effectively assumed that the samples were made from slow-cooled billets and that a 10:1 extrusion ratio was applied, by grouping them as Dataset G11 in Section 5.2 with creep samples prepared that way.

3.3.4.2 Thermal creep of Zircaloy and Zr-2.5Nb, showing DSA

Lucas and Pelloux (1981) determined that the thermal creep strain of Zircaloy-2 is quite sensitive to the original texture and the material heat treatment. They observed transitions in creep rate behaviour at a certain time during the tests, which they attributed to strain aging.

Christodoulou et al. (2002) observed differences in creep rate of Zr-2.5Nb samples of similar texture\textsuperscript{13} and dislocation density and subjected to similar conditions\textsuperscript{14}. They attributed their observations to Dynamic Strain Aging (DSA)\textsuperscript{15}. This phenomenon is well

\textsuperscript{12} The apparent drop in true stress values is ascribed to uncertainty introduced with digitization of engineering stress and strain values from Christodoulou et al.

\textsuperscript{13} Only one texture value is given and variation between samples is not stated. It is evident from Figure G-1 that there is significant texture variation between Zr-2.5Nb samples, and it is shown in Appendix G.1 how manufacturing variance is correlated with texture.

\textsuperscript{14} Shown in Figure G-22

\textsuperscript{15} Dislocation interaction with solute atoms diffusing (temperature dependent) through the material are believed to cause DSA (Dynamic Strain Aging), as different impurity concentrations and distributions would result in differences in diffusion rates.
documented for Zr-alloys, e.g., Lucas & Pelloux (1981). However, there is uncertainty if the difference observed by Christodoulou at al (2002) should be attributed to DSA, given the lack of association between the samples and reported texture. It is hypothesized here that the discrepancies they observed may have been the result of texture differences between samples instead, resulting in Assumption 7) in Section 8.2. Li (2009) carried out thermal creep tests with pressurized capsules made from different Zr-2.5Nb billets with documented texture information, which were then processed in a variety of ways to evaluate the impact on thermal creep behaviour. These thermal creep results for Zr-2.5Nb are explored and summarized in Appendix G\textsuperscript{16}, where correlation with texture is explored in detail and where expected trends are identified\textsuperscript{17}. Figure 4\textsuperscript{18}, shows the separation of results as a result of differences in the sample texture for tests performed on material extruded at 650\textdegree C at a ratio of 4:1. Li (2009) reported better repeatability for repeated tests than Christodoulou et al. (2002).

\textsuperscript{16} Section G.3
\textsuperscript{17} Trends between strain and texture from the Li (2009) thermal creep experiments are tabulated in Table G-11.
\textsuperscript{18} Reproduced from Figure G-25.
Based on DSA observed in other materials, e.g., 9Cr-1Mo where strain rate insensitivity is observed for tests performed at temperature below 460°C only, Ho & Krempl (2000) enhanced VBO to account for DSA, as described in Section 4.3.2. Different approaches were attempted with ATXVBO using Equations (12) and (13) provided in that section to investigate the effects of DSA.

3.4 Slip parallel to basal planes

As a result of its aspect ratio and critical resolved shear stress, the dominant deformation mechanism of Zr is prismatic slip parallel to basal planes rather than basal or pyramidal slip or twinning, while it is known that some of these other mechanisms are required to explain deformation at higher temperatures (Tenckhoff, 1988) and compressive or larger strain values (Ballinger, Lucas, & Pelloux, 1984) identified in
Section 3.3.3. Experimental thermal creep data is processed in Appendix G\textsuperscript{19}, to meet Objective 3) in Chapter 2, i.e., to investigate if slip occurs predominantly parallel to the HCP basal planes in Zr alloys subjected to tensile straining. A qualitative discussion of thermal creep test results confirm that this behaviour, as postulated by Tenckhoff (1988), holds true for Zr-2.5Nb material subjected to thermal creep testing performed at 350\textdegree C. This observation for small deformation supports modeling the material behaviour with a small deformation phenomenological model that does not differentiate between deformation mechanisms in its formulation and where no provision is introduced to accommodate twinning, validating Assumption 1) in Section 8.2.

\textsuperscript{19} See Section G.3 and Table G-11
CHAPTER 4. SELECTION AND EXPANSION OF AVBO TO INCORPORATE TEXTURE AND TEMPERATURE AS INPUTS

Tenckhoff (1988) predicted the predominance of prismatic slip parallel to the basal planes for Zr HCP crystals (Section 3.4). Christodoulou et al. (1996) assumed in their self-consistent modelling that thermal creep is dominated by prismatic and pyramidal slip. Murty et al. (1994) and Li (2009) introduced basal slip in their self-consistent models that predict Zr alloy as discussed in Section 4.1. As this is a phenomenological evaluation, no attempt is made to capture any particular slip or twinning system aspect in the model as motivated in Section 3.4, despite such attempts with other phenomenological models. Suggestions for including twinning to capture compressive strains are made as Recommendation 5) in Chapter 9, should the application of interest necessitate that.

This chapter motivates the selection of AVBO and the need to modify it to include texture and temperature dependency in Section 4.1. Section 4.2 provides a historical perspective of VBO and AVBO and Section 4.3 introduces the new variant ATXVBO that accounts for non-evolving texture and temperature as input parameters.

4.1 Unified phenomenological models and Zr alloys – Selecting AVBO

Deformation predictions for Zr alloys have been published for a few unified phenomenological models. Miller (1977) (1987) predicted inelastic deformation of Zircaloy with an isotropic version of the MATMOD model not relying on an assumed yield locus. He accounted for dislocation movement phenomena in formulating MATMOD, introducing elements of self-consistent modelling as well. There are two
anisotropic versions of MATMOD, MATMOD-Z (Oldberg, Miller, & Lucas, 1979) and MATMOD-4V (Helling & Miller, 1987). Both anisotropic versions introduced a yield surface. Delobelle et al. (1996) developed an anisotropic yield locus based theory somewhat similar to MATMOD, but assumed that the inelastic strain rate is a function of back stress in its flow law, whereas Miller considered it to be a function of stress. No unified model was used for a Zr alloy that considered anisotropy while not relying on an assumed yield surface. Therefore, Objective 1) in Chapter 2 could not be satisfied from literature.

Attempts to model the deformation of HCP material with VBO or AVBO are limited, with no attempt to model Zr-alloys. A Ti-alloy was modelled with VBO (Krempl, Ruggles, & Yao, 1987), not exploring anisotropy. VBO was inspired by experimental observations of the overstress phenomenon on a macroscopic level and no attempt was made to capture dislocation phenomena in its derivation. VBO was subsequently derived from an idealized viscoplastic material model that contains springs, dashpots and sliders, as summarized in Appendix A\textsuperscript{20}. Later variations introduced improvements to address material observations. For example, Ho and Krempl (2000) added functionality to describe DSA\textsuperscript{21}. It is therefore of interest to evaluate the merits of the more general phenomenological version AVBO to model the behaviour of Zr-alloys as also explored in Appendix A.

\textsuperscript{20} Section A.1
\textsuperscript{21} Section A.2.4.2
4.1.1 Microstructure and texture correlation – the case for VBO, AVBO and ATXVBO

It has been demonstrated in Section 3.3.2 that texture is correlated to grain size, billet heat treatment as well as extrusion temperature and ratio, providing adequate motivation to only rely on texture (and temperature) as input parameters.

Only one of the phenomenological models used for predicting anisotropic material behaviour mentioned in Sect. 4.1 allows for the prediction of deformation for a texture that is different than the texture of the material used to fit the constants. Oldberg et al. (1979) took account of only the radial Kearns factor in MATMOD-Z and used it to determine the coefficients of the elastic Hill’s equation. They let one of the elastic Hill’s coefficients evolve in the inelastic stress definitions to capture yield surface distortion. MATMOD-4V (Helling & Miller, 1987), allowed distortion of the yield surface differently, but they did not introduce texture as a variable and did not validate their model against Zr alloys. In summary, none of the unified models has the ability to prescribe the texture completely in a phenomenological model, functionality that is being introduced with this study.

The relevant variants of VBO and AVBO are explained in detail in Appendix A and summarized in Section 4.2, while ATXVBO is introduced with temperature and texture as input variables in Section 4.3. Although microstructural effects other than texture are not introduced into ATXVBO, it is investigated in Section 7.1.5 whether ATXVBO lends itself to addressing such variances.
4.1.2 Temperature dependency

Polynomial functions have been employed to capture temperature dependency in VBO and AVBO (Lee & Krempl, 1991) (Yeh & Krempl, 1993). That approach is followed in this study. The choice of linear and quadratic relations was motivated by observations of earlier users of VBO. In order to inspect the temperature dependency for Zr-2.5Nb, the stress versus strain plots provided at different temperatures in Figure 3 were recast as stress versus temperature in Appendix G at different strain levels. Significant linear dependency of stress with temperature is observed, confirming the linear thermal dependency Assumption 3) used during the derivation of ATXVBO. The exception is for H in the equilibrium stress rate Equation (11) to take account of DSA rate sensitivities, as discussed in Sections 3.3.4.2 and 4.3.2. The attempted validation of Assumption 3) on linear and quadratic temperature dependence is done in Section 8.2, where it is concluded that further effort is required to better capture temperature effects with ATXVBO.

4.2 VBO and AVBO

The origins and main variants of VBO are summarized in Appendix A. It compares variants of VBO equations and explains why certain ones were selected for generalization to AVBO. The equations for AVBO (no temperature or texture sensitivity) are also presented. For a more concise presentation and consistent with Sütçü (1985), the AVBO variant selected utilizes the Representation Theorem (presented in Appendix B), used in

22 Figure G-19
lieu of tensor transformations to describe the stress-strain response in directions other than the material preferred directions. Lee (1989) formulated his version of AVBO with tensor transformations instead. Other versions of VBO are available, including TVBO with temperature as variable (Lee K. -D., 1989) and finite deformation versions (FVBO and AFVBO) (Colak, 2001), however, these versions are not relevant for this study.

The equations for the newly derived version of AVBO, ATXVBO, are provided in Section 4.3, where the objective is to predict the stress state at any constant temperature or texture. Terms could be added to accommodate a transient temperature profile (Lee K. -D., 1989) but it is not included here. Note that both Sütçü and Lee used stress and strain components and not their deviators in their formulations of AVBO unlike VBO23.

4.3 ATXVBO - AVBO with fixed texture and temperature values as input parameters

Texture and single crystal properties are employed in a new way to determine polycrystal material properties required for AVBO. Material property concepts are introduced in Section 4.3.1 as background information before the equations are presented in Section 4.3.2. Anisotropic tensor ratios and DSA modeling aspects are discussed in Section 4.3.4 and Section 4.3.5 summarizes strategies to minimize the number of constants. Appendix E provides a summary of all the ATXVBO equations.

23 Also adopted by others who have used their models, e.g., Chow (1993), Krempl (1996) and Colak (2001).
4.3.1 Material constants required for ATXVBO

Section 4.3.1.1 explains how texture and temperature are assigned. The methodology to derive the elastic properties is summarized in Section 4.3.1.2 and is presented in detail in Appendix C: It was obtained from literature. Section 4.3.1.2 summarizes the approach to derive the inelastic polycrystal property equations, with a detailed derivation in Appendix D: This is original content.

4.3.1.1 Scalar and tensor constants and temperature dependency

In the equations below, scalar and tensor constants are treated differently. For scalar constants, based on the observations discussed in Section 4.1.2, it is assumed that there is linear temperature dependency. Texture is also assumed to vary in a linear fashion. For instance, the isotropic stress constant $A_c$ utilised in Equation (19) is described as

$$A_c[T, f_R, f_T] = \left(A_c^{(00)} + A_c^{(01)} f_R + A_c^{(02)} f_T\right) + \left(A_c^{(10)} + A_c^{(11)} f_R + A_c^{(12)} f_T\right) T$$

(2)

The exception is $H$, described in Equations (11) to (13). Since DSA is a diffusion-dominated phenomenon, its behaviour is non-linear with temperature and a quadratic dependency is assumed, as described in Section 4.1.2. Tensorial properties are discussed in Sections 4.3.1.2 and 4.3.1.3.

4.3.1.2 Elastic properties using single crystal properties and Kearns factors

Appendix C provides a literature review on methods to derive elastic material properties for Zr-alloys utilizing single crystal properties and texture information. A pole figure captures the X-ray (or neutron or electron) diffraction intensity distribution of crystal orientation as an area representation. Relationships that express the area...
representation as a volume, using spherical harmonic equations, ODFs with ODCs, are then used to describe texture orientation in space, as discussed in Section 3.2. Upper bound compliance tensor values are predicted by assuming compatibility (equal strain) of the single and polycrystals following the Voigt approach, while lower bound compliance tensors values are predicted by assuming equilibrium (equal stress) of the single and polycrystals with the Reuss approach, thus introducing some aspects of self-consistent modelling into ATXVBO. The Hill stiffness, as introduced in ATXVBO, is the average of the upper and lower bound compliances. Since relationships exist between the Kearns factors and ODCs, Equation (1), the compliance or stiffness can be expressed as a function of the single crystal stiffness and Kearns factors only, with no need to use the ODCs.

4.3.1.3 Inelastic properties using single crystal properties and Kearns factors

It is being postulated that equivalent single crystal-like tensors exist that can be used with the ODCs or Kearns factors to calculate polycrystal tensors. Appendix D provides a detailed account on how the material properties are calculated. The parallels between the elastic and inelastic single crystal tensors are provided in Table 1, while the polycrystal tensors equivalencies are highlighted in Table 224.

24 Figure D-1 shows the computed entities required for the various ODEs that the properties are needed for, while the sequence for computing the elastic and inelastic polycrystal property tensors are shown in Figure D-2.
4.3.2 The applicable VBO and AVBO as well as ATXVBO equations

Frequent references are made to sections and equations in Appendix A in this chapter where a detailed summary of VBO, AVBO and ATXVBO equations is provided.

The total strain rate is expressed, in either true or deviatoric strain, respectively, as:

\[ \dot{\varepsilon} = \dot{\varepsilon}^{\text{el}} + \dot{\varepsilon}^{\text{in}} \text{ or } \dot{\varepsilon} = \dot{\varepsilon}^{\text{el}} + \dot{\varepsilon}^{\text{in}} \]  

\( (3) \)

\( \dot{\varepsilon} \) is the total strain rate and \( \dot{\varepsilon} \) its deviator. The deviatoric elastic strain rate \( \dot{\varepsilon}^{\text{el}} \) and strain rate \( \dot{\varepsilon}^{\text{el}} \) are expressed for VBO, from Equations (A-11) and (A-12) as:

\[ \dot{\varepsilon}^{\text{el}} = \frac{1 + \nu^{\text{el}}}{E} \dot{\sigma}^{d} \]

\( (4) \)

\[ \dot{\varepsilon}^{\text{el}} = \frac{1 + \nu^{\text{el}}}{E} \dot{\sigma}^{d} + \frac{1 - 2\nu^{\text{el}}}{3E} \delta_{ij} \text{tr}(\dot{\sigma}) I \]

\( (5) \)

For the anisotropic AVBO\(^{25} \) (and ATXVBO), with the loads applied in the material preferred directions, from Equation (A-79), the elastic strain rate is:

\[ \dot{\varepsilon}^{\text{el}} = S \dot{\sigma} \]

\( (6) \)

\( S \) is the compliance and \( \dot{\sigma} \) the stress rate. The Representation Theorem is used to express the elastic strain rate for any arbitrary stress state, as described in Section A.2. From Equation (A-81), with \( S_y \) defined in Equation (A-82) and \( M_y \) in Equation (B-3), the strain rate is

\[ \dot{\varepsilon}^{\text{el}} = S_y M_y + S_{y+3} (M_y \dot{\sigma} + \dot{\sigma} M_y) \]

\( (7) \)

\(^{25} \) All versions of AVBO use stress rather than deviatoric stress. See Section A.1.4 where deviatoric stress and strain components are introduced as the VBO equations are derived from the uniaxial equations derived from the modified SLS in Section A.1.1.
VBO has its origins in observations made about the relation between inelastic strain rate and overstress. The deviatoric inelastic strain rate $\dot{\varepsilon}^{\text{in}}$ is expressed for VBO, from Equation (A-13) as

$$\dot{\varepsilon}^{\text{in}} = \frac{(1 + n^{\text{in}})}{E \kappa[\Gamma]} o^d$$

where $o^d$ is the deviatoric overstress $\sigma^d - g^d$, with $\sigma^d$ the deviatoric stress tensor and $g^d$ the deviatoric equilibrium stress tensor. $E$ is the modulus of elasticity. $\kappa$ (Equation (A-16)) is the viscosity function which relies on the effective overstress $\Gamma$ described by Equation (20). The equilibrium stress describes the stress state achieved at very low strain rates. For AVBO and ATXVBO, with loads applied in the material preferred directions, the inelastic strain rate is (Equation (A-83)):

$$\dot{\varepsilon}^{\text{in}} = \frac{S_1 B^\varepsilon (\sigma - g)}{\kappa[\Gamma]}$$

$S_1$ is the first component of the compliance tensor, $B^\varepsilon$ an inelastic material property tensor (Equation (A-84)), $\sigma$ the stress and $g$ the equilibrium stress. Now $\Gamma$ is defined by Equation (22). For an arbitrary stress state, from Equation (A-86), with $B^\varepsilon_y$ defined in Equation (A-87), the strain rate is:

$$\dot{\varepsilon}^{\text{in}} = \frac{1}{E_1 \kappa} \left( B^\varepsilon_y M_y + B^\varepsilon_{y+3} (M_y (\sigma - g) + (\sigma - g) M_y) \right)$$

$E_1$ is the first component of the anisotropic elastic modulus, the reciprocal of $S_1$.

Various variations of the equilibrium stress rate exist as summarized in Appendix A.1.6. Although not explicitly stated by Sütçü (1985), it is demonstrated in Section A.1.6.2 that the version of VBO used for generalization to AVBO is his modified
Yao version, effectively adopted by Lee & Kreml (1991). The capability to describe DSA in VBO, significant for Zr-alloys, is captured with a modification of the isotropic stress term $A$ in the dynamic recovery term (Section A.1.6.6) to arrive at Equation (A-57) for the deviatoric equilibrium stress rate:

$$
\dot{\gamma}^d = E\bar{\psi}[\Gamma]\left(\frac{\dot{\epsilon}^{el}}{1 + \nu^{el}} + \frac{\dot{\epsilon}^{in}}{1 + \nu^{in}} - \frac{\Theta}{A + H\Gamma} \left(1 - \frac{E_t}{E\bar{\psi}[\Gamma]}\right) \frac{\dot{\epsilon}^{in}}{1 + \nu^{in}}\right) \quad (11)
$$

$\bar{\psi}$ describes the shape function, $A$ the isotropic stress, $H$ is a coefficient to describe DSA and $E_t$ the tangent modulus while $\nu^{el}$ and $\nu^{in}$ are elastic and inelastic Poisson ratios. $\Theta$ is an effective stress defined with Equation (21) based on $\dot{\gamma}^d - f^d$, The equation for $H$ for AET and AIT described in Section 4.3.3 is shown as Equation (12), from Equations (A-55),

$$
H = H_3, \quad (12)
$$

while for AIT, DSA, Equation (13) repeated from Equation (A-53), introduces sensitivity to $\dot{p}$, the accumulated effective inelastic strain rate:

$$
H[\dot{p}] = H_3 \frac{1}{H_1 \sqrt{2\pi}} e^{\frac{-(\ln \dot{p} - H_2)^2}{2(H_1)^2}}. \quad (13)
$$

For AVBO and ATXVBO, with loads applied in the material preferred directions, from Equation (A-97), the equilibrium stress rate is:

$$
\frac{\dot{\gamma}}{E_1\bar{\psi}[\Gamma]} = D^g \left(\dot{\epsilon} - \frac{\Theta}{A + H\Gamma} \left(1 - \frac{P_1}{E_1\bar{\psi}[\Gamma]}\right) \dot{\epsilon}^{in}\right) \quad (14)
$$

$D^g$ is an inelastic material property tensor (Equation (A-91)), where $f^d$ is the deviatoric kinematic stress defined below and $P_1$ is a constant and the equivalent of $E_t$ for AVBO.
Now $\Theta$ is defined by Equation (23). For an arbitrary stress state, from Equation (A-95), with $D^g_y$ defined in Equation (A-96), the equilibrium stress rate is:

$$
\dot{\mathbf{g}} = E_1 \overline{\psi} \left( D^g_y \mathbf{M}_y + D^g_{y+3} (\mathbf{M}_y \dot{\mathbf{x}} + \dot{\mathbf{x}} \mathbf{M}_y) \right)
$$

$$
\dot{\mathbf{x}} = \dot{\mathbf{e}} - \frac{\Theta}{A + H} (1 - \varphi) \dot{\mathbf{e}}_{\text{in}}
$$

$\dot{\mathbf{x}}$ is a combined inelastic strain rate that permits employing the Representation Theorem and is defined with Equation (A-94). $\varphi$ is an adjusted normalized shape function defined by Equation (A-90).

Kinematic stress introduces the ability to model work hardening and its rate is expressed from Equation (A-61) as:

$$
\dot{\mathbf{f}}^d = \frac{2}{3} E_t \dot{\mathbf{e}}_{\text{in}} = \frac{1}{(1 + \nu_{\text{in}})} E_t \dot{\mathbf{e}}_{\text{in}}
$$

For AVBO and ATXVBO, with loads applied in the material preferred directions, from Equation (A-99), the kinematic stress rate is:

$$
\dot{\mathbf{f}} = P_1 \mathbf{D}^f \dot{\mathbf{e}}_{\text{in}}
$$

$\mathbf{D}^f$ is an inelastic material property tensor (Equation (A-103)). For an arbitrary stress state, from Equation (A-101), with $D^f_y$ defined in Equation (A-102), the kinematic stress rate is:

$$
\dot{\mathbf{f}} = P_1 \left( D^f_y \mathbf{M}_y + D^f_{y+3} (\mathbf{M}_y \dot{\mathbf{e}}_{\text{in}} + \dot{\mathbf{e}}_{\text{in}} \mathbf{M}_y) \right)
$$

The isotropic stress rate $\dot{\mathbf{A}}$ is (Equation (A-71))

$$
\dot{\mathbf{A}} = A_c (A_f - A) \dot{\mathbf{p}}.
$$
A_c (dimensionless) controls the speed at which the final solution A_f (dimension of stress) is being approached. Both A_c and A_f are constants.

Two scalar effective stress definitions are required. In the case of VBO, \( \Gamma \) captures \( \sigma^d - g^d \) dependency and \( \Theta \) captures \( g^d - f^d \) dependency, from Equations (A-76) and (A-77), respectively:

\[
\Gamma^2 = (1 + \nu^{\text{in}})(\sigma^d - g^d) \cdot (\sigma^d - g^d) \tag{20}
\]

\[
\Theta^2 = (1 + \nu^{\text{in}})(g^d - f^d) \cdot (g^d - f^d) \tag{21}
\]

For AVBO and ATXVBO these equations become, from Equations (A-106) and (A-107):

\[
\Gamma^2 = \left( \begin{vmatrix} B^e \cdot (\sigma - g) \end{vmatrix} \right) \cdot \left( \begin{vmatrix} B^e \cdot (\sigma - g) \end{vmatrix} \right) \tag{22}
\]

\[
\Theta^2 = \left( \begin{vmatrix} B^e \cdot (g - f) \end{vmatrix} \right) \cdot \left( \begin{vmatrix} B^e \cdot (g - f) \end{vmatrix} \right) \tag{23}
\]

4.3.3 Plastic compressive, direction sensitive hardening and cyclic loading

Based on the observations in Section 3.3.3, texture evolution needs not be considered in ATXVBO unless compressive plastic straining is also experienced. The test data used for optimization as summarized in Section 5.2 are all of a tensile nature and do not include cycling. However, the capability to model differences in hardening behaviour in non-test directions to account for changes of R as deformation progresses (Section 3.3.3) requires some attention. As indicated in Section A.1.8, cyclic hardening or softening is accomplished in VBO (and AVBO) with the scalar isotropic stress rate \( \Lambda \), Equation (19), which is a function of the effective inelastic strain rate. Differences in hardening or softening characteristics in different directions, as suggested by Ballinger et al.(1984),
require tensorial dependency, already captured in the kinematic stress rate $\dot{f}$, Equation (17). However, to capture different hardening responses for compression and tension will require additional functionality in ATXVBO. This observation is captured as Limitation 3) in Section 8.4 and Recommendation 5) in Chapter 9.

### 4.3.4 Strategies with respect to elastic and inelastic anisotropy ratio equivalency and DSA strain rate sensitivity

Sütçü (1985) identified elastic and inelastic lateral ratios, which are normalized versions of the anisotropy tensors $S, B^e, D^b$ and $D^f$, where normalization is done against $S_1, B_1^e, D_1^b$ and $D_1^f$, respectively (see Section A.2.3). Sütçü and Krempl (1990) introduced a simplifying assumption that the inelastic anisotropy ratios are equal to elastic anisotropy ratios. In this study, as indicated in Chapter 1, Contribution 2), the validity of the Sütçü and Krempl (1990) assumption is tested for Zr-2.5Nb. The terminology AET is used to identify their approach with respect to the assumption of equivalent inelastic anisotropy ratios. AIT and AIT, DSA are used if inelastic anisotropic tensor ratios are determined for all inelastic ODEs. AET and AIT rely on $H$ as expressed in Equation (12) while AIT, DSA rely on Equation (13) to account for dynamic strain aging effects: AIT, DSA assumes that DSA is inelastic strain rate dependent, captured as Assumption 8) in Section 8.2 and described in Section A.1.6.4. All three approaches, AET, AIT and AIT, DSA were used during optimization, validation and sensitivity evaluations.
4.3.5 Economy in total number of constants

A comparison of the number of constants for variations of VBO, AVBO and ATXVBO are provided in Table 3. A significant reduction in the number of constants required for AVBO has been achieved by introducing the single crystal tensors $\mathbf{s}$, $\mathbf{b}^{sc}$, $\mathbf{d}^{sc}$ and $\mathbf{d}^{sp}$ and associated polycrystal tensors $\mathbf{S}$, $\mathbf{B}^{e}$, $\mathbf{D}^{g}$ and $\mathbf{D}^{f}$ for ATXVBO. Each of the four redefined polycrystal tensors $\mathbf{S}$, $\mathbf{B}^{e}$, $\mathbf{D}^{g}$ and $\mathbf{D}^{f}$ requires ten constants, two constants associated with each of the five single crystal components to account for linear temperature dependency. When polycrystal properties are used instead, as with AVBO, 18 constants are required for each of the four polycrystal tensors: For instance, see Equation (A-80) for $\mathbf{S}$, with two constants to describe the temperature dependency for each of the nine components. The polycrystal approach increases the total number of constants by $(18-10) \times 4 = 32$, from 67 for ATXVBO to 99 for AVBO. It also requires optimization of all constants for each texture state, not necessary with the single crystal approach.

The simplifying assumption of Sütçü and Kreml (1990) regarding similarity of anisotropy ratios (AET approach, Section 4.3.3) brings a reduction of 16 in the number of constants required for $\mathbf{B}^{e}$, $\mathbf{D}^{g}$ and $\mathbf{D}^{f}$ for AVBO, with a reduction to 51 (= 99-3x16) equations. If the single crystal approach (i.e. ATXVBO) is being used instead, the reduction of eight components for each of $\mathbf{b}^{sc}$, $\mathbf{d}^{sc}$ and $\mathbf{d}^{sp}$ means that the total amount of constants is reduced to 67-3x8=43 (ATXVBO with AET approach).

The 67 constants for ATXVBO (AIT, DSA) are listed in Table 8 as obtained through optimization for a number of experimental datasets (Section 5.2). 40 of the constants are
required to describe the state of anisotropy with the single crystal tensors $s$, $b_{\epsilon}^{sc}$, $d_{g}^{sc}$ and $d_{f}^{sc}$. 
CHAPTER 5. OPTIMIZATION OF CONSTANTS

This chapter discusses how constant values are determined through numeric optimization. Section 5.1 describes the use of a genetic algorithm for that purpose. Experimental data are identified in Section 5.2 while their suitability is evaluated in Section 5.3. The implementation of the equations presented in Chapter 4\textsuperscript{26} is discussed in Section 5.4. Optimization activities are reported in detail in Section 5.5. The various inputs and outputs for optimization are summarized in Table 6, Lines 1) to 4).

5.1 Strategy to determine constants

One possible approach is to derive the constants through a series of different tests designed to enable solving of a few of the constants at a time. Given that there are 67 constants required for ATXVBO (Section 4.3.3), this approach was not found feasible given the limited number of suitable plastic deformation and thermal creep experimental datasets available with texture information for Zr-2.5Nb.

It is also possible to determine all constants simultaneously using an optimization strategy. Constants are determined by minimizing residuals between measured and predicted results. The genetic algorithm has been applied with success by Dusuncelli et al. (2010) to optimize constants for large deformation AVBO of polymers. Genetic algorithms improve consecutive iteration guesses of the constants by pairing the previous best guesses, identified as the candidates that produce the smallest residuals. During the

\textsuperscript{26} The polycrystal formulations for coding with MATLAB™ was obtained from Sections C.3.2.2 and D.3, the ODEs and other equations from Appendix E and the sequence of implementation in Appendix F.
pairing, it also introduces a mutation of some of the new guesses to prevent inbreeding. Another strategy is introduced to ensure that the global minimum rather than a local minimum is found during the comparison of residuals: New guesses are introduced during each iteration. Appendix H demonstrates, with the introduction of single crystal based material properties, how constants can in principle be determined through optimization with single plastic deformation and thermal creep datasets.

5.2 Experimental data selected for optimization of constants

This section identifies and motivates the selection of suitable data to be used for the optimization of constants for Zr-2.5Nb. Four combination sets are identified here for different optimization datasets, G11, G9 and G4 and G11(3). The sets are summarized in Table 4 and are made up with data described in Section 3.3.4. The plastic deformation experimental data obtained from plate samples are more likely to have accurately documented texture information. As a result, Dataset G11 was selected as primary set for optimization purposes, recognizing the uncertainty in not knowing the billet cooling method and extrusion ratio for the plastic deformation data (Section 3.3.4.1). Dataset G11 includes two sets of uniaxial plastic deformation experimental test results for samples cut from plate, one tested at 250°C in the longitudinal direction and the other tested at 100°C in the transverse direction. Dataset G11 also includes one thermal creep set of results from a bi-axially loaded pressurized capsule tested at 350°C. Dataset G9 substitutes one plastic deformation plate result set with tube results with uncertainty on the texture values, described in Section 3.3.4.1 – one of the texture states reported by Christodoulou et al. (2000) were arbitrarily assigned for the tube material (Section 5.3).
Dataset G4 substitutes the thermal creep set in Dataset G11 with results for a sample that was prepared from material extruded at 650°C instead of 815°C. Dataset G11(3) includes an additional plate plastic deformation sample tested at 150°C, to investigate the effect of the input temperature further.

5.3 Potential limitations of experimental data selected for optimization

For the plastic deformation experiments mentioned in Section 3.3.4.1, the texture for each specimen is only known within a range. Any test shown for tube material could have had the texture of Tube A, B, C or D as discussed in Appendix G. As also hypothesized there, the single texture reported for plate material suggests that all samples were cut from a single plate, thus suggesting specimen specific texture was reported in that case. Therefore, the plate data is selected for optimization purposes in this study. Note, as also pointed out in Section 3.3.4.1, that some uncertainty is introduced with the selection of this plate material data, as the billet cooling strategy is not known and extrusion ratio not reported.

As described in Section 3.3.4.2, Li (2009) documented the texture for each thermal creep test performed with Zr-2.5Nb tubes. As the various capsules were extruded at different temperatures and ratios, this data lends itself well to this study.

Four combination datasets, G11, G9, G4 and G11(3), were identified for optimization of constants as motivated in Section 5.2. The uncertainty in the plastic deformation data casts some uncertainty over the validity of the derived constants presented in Table 8,

27 Section G.2
further discussed in Section 5.2 and identified as an opportunity for improvement in Chapter 9, Recommendation 2).

5.4 Analysis methodology

The analysis was performed with MATLAB™ Version 7.8.0.347 (R2009a) on a Windows 7 PC platform. The multi-objective genetic algorithm “gamultiobj” in the MATLAB Optimization Toolbox was used for optimization. Although not documented here, some validation of the numeric tools were performed first through implementation of the VBO equations of Majors (1993). The published data for 9Cr-1Mo steel (Ruggles, Cheng, & Krempl, 1994) were optimized successfully with the MATLAB “ga” routine. Using Majors’ constants, his results for the same data were also duplicated successfully.

5.5 Multi-objective optimization with plastic deformation and thermal creep data

Four combined plastic deformation and thermal creep experimental Zr-2.5Nb datasets, G11, G9, G4 and G11(3) were used for optimization, as motivated in Section 5.2 and summarized in Table 4. Three solution strategies, AET (equivalent inelastic anisotropy ratios), AIT (independent inelastic anisotropic tensor ratios) and AIT, DSA (independent inelastic anisotropic tensor ratios as well as inelastic strain rate dependency) were attempted, as defined in Section 4.3.3.

Pareto fronts were generated to document the fitness values for each dataset and solution strategy combination, as discussed in Section 5.5.1. As motivated in Section 5.2, Dataset G11 is expected to offer the best texture information and consistency in
manufacturing history and its optimization results are presented in Section 5.5.2. The results for Datasets G9, G4 and G11(3) are summarized in Section 5.5.3 for comparison purposes.

Over and above the Pareto fronts, stress correlation and stress versus strain plots for plastic deformation evaluation cases are provided as well. Similarly, strain correlation and strain versus time plots are provided for thermal creep cases. The correlation plots compare the experimental and predicted stress and strain values, respectively. An example of a strain correlation plot is provided as Figure 5: The correlation plots are included to show the fitness during optimization in a condensed manner and to allow an easy comparison between the fitness values obtained from different optimization attempts. The straight line indicates perfect correlation.
Figure 5. Explanation of correlation plots to show quality of optimization.
5.5.1 Pareto fronts

The concept of a Pareto front, a plot of non-correlated fitness values obtained from a multi-objective optimization (MOO) run, is explained in Appendix H\textsuperscript{28}. The front provides a series of optimum solutions for plastic deformation $f_{pl}$ versus creep $f_{cr}$ fitness values. The Pareto fronts obtained for combination Datasets G11, G9 and G4 using the AET, AIT and AIT, DSA strategies defined in Section 4.3.4, are compared in Figure 6. Pareto fronts for each of Datasets G11, G9, G4 and G11(3) are provided in Figure 7, Figure 11, Figure 14 and Figure 17, respectively. Care was taken during the optimization to ensure that an ample number of generations were allowed for the fronts to stabilize\textsuperscript{29}. The best solution with the lowest combined fitness values was obtained for Dataset G11 using the AIT, DSA strategy. The solutions on the Pareto fronts selected by inspection for further evaluation are identified in Figure 7, Figure 11, Figure 14 and Figure 17 and are discussed below in separate sections.

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\textsuperscript{28} Section H.3

\textsuperscript{29} With the exception of G11(3) – See Section 5.5.3.3.
Figure 6. Comparison of Pareto fronts obtained for Datasets G11, G9 and G4 using AET, AIT and AIT, DSA ATXVBO strategies.
5.5.2 Optimization results for Dataset G11

MOO solutions were obtained for each of the AET, AIT and AIT, DSA strategies using Dataset G11. The optimum solutions for further evaluation on the fronts are “AET Sol 44,” “AIT Sol 2” and “AIT, DSA Sol2” as identified in Figure 7. The best overall fitness was obtained with AIT, DSA.

![Three Pareto fronts obtained with different MOO strategies using Dataset G11 in Table 4.](image)

5.5.2.1 Results and discussion for G11, “AET Sol 44”

To further evaluate the merit of the selected solution, correlation plots for stress and strain for AET are provided in Figure 8(a). The corresponding stress versus strain plot (plastic deformation cases) and strain versus time plot (thermal creep cases) are provided as Figure 8(b) and Figure 8(c), respectively.
Figure 8(a). Correlation stress and strain plots, Dataset G11, AET Sol 44.
Figure 8(b). Stress versus strain, Dataset G11, AET Sol 44. Figure G-18
The stress correlation in Figure 8(a) is not good, with scatter above and below the straight line that indicates perfect correlation. The correlation with the creep results is very good. There is an apparent insensitivity to test temperature in the stress versus strain plots in Figure 8(b) and the equilibrium stress \( \sigma \) does not exhibit a transition from elastic to inelastic deformation as observed for the stress \( \sigma \). There is negligible kinematic stress \( f \), which is the case for all results obtained in this study. The strain versus time plot in Figure 8(c) reflects the good correlation observed in the lower Figure 8(a).
5.5.2.2 Results and discussion for G11, “AIT Sol 2”

The correlation plot, stress versus strain and strain versus time plots for the AIT strategy are provided in Figure 9(a), Figure 9(b) and Figure 9(c), respectively.

![Correlation stress and strain plots, Dataset G11, AIT Sol 2.](image-url)
Figure 9(b). Stress versus strain, Dataset G11, AIT Sol 2.
Figure 9(c). Strain versus time, Dataset G11, AIT Sol 2.

Figure 9. Stress and strain optimization correlation plots, stress versus strain plots and strain versus time plots for Strategy AIT Sol 2 in Figure 7 for Dataset G11 in Table 4.

When compared to the results from “AET Sol44” in Section 5.5.2.1, the stress correlation is somewhat better with some sensitivity to test temperature but the equilibrium stress $g$ still does not exhibit a transition from elastic to inelastic deformation, in fact, it predicts negligible equilibrium stress, especially a slightly negative trend in the axial direction. The correlation with the creep results is again very good.
5.5.2.3 Results and discussion for G11, “AIT, DSA Sol 2”

The correlation plot, stress versus strain and strain versus time plots for the AIT, DSA strategy are provided in Figure 10(a), Figure 10(b) and Figure 10(c), respectively.

Figure 10(a). Correlation stress and strain plots, Dataset G11, Solution AIT, DSA Sol 2.
Figure 10(b). Stress versus strain, Dataset G11, Solution “AIT, DSA Sol 2”
Figure 10(c). Strain versus time, Dataset G11, Solution “AIT, DSA Sol 2”.

Figure 10. Stress and strain optimization correlation plots, stress versus strain plots and strain versus time plots for Strategy AIT, DSA Sol 2 in Figure 7 for Dataset G11 in Table 4.

When compared to the results from “AIT Sol 2” in Section 5.5.2.2, the stress correlation is good, there is good sensitivity to test temperature in the stress versus strain plot, where the equilibrium stress now exhibits results of similar magnitude in the axial and transverse directions while exhibiting the expected transition from elastic to inelastic deformation. The correlation with the creep results is again good, with a little more under-prediction of the inelastic strain at higher strain values.
5.5.2.4 Conclusions from optimization results obtained for Dataset G11

The plastic deformation and thermal creep behaviour of Zr-2.5Nb material can be replicated with ATXVBO. A noticeable improvement of the stress $\sigma$ prediction is obtained when the AIT strategy is used instead of the AET strategy, if equal anisotropy ratios are not assumed. The calculated equilibrium stress $g$ shows reasonable values and an expected shape with transition from elastic to inelastic behaviour with the AIT, DSA strategy, where inelastic strain rate sensitivity is introduced into the equilibrium stress equation (Section 4.3.3). The stress-strain predictions are almost bi-linear in appearance. The bi-linear behaviour could potentially be the result of having used samples for plastic deformation and creep testing with manufacturing differences: The assumptions made in Section 5.2 regarding the billet cooling method for the plastic deformation samples (slow cooled assumed) and their extrusion ratio (assumed 10:1) may not be true.

5.5.3 Optimization results with other datasets for comparison to Dataset G11

Results for Datasets G9, G4 and G11(3) are included for comparison purposes against Dataset G11.

5.5.3.1 Optimization results for Dataset G9

Dataset G9 includes one set of tube experimental results with arbitrarily assigned texture for plastic deformation for reasons explained in Sections 5.2 and 5.3. Two solutions, “AET Sol 24” and “AIT Sol 1” were selected from the family of optimized solutions in Figure 11. The correlation plots, stress versus strain and strain versus time plots for “AET Sol 24” are provided in Figure 12(a), Figure 12(b) and Figure 12(c),
respectively. Similarly, the correlation plot, stress versus strain and strain versus time plots for “AIT Sol 1” are provided in Figure 13(a), Figure 13(b) and Figure 13(c). The results for all seven figures are discussed after Figure 13.

Figure 11. Two Pareto fronts obtained with different MOO strategies using Dataset G9 in Table 4.
Figure 12(a). Correlation stress and strain plots, Dataset G9, “AET Sol 24”.
Figure 12(b). Stress versus strain, Dataset G9, “AET Sol 24”.

Stress (MPa) vs. Strain

- Tube sample
- Plate sample

Parameter predictions:
- \( \sigma(L) \), Chr2000Fig5a, Axial, 300°C, 0.00011/s, \( f_R=0.365, f_T=0.557, f_L=0.077 \)
- \( g(L) \), Chr2000Fig5a, Axial, 300°C, 0.00011/s, \( f_R=0.365, f_T=0.557, f_L=0.077 \)
- \( f(L) \), Chr2000Fig5a, Axial, 300°C, 0.00011/s, \( f_R=0.365, f_T=0.557, f_L=0.077 \)
- \( \sigma(T) \), Chr2000Fig6b, Trans, 100°C, 0.0011/s, \( f_R=0.67, f_T=0.162, f_L=0.168 \)
- \( g(T) \), Chr2000Fig6b, Trans, 100°C, 0.0011/s, \( f_R=0.67, f_T=0.162, f_L=0.168 \)
- \( f(T) \), Chr2000Fig6b, Trans, 100°C, 0.0011/s, \( f_R=0.67, f_T=0.162, f_L=0.168 \)
Figure 12(c). Strain versus time, Dataset G9, “AET Sol 24”.

Figure 12. Optimization correlation stress and strain plots obtained with constants from Table 8 for solution “AET Sol 24” in Figure 7(b) for Dataset G9 in Table 4.
Figure 13(a). Correlation stress and strain plots, Dataset G9, “AIT Sol 1”.

- Stress exp (MPa)
- Stress calc (MPa)
- Strain exp
- Strain calc

- Chr 2000 Fig 5a, Axial, 300°C, 0.0001 1/s, fR=0.365, fT=0.557, fL=0.077
- Chr 2000 Fig 6b, Trans, 100°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
- WLi, IV-30, MPT66-05, 142.8MPa (L), 300MPa (T), 350°C, Biaxial, fR=0.359, fT=0.554, fL=0.087
Figure 13(b). Stress versus strain, Dataset G9, “AIT Sol 1”.

- Chr 2000 Fig 5a, Axial, 300°C, 0.0001 1/s, fR=0.365, fT=0.557, fL=0.077
- Chr 2000 Fig 6b, Trans, 100°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
- Prediction: σ(L), Chr2000Fig5a,Axial,300°C,0.00011/s,fR=0.365,fT=0.557,fL=0.077
- Prediction: g(L), Chr2000Fig5a,Axial,300°C,0.00011/s,fR=0.365,fT=0.557,fL=0.077
- Prediction: f(L), Chr2000Fig5a,Axial,300°C,0.00011/s,fR=0.365,fT=0.557,fL=0.077
- Prediction: σ(T), Chr2000Fig6b,Trans,100°C,0.0011/s,fR=0.67,fT=0.162,fL=0.168
- Prediction: g(T), Chr2000Fig6b,Trans,100°C,0.0011/s,fR=0.67,fT=0.162,fL=0.168
- Prediction: f(T), Chr2000Fig6b,Trans,100°C,0.0011/s,fR=0.67,fT=0.162,fL=0.168
Figure 13(c). Strain versus time, Dataset G9, “AIT Sol 1”.

Figure 13. Optimization correlation stress and strain plots obtained with constants from Table 8 for solution “AIT Sol 1” in Figure 7(b) for Dataset G9 in Table 4.

A comparison of Figure 13(a) and (b) with Figure 12(a) and (b) shows a noticeable improvement of the stress $\sigma$ prediction when the AIT strategy is used instead of the AET strategy, consistent with Dataset G11. Unfortunately, the same observations cannot be made regarding the equilibrium stress $\sigma$: Although the transition from the elastic to inelastic regions is apparent for the tube material in Figure 13(b) with AIT, it now exhibits an even higher negative trend than what was observed for Dataset G11 in Figure 9(b). The poor equilibrium stress prediction for the tube sample suggests that the
texture values guessed, given the uncertainty of reported texture of the samples, are not the correct ones and that true texture values are a pre-requisite for ATXVBO.

### 5.5.3.2 Optimization results for Dataset G4

With Dataset G4, the data of the plastic deformation and thermal creep samples are not from material extruded at the same temperature, with the creep sample prepared from material extruded at 650°C, as explained in Section 5.2. Two solutions, “AET Sol 77” and “AIT Sol 2” were selected from the family of optimized solutions in Figure 14. The correlation plots, stress versus strain and strain versus time plots for “AET Sol 77” are provided in Figure 15(a), Figure 15(b) and Figure 15(c), respectively. Similarly, the correlation plot, stress versus strain and strain versus time plots for “AIT Sol 2” are provided in Figure 16(a), Figure 16(b) and Figure 16(c). The results for all seven figures are discussed after Figure 16.

![Figure 14. Two Pareto fronts obtained with different MOO strategies using Dataset G4 in Table 4.](image-url)
Figure 15(a). Correlation stress and strain plots, Dataset G4, “AET Sol 77”.
Figure 15(b). Stress versus strain, Dataset G4, “AET Sol 77”.

Prediction: \( \sigma(L), \) Chr2000Fig6a, Axial, 250°C, 0.0011/s, \( f_R=0.67, f_T=0.162, f_L=0.168 \)
Prediction: \( g(L), \) Chr2000Fig6a, Axial, 250°C, 0.0011/s, \( f_R=0.67, f_T=0.162, f_L=0.168 \)
Prediction: \( f(L), \) Chr2000Fig6a, Axial, 250°C, 0.0011/s, \( f_R=0.67, f_T=0.162, f_L=0.168 \)
Prediction: \( \sigma(T), \) Chr2000Fig6b, Trans, 150°C, 0.0011/s, \( f_R=0.67, f_T=0.162, f_L=0.168 \)
Prediction: \( g(T), \) Chr2000Fig6b, Trans, 150°C, 0.0011/s, \( f_R=0.67, f_T=0.162, f_L=0.168 \)
Prediction: \( f(T), \) Chr2000Fig6b, Trans, 150°C, 0.0011/s, \( f_R=0.67, f_T=0.162, f_L=0.168 \)
Figure 15(c). Strain versus time, Dataset G4, “AET Sol 77”.

Figure 15. Optimization correlation stress and strain plots obtained with constants from Table 8 for solution “AET Sol 77” in Figure 7(c) for Dataset G4 in Table 4.
Figure 16(a). Correlation stress and strain plots, Dataset G4, “AIT Sol 2”.

Chr 2000 Fig 6a, Axial, 250°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
Chr 2000 Fig 6b, Trans, 150°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168

WLi, IV-36, MPT73-02, 145.2MPa (L), 300MPa (T), 350°C, Biaxial, fR=0.382, fT=0.538, fL=0.08
Figure 16(b). Stress versus strain, Dataset G4, “AIT Sol 2”.

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Figure 16(c). Strain versus time, Dataset G4, “AIT Sol 2”.

Figure 16. Optimization correlation stress and strain plots obtained with constants from Table 8 for solution “AIT Sol 2” in Figure 7(c) for Dataset G4 in Table 4.

Unlike Datasets G11 and G9, little if any improvement of the stress values is observed for Dataset G4 when the AIT strategy is used instead of the AET strategy, from a comparison between Figure 15(a) and (b) with Figure 16(a) and (b); in fact, both strategies show poor correlation with the experimental data. The strain prediction is somewhat improved with AIT, as seen with Figure 15(c) and Figure 16(c). The equilibrium stress shows no clear distinction between elastic and inelastic regions but positive magnitudes are obtained for both cases. These results suggest that data from
samples extruded at different temperatures cannot be combined into one dataset for optimization purposes.

5.5.3.3 Optimization results for Dataset G11(3)

A third plastic deformation set is included in this expanded version of Dataset G11, with the inclusion of experimental results obtained at 150°C, over and above the results at 100°C and 250°C already included, to investigate test temperature aspects further (Section 5.2). The Pareto fronts in Figure 17 are for different optimization population sizes and numbers of generations. The correlation plots as well as stress versus strain plots for “AIT, DSA Sol 10” are provided in Figure 18(a) and Figure 18(b).

![Figure 17. Pareto front for Dataset G11(3).](image)
Figure 18(a). Correlation stress and strain plots, Dataset G11(3), “AIT, DSA Sol 10”.
Figure 18(b). Stress versus strain, Dataset G11(3), “AIT, DSA Sol 10”.

Figure 18. Optimization correlation stress and strain plots obtained with constants from Table 8 for solution “AIT, DSA Sol 10” in Figure 7 for Dataset G11(3) in Table 4.

Although the shape of the 400 population, 15 generation solution in Figure 17 is smooth, it cannot be considered to be the optimum solution, as the fitness curve is higher (i.e. poorer fitness) than the one with a population of 500 obtained after 20 generations.

The shape of the latter Pareto front is not smooth, suggesting that a higher number of
generations should have resulted in even better fitness values. The stress correlation plot in Figure 18(a) for “AIT, DSA Sol 10” is significantly poorer than the one predicted for G11, “AIT, DSA Sol 2” in Figure 10(a). This is also evident in the stress versus strain plot in Figure 18(b) as opposed to Figure 10(b): There is now inconsistent success in predicting the stress at different temperatures. The equilibrium stress curves in Figure 18(b) show a proper transition from elastic to inelastic behaviour, with consistent positive magnitude. This attempt suggests that the AIT, DSA ATXVBO strategy is unable to capture temperature effects well.

5.5.3.4 Conclusions from optimization results obtained for Datasets G9, G4 and G11(3)

As observed with Dataset G9, equilibrium stress (and therefore stress) predictions require accurate texture values as input. The results obtained with Dataset G4 show that all data used for the optimization must have had a similar extrusion temperature and that material from different manufacturing routes cannot be combined for optimization purposes. The attempts with Dataset G11(3) indicate that the current formulation of ATXVBO has difficulty to optimize data at all temperatures, suggesting that ATXVBO has to be revised to permit different behaviour in terms of strain rate dependency at different temperatures.
CHAPTER 6. VALIDATION OF ATXVBO AND CONSTANTS

ATXVBO runs were launched for a number of plastic deformation and thermal creep datasets not used for optimization purposes in Chapter 5 to validate ATXVBO with its constants obtained through optimization. The availability of more thermal creep experimental data with known texture allowed more creep than plastic deformation validation activities. Plastic deformation validation is discussed in Section 6.1 and thermal creep in Section 6.2. The various inputs and outputs for validation are summarized in Table 6, Lines 5) to 12).

6.1 Plastic deformation Dataset A2

Given the uncertainty of the texture of the plastic deformation datasets (Section 3.3.4.1), only limited validation could be performed: Some of the plate samples with higher certainty of the texture were selected for optimization. The remainder of the plate samples, as well as tube samples with an arbitrarily selected texture from the values reported by Christodoulou et al. (2000) were used in the validation runs in Figure 19: Figure 19(a) shows the response obtained with the AET strategy, Figure 19(b) the results with AIT, DSA and Figure 19(c) again for AIT, DSA, but limiting the data to sets obtained at the temperatures used in the optimization Dataset G11.
Figure 19(a). Correlation stress plots, Dataset A2, “AET Sol 44”.
Figure 19(b). Correlation stress plots, Dataset A2, “AIT, DSA Sol 2”.

- Plate samples
  - Chr 2000 Fig 5a, Axial, 250°C, 0.0001 1/s, fR=0.365, fT=0.557, fL=0.077
  - Chr 2000 Fig 5a, Axial, 300°C, 0.0001 1/s, fR=0.365, fT=0.557, fL=0.077
  - Chr 2000 Fig 5b, Trans, 250°C, 0.0001 1/s, fR=0.365, fT=0.557, fL=0.077
  - Chr 2000 Fig 5b, Trans, 300°C, 0.0001 1/s, fR=0.365, fT=0.557, fL=0.077
  - Chr 2000 Fig 6a, Axial, 100°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6a, Axial, 150°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6a, Axial, 200°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6a, Axial, 250°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6b, Trans, 100°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6b, Trans, 150°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6b, Trans, 200°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6b, Trans, 250°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168

- Tube samples
  - Chr 2000 Fig 5a, Axial, 250°C, 0.0001 1/s, fR=0.365, fT=0.557, fL=0.077
  - Chr 2000 Fig 5a, Axial, 300°C, 0.0001 1/s, fR=0.365, fT=0.557, fL=0.077
  - Chr 2000 Fig 5b, Trans, 250°C, 0.0001 1/s, fR=0.365, fT=0.557, fL=0.077
  - Chr 2000 Fig 5b, Trans, 300°C, 0.0001 1/s, fR=0.365, fT=0.557, fL=0.077
  - Chr 2000 Fig 6a, Axial, 100°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6a, Axial, 150°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6a, Axial, 200°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6a, Axial, 250°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6b, Trans, 100°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6b, Trans, 150°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6b, Trans, 200°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
  - Chr 2000 Fig 6b, Trans, 250°C, 0.001 1/s, fR=0.67, fT=0.162, fL=0.168
Figure 19(c). Correlation stress plots, Dataset A2, “AIT, DSA Sol 2”, for experiments performed at 100°C and 250°C.

Figure 19. Validation stress correlation plots for Dataset A2 (Table G-4 and Figure G-18), obtained with constants from Table 8 for solutions “AET Sol 44” and “AIT,DSA Sol 2” in Figure 7 obtained through optimization with Dataset G11 (Table 4).
6.1.1 Conclusions from results obtained with plastic deformation data

Significant scatter around the optimum straight line is observed in both Figure 19(a) and Figure 19(b). However, Figure 19(c) shows good correlation for the plate material and not for the tube material, indicating that the tube texture was guessed wrong and confirming the importance of possessing quality texture data as input. The poor correlation at temperatures other than the optimization set temperatures indicates an inability of ATXVBO as currently defined to capture temperature effects of the material.

6.2 Thermal creep datasets

The thermal creep experimental results for Zr-2.5Nb used for optimization in Section 5.2 were derived from a detailed evaluation of available data in Appendix G. The validation sets for thermal creep, F3, F4, F9, F5, F6 and F6a, are defined in Table 5\textsuperscript{30} where the variation in manufacturing steps between them are recognized in their definitions, consistent with the key differences considered by Holt and Aldridge (1985)\textsuperscript{31}. Apart from recognizing the correlation between manufacturing differences and texture, significant correlation between thermal creep strain and texture for these datasets are identified from another detailed evaluation in Appendix G\textsuperscript{32, 33}. It was established there that the results for the six datasets can be explained (with noted exceptions) by slip parallel to the HCP crystal basal planes as found to be predominant for HCP materials in

\textsuperscript{30} Repeated from Table G-10
\textsuperscript{31} See Section G.1 and Table G-1, Table G-2 and Table G-3
\textsuperscript{32} See Section G.3
\textsuperscript{33} See Table G-11
Section 3.4 for the data considered. Conversely, good correlation between these experimental strain results and ATXVBO predicted strain results will validate that the developed theory is able to capture the texture effects as observed and that the effects of twinning need not be captured in the definition of ATXVBO for small tensile strains. All datasets are evaluated separately in Sections 6.2.1 to 6.2.6 and conclusions are provided for all sets in Section 6.2.7.
6.2.1 Dataset F3: Slow cooled billet, extruded at 650°C at a ratio of 4:1

It is observed from experiments (Table G-11, using Figure G-25) that MPT65-01 and MPT79-02 do not follow the expected trend for slip.

A stress correlations plot for “AIT, DSA Sol 2” is provided in Figure 20, with its strain versus time plot in Figure 21. These figures show that the transverse strain is consistently under predicted with little scatter, with the exception of MPT65-01 and MPT79-02 which under-predicts the strain even more.

![Validation strain correlation plots for Dataset F3 (Slow cooled billets, Extr. temp. = 650°C, Extr. ratio = 4:1) in Table G-10 and Figure G-25, obtained with constants from Table 8 for solution “AIT, DSA Sol 2” in Figure 7 for Dataset G11 in Table 4.](image-url)
Figure 21. Validation strain versus time for Dataset F3 (Slow cooled billets, Extr. temp. = 650°C, Extr. ratio = 4:1) in Table G-10 and Figure G-25, obtained with constants from Table 8 for solution AIT, DSA Sol 2 in Figure 7 for Dataset G11 in Table 4.
6.2.2 Dataset F4: Slow cooled billet, extruded at 650°C at a ratio of 10:1

No conclusive trend emerges between texture and strain from experiments for this creep dataset (Table G-11, using Figure G-26).

Stress correlation and transverse stress versus time plots are provided for constants optimized with Dataset G11 and Dataset G4, respectively. Dataset G4 is also included, as it includes data extruded at different temperatures: Plastic deformation samples were made from material extruded at 815°C and creep samples at 650°C (as for creep set F4 being evaluated here). The correlation plot for the G11 based constants are provided in Figure 22(a) and the strain versus time plot in Figure 23(a). The similar plots for the G4 based constants are provided in Figure 22(b) and Figure 23(b). Note that the AIT, DSA strategy was used for G11 and the AIT strategy for G4. The predictions with constants from optimization set G11 show that the transverse strain is consistently under-predicted, with significant scatter or pluming in the correlation. The predictions for optimization set G4 show that correlation between actual and predicted strain is now reasonable, but the scatter is more pronounced.
Figure 22. Validation strain correlation plots for Dataset F4 (Slow cooled billets, Extr. temp. = 650°C, Extr. ratio = 10:1) in Table G-10 and Figure G-26(a), obtained with constants from Table 8 for solution “AIT, DSA Sol 2” in Figure 7 for Dataset G11 and “AIT Sol 2” in Figure 14 for Dataset G4 in Table 4.
Figure 23. Validation strain versus time for Dataset F4 (Slow cooled billets, Extr. temp. = 650°C, Extr. ratio = 10:1) in Table G-10 and Figure G-26(a), obtained with constants from Table 8 for solution “AIT, DSA Sol 2” in Figure 7 for Dataset G11 and “AIT Sol 2” in Figure 14 for Dataset G4 in Table 4.
6.2.3 Dataset F9: Slow cooled billet, extruded at 815°C at a ratio of 10:1

As expected, the experimental data (Table G-11) indicates an increase in transverse strain as the applied pressure is increased (Figure G-27). However, the increase in strain is not proportional. The strain measurements in the longitudinal direction are questionable.

Stress correlation and transverse stress versus time plots are provided in Figure 24 and Figure 25, respectively. Dataset F9 represents the same manufacturing parameters as used in optimization Dataset G11: In fact, it contains one of the experimental results used for optimization (MPT66-05 as indicated in Figure 25). The transverse strain is predicted reasonably well, with MPT66-02 showing a more pronounced under-prediction. The experimentally observed non-proportional increase of transverse strain with pressure is not reflected in the predictions. It is possible that the transverse measurement of MPT66-04 may have been faulty, suggested by the jump in longitudinal measurement in Figure G-27, which could explain this observation.
Figure 24. Validation strain correlation plot for Dataset F9 (Slow cooled billets, Extr. temp. = 815°C, Extr. ratio = 10:1) in Table G-10 and Figure G-27, obtained with constants from Table 8 for solutions AET Sol 44 and AIT, DSA Sol 2 in Figure 7 for Dataset G11 in Table 4.
Figure 25. Validation strain versus time for Dataset F9 (Slow cooled billets, Extr. temp. = 815°C, Extr. ratio = 10:1) in Table G-10 and Figure G-27, for solution AIT, DSA Sol 2 in Figure 7 for Dataset G11 in Table 4.
6.2.4 Dataset F5: Slow cooled billet, extruded at 975°C at a ratio of 10:1

No consistent correlation is observed between strain measurements and texture in Figure G-28 (Table G-11) for this material, which was not extruded in the α+β phase (see Section 3.1).

The ATXVBO prediction for this material shows a significant bias from the perfect correlation straight line (Figure 26) with significant scatter.

Figure 26. Validation strain correlation plots for Dataset F5 (Slow cooled billets, Extr. temp. = 975°C, Extr. ratio = 10:1) in Table G-10 and Figure G-28, obtained with constants from Table 8 for solutions AET Sol 44 and AIT, DSA Sol 2 in Figure 7 for Dataset G11 in Table 4.
6.2.5 Dataset F6: \(\beta\)-quenched billet, extruded at 815\(^\circ\)C at a ratio of 10:1 –

**Samples subjected to internal pressure only**

Consistent response is observed from the experimental results in Figure G-29 for the two tests performed at the same conditions, with some postulated measurement errors in the axial direction (Table G-11).

The ATXVBO prediction in Figure 27, for the material that was \(\beta\)-quenched at the billet stage with resulting small grain size, is consistent but biased from the perfect correlation straight line. The optimization Dataset G11 used data that was slow cooled with resulting larger grain size.
Figure 27. Validation strain correlation plots for Dataset F6 (β-quenched billets, Extr. temp. = 815°C, Extr. ratio = 10:1) in Table G-10 and Figure G-29, obtained with constants from Table 8 for solutions AET Sol 44 and AIT, DSA Sol 2 in Figure 7 for Dataset G11 in Table 4.
6.2.6 Dataset F6a: $\beta$-quenched billet, extruded at 815°C with 30% cold work or 700°C with 70% cold work - Samples subjected to internal pressure as well as tensile and compressive loads

It is observed in Figure G-30 that the experimental results for the capsules made from material that was extruded at 815°C with 30% CW shows variation in strain as expected with changes in axial load, with the exception of MPT63-05 which appears to underestimate the transverse strain (Table G-11). There is no consistency in transverse response with respect to variation in axial load for the material that was extruded at 700°C with 70% CW (Figure G-31).

The predicted correlation for the material extruded at 815°C with 30% CW is shown in Figure 28(a) while the prediction for the material extruded at 700°C with 70% cold work is provided in Figure 28(b). Consistent with the observation in Section 6.2.5, regarding the bias for material with a small grain size using the constants obtained for a larger grain size, the transverse strain is consistently under-predicted in Figure 28(a) with the exception of MPT63-05. The prediction does not mask the unexpected behaviour observed in the experimental results for this sample. The results for the 700°C with 70% cold work specimens fail to predict the material response with constants obtained with Optimization Dataset G11.
Figure 28. Validation strain correlation plots for Dataset F6a (β-quenched billets, Extr. temp. = 815°C or 700°C, Extr. ratio = 10:1 or 12:1, Cold work = 30% or 70% in Table G-10 and Figure G-30 or Figure G-31), obtained with constants from Table 8 for solutions AET Sol 44 and AIT, DSA Sol 2 in Figure 7 for Dataset G11 in Table 4.
6.2.7 Conclusions from results obtained with thermal creep data

The evaluation of Dataset F9 shows that ATXVBO predicts the strain reasonably well for other creep samples which had been manufactured in the same way as the one used for optimization purposes.

The consistent under-prediction for Dataset F6 and F6a captures the behaviour observed in Figure G-32, that there is a significant difference in response for material with a different billet cooling strategy than the optimization set. Separate optimization is required for each grain size. This aspect is further explored in Section 7.1.2.

The differences between the results obtained for the extrusion temperature and ratio for Dataset F3 (650°C and 4:1) and the optimization set G11 (815°C and 10:1) again show the need for separate optimization for different extrusion parameters. The differences between the extrusion temperature for Dataset F4 (650°C) and the optimization set G11 (815°C), both subjected to a 10:1 extrusion ratio, more specifically show the need for separate optimization for different extrusion temperatures. Having optimized with plasticity data for specimens extruded at 815°C (none available at 650°C) and creep data with specimens extruded at 650°C improved the predictability somewhat but still not satisfactorily. It is to be proven through a separate optimization exercise if ATXVBO would be able to predict the response of material that had been extruded above its α+β phase. The effect of extrusion temperature is further explored in Section 7.1.3 and the effect of extrusion ratio in Section 7.1.4.
CHAPTER 7. SENSITIVITY

It is demonstrated that ATXVBO is able to model the material behaviour of the HCP material subjected to a variety of material and loading conditions. Sensitivity to texture, grain size and extrusion conditions are explored in Section 7.1 which concludes with an evaluation of avenues to deal with observed biases. Section 7.2 investigates the ability of ATXVBO to predict the anisotropic Poisson effect. Section 7.3 explores how ATXVBO responds to loads applied in material non-preferred directions.

7.1 Material variability

The cases evaluated here, with cross references to manufacturing and test data are summarized in Table 734. The effects of texture, grain size as a result of different billet cooling strategies, extrusion temperature and extrusion ratio are explored in Sections 7.1.1 to 7.1.4. Section 7.1.5 explores alternatives to potentially adjust the predictions or constants without re-optimization to account for differences in manufacturing. Conclusions on these sensitivity evaluations are provided in Section 7.1.6.

7.1.1 Texture

The texture of the experimental datasets selected for optimization and validation purposes are compared in Section 3.335. It is observed in Section 3.3.1 that $f_R$ ranges

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34 Experimentally observed correlations between deformation and material manufacturing aspects and characteristics used during this evaluation are summarized in Table G-12.

35 Supporting information in Section G.1
between 0.2 and 0.445, \( f_T \) between 0.523 and 0.64 and \( f_L \) between 0.040 and 0.088 for pressure tubes. Highest stress values are expected in a direction normal to the basal plane (Section 3.4). Since good correlation is observed between experimental and values predicted for Zr-2.5Nb with ATXVBO using constants obtained for material subjected to the same manufacturing steps (Sections 5.5.2.4 and 5.5.3.4), it is concluded that ATXVBO is able to capture the experimentally observed textural sensitivity.

It is now shown in Figure 29 (AET Sol 44) and Figure 30 (AIT Sol 2 and AIT, DSA Sol 2) how sensitive Zr-2.5Nb material is to a change in texture, where a range of \( \Delta f_R = \pm 0.05 \), \( \Delta f_t = \pm 0.05 \) and \( \Delta f_L = \pm 0.05 \) is introduced in consecutive ATXVBO runs to the texture of a plate sample that had been used during optimization. A run with typical tube texture is also included. Figure 30 a) for AIT Sol 2 predicts softening in the axial direction only, which has not been observed in any of the experimental results, confirming the need to include strain rate sensitivity at a temperature of 250\(^\circ\)C. Figure 31 shows a similar plot for G11(3) Solution AIT Sol 10. The concentration of the results in the transverse direction suggests insensitivity to texture or perhaps strain rate at 100\(^\circ\)C: It was observed in Section 5.5.3.3 that the inclusion of a third plasticity dataset did not lead to an improvement in the overall correlation; it was concluded that ATXVBO as formulated is not yet able to capture temperature effects well. This shortcoming might have caused this contraction of results in the transverse direction.
Figure 29. Stress versus strain for AET Sol 44 in Figure 7 accounting for variation in texture from the values used during optimization with Dataset G11.
a) Solution AIT Sol 2 in Figure 7.
b) Solution AIT, DSA Sol 2 in Figure 7.

Figure 30. Stress versus strain for AIT Sol 2 and AIT, DSA Sol 2 accounting for variation in texture from the values used during optimization with Dataset G11.
Figure 31. Stress versus strain for Dataset G11(3) with AIT, DSA Sol 10 described in Table 4.
7.1.2 Billet cooling strategy and grain size

It is shown in Appendix G\textsuperscript{36} that significantly less strain is observed for the material with larger grain size determined by the slow billet cooling as described in Section 3.1 Bullet 5).

The separation between the $\beta$-quenched results in Section 6.2.5 and the slow cooled results in Section 6.2.3 is clearly observed in Figure 32: Strain is consistently under-predicted for the $\beta$-quenched MPT63-03 and MPT63-08 samples.

![Validation strain correlation plots for Dataset “SC vs. $\beta$” (Slow cooled or $\beta$-quenched billets, Extr. temp. = 815°C, Extr. ratio = 10:1, Cold work = 27-30%) in Table G-10 and Figure G-32, obtained with constants from Table 8 for solution AIT, DSA Sol 2 in Figure 7 for Dataset G11 in Table 4.]

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\textsuperscript{36} Section G.1.2 explores sensitivity of texture to grain size. The effect of texture on thermal creep is shown in Figure G-32 and discussed in Table G-11.
7.1.3 Extrusion temperature

As seen in Figure 33, the experimentally observed distinction with respect to extrusion temperature is captured by ATXVBO, showing a bias away from the perfect correlation straight line for data from specimens that were not extruded at 815°C. Appendix G\textsuperscript{37} argues that although their results are very similar, separation would be expected between MPT72-02 and MPT73-02, given their dissimilar values of $f_T$, 0.582 and 0.538\textsuperscript{38}. ATXVBO predicts a noticeable difference between their responses.

![Strain correlation plots for Dataset “Extr temp.” (Slow cooled billets, Extr. temp. = 650, 815 or 975°C, Extr. ratio = 10:1, Cold work = 27-30%) in Table G-10 and Figure G-33, obtained with constants from Table 8 for solution AIT, DSA Sol 2 in Figure 7 for Dataset G11 in Table 4.]

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\textsuperscript{37} Section G.1.3 and Figure G-33 shows distinct separation between results obtained with samples subjected to different extrusion temperatures and good repeatability at the same extrusion temperature.

\textsuperscript{38} Discussed in Table G-11
7.1.4 Extrusion ratio

The only experimental data available that permits a comparison of different extrusion ratios are for data extruded at 650°C, not the 815°C used during optimization with Dataset G11. ATXVBO with AIT, DSA yields a consistent correlation of predicted versus measured strain (Figure 34) with a distinct bias from the perfect correlation straight line, not showing separation for transverse strain, as with the experiments\(^39\).

![Figure 34. Transverse strain correlation plots for Dataset “Extr rat” (Slow cooled billets, Extr. temp. = 650°C, Extr. ratio = 10:1 and 4:1, Cold work = 27-30%) in Table G-10 and Figure G-34, obtained with constants from Table 8 for solution AIT, DSA Sol 2 in Figure 7 for Dataset G11 in Table 4.](image)

\(^39\) Section G.1.4 explores sensitivity of texture to extrusion ratio at 650°C given the available data (see Figure G-34). A clear distinction is observed between data subjected to a ratio of 10:1 versus 4:1 in the axial direction but not the predominantly loaded transverse direction. The apparent absence of a bias in Figure 22(b) (optimization Dataset G4 with 650°C creep data) suggests that the bias can be attributed to not using constants with the same manufacturing history.
7.1.5 Adjustment for material variability

The prediction versus experimental result biases from the perfect correlation straight line observed in the various validation and sensitivity evaluations above for samples subjected to different billet cooling strategies, extrusion temperatures or extrusion ratios are explored further. Two thermal creep datasets, F3 and F4, for material extruded at 650°C and extrusion ratios of 4:1 and 10:1, respectively\(^{40}\), are explored. As before, constants obtained with optimization Dataset G11 (Table 4) for material extruded at 815°C at a ratio of 10:1 was used. The validation correlation plots for the two datasets, that show the biases before any attempted adjustment, are provided in Figure 20 and Figure 22(a), while the strain-time plots are provided in Figure 21 and Figure 23(a).

One possibility to adjust the results for a better prediction is to do a bias shift of the stress or strain results. This has been done in Figure 35 for the strain prediction for F3 in Figure 21. Figure 35 shows the experimental creep strain values and the results of having applied a multiplication of 2.2 to the predicted strain results in Figure 21.

\(^{40}\) Details in Table G-10.
Figure 35. Transverse strain versus time for Dataset F3 (Slow cooled billets, Extr. temp. = 650°C, Extr. ratio = 4:1) from Figure 21 but with a factor of 2.2 applied to the strain predictions.

The bias has been addressed, but the “plume” of the result set has opened up. The correlation between the individual prediction plots and test results are inconsistent and not following a trend.
Alternatively, the value of $k_3$ in the viscosity function Equation (A-16), that characterizes the overstress, is adjusted, by a factor of 1.1 for both Datasets F3 and F4, with strain correlation plots in Figure 36 and Figure 37, and strain versus time plots in Figure 38 and Figure 39, respectively.

It is evident for both Datasets F3 and F4 that the correlation between individual sample and predicted values are not good, with inconsistency in terms of over and under-prediction in a rather wide plume. A comparison of Figure 35 and Figure 38 shows that the width of the plume has again increased with the second approach to change $k_3$ only. Re-optimization would be a better avenue to pursue in this case where extrusion conditions are different.
Figure 36. Strain correlation for Dataset F3 (Slow cooled billets, Extr. temp. = 650°C, Extr. ratio = 4:1) with a factor of 1.1 applied to constant k₃ for “G11 AIT, DSA Sol 2” for comparison to Figure 20.

Figure 37. Strain correlation for Dataset F4 (Slow cooled billets, Extr. temp. = 650°C, Extr. ratio = 10:1) with a factor of 1.1 applied to constant k₃ for “G11 AIT, DSA Sol 2” for comparison to Figure 22.
Figure 38. Transverse strain versus time for Dataset F3 (Slow cooled billets, Extr. temp. = 650°C, Extr. ratio = 4:1) with a factor of 1.1 applied to constant $k_3$ for “G11 AIT, DSA Sol 2” for comparison to Figure 21.
Figure 39. Transverse strain versus time for Dataset F4 (Slow cooled billets, Extr. temp. = 650°C, Extr. ratio = 10:1) with a factor of 1.1 applied to constant $k_3$ for “G11 AIT, DSA Sol 2” for comparison to Figure 21.

7.1.6 Conclusions from investigation into material variability

From the various evaluations of texture variation with different analysis strategies in Section 7.1.1, it is concluded that strain rate sensitivity is captured well for the evaluation of Zr-2.5Nb at 250°C, while not the case for predictions at 100°C. This might mean that Equation (13) should be used for H (Section 4.3.2) at higher temperatures, with another
approach at lower temperatures. It is reconfirmed in Section 7.1.2 that constants need to be optimized for each billet cooling strategy to capture the effect of grain size.

Section 7.1.3 confirms the need for separate optimization for different extrusion temperatures, while Section 7.1.4 suggests that the effect of the extrusion ratio might be small for material extruded at 650°C; creep data for material extruded at the typical 815°C at different extrusion ratios was not available to verify this observation. It is demonstrated Section 7.1.5 that an adjustment of the strain results obtained with constants for another extrusion temperature, or an adjustment of the constant $k_3$, that governs the size of the overstress $g$, does not yield a good prediction and that optimization has to be undertaken for each set of billet cooling and extrusion conditions.

### 7.2 Poisson contraction during axial loading: P and R evaluation

As indicated in Section 3.3.3, Ballinger, Lucas and Pelloux (1984) observed a nonlinear evolution of the ratio of the strain components in the non-test directions. It is established here how ATXVBO predicts strain in the non-test directions. Murty, Jallepalli, & Mahmood (1994) compared the anisotropic response of Zr alloys tested against values predicted with a yield locus based self-consistent model, employing coefficients of anisotropy $R$ (24) and $P$ (25) to characterise the anisotropic response. $R$ is the ratio of transverse direction to normal direction strain increments for a plate uniaxially tested in the rolling direction. $P$ is the ratio of rolling direction to normal direction strain increments for a plate uniaxially tested in the transverse direction.

\[
R = \frac{\Delta \varepsilon_T}{\Delta \varepsilon_R} \quad \text{with} \quad \sigma_T = \sigma_R = 0 \text{ and } \sigma_L \neq 0
\]  

(24)
The experimental values reported by Murty, Jallepalli, & Mahmood are for Zircaloy-4, both for CWSR (Cold Worked Stress-Relieved) and Recrystallized (Rx) material, as well as three other alloys containing different amounts of alloy elements Nb, Sn, Fe, Cr, Mo and Ni, either in the CWSR or Rx condition. The details of the heat treatment and reduction history during manufacturing are not known. The temperature at which the tests were conducted is not known either – room temperature is assumed.

7.2.1 P and R at different textures

The experimental results of Murty, Jallepalli & Mahmood are compared in Figure 40 (250°C) and Figure 41 (100°C) to ATXVBO predictions for Zr-2.5Nb with the same texture, employing AET, DSA and AIT, DSA defined in Section 4.3.3. A further similar comparison is made in Figure 42 and Figure 43, where the texture variation considered in Figure 29 and Figure 30 is used for Zr-2.5Nb instead. Figure 44 and Figure 45 repeat the comparison between ATXVBO and the data of Murty, Jallepalli & Mahmood, however, this time shown as a function of $f_{T-f_R}$ for the same three strategies.
Figure 40. $R$ predicted for Zr-2.5Nb at various textures and 250ºC with ATXVBO using AET, AIT and AIT, DSA solutions identified in Figure 7, compared to test data for Zr alloys (Murty, Jallepalli, & Mahmood, 1994).
Figure 41. P predicted for Zr-2.5Nb at various textures and 100°C with ATXVBO using AET, AIT and AIT, DSA solutions identified in Figure 7, compared to test data for Zr alloys (Murty, Jallepalli, & Mahmood, 1994).
Figure 42. R predicted for Zr-2.5Nb at various textures and 250°C with ATXVBO using AET, AIT and AIT, DSA solutions identified in Figure 7, compared to test data for Zr alloys (Murty, Jallepalli, & Mahmood, 1994).
Figure 43. P predicted for Zr-2.5Nb at various textures and 100°C with ATXVBO using AET, AIT and AIT, DSA solutions identified in Figure 7, compared to test data for Zr alloys (Murty, Jallepalli, & Mahmood, 1994).
Figure 44. $R$ predicted for Zr-2.5Nb at various values of $fT-fR$ and $250^\circ C$ using AET, AIT and AIT, DSA solutions identified in Figure 7, with textures of Zircaloy alloys reported by Murty, Jallepalli, & Mahmood (1994).
Figure 45. $P$ predicted for Zr-2.5Nb at various values of $f_T-f_R$ and $100^\circ C$ using AET, AIT and AIT, DSA solutions identified in Figure 7, with textures of Zircaloy alloys reported by Murty, Jallepalli, & Mahmood (1994).

It is observed in Figure 40 to Figure 43 that $P$ and $R$ are insensitive to changes in texture for predictions following the AET approach. For the AIT approach, results were not obtained for $R$ at $250^\circ C$ for some of the textures using the constants obtained for “AIT Sol 2”. The predictions of $R$ at $250^\circ C$ obtained with “AIT, DSA Sol 2” on the
other hand are consistent with those observed for the other Zr-alloys determined experimentally by Murty et al. At 100°C the predictions of P show an opposite trend: The predictions using “AIT, DSA Sol 2” show no texture sensitivity, while the predictions with “DSA Sol 2” do show sensitivity though not as consistent with the values obtained at room temperature by Murty et al..

7.2.2 P and R at different test temperatures

To further explore the effect of temperature, R and P were evaluated for a range of temperatures in Figure 46 and Figure 47. A comparison was made against experimental data of Wang and Murty (1998), who tested CWSR Zircaloy-4 specimens, annealed at a temperature of 515°C, between room temperature and 500°C. The textures of their plate specimens are not reported but a comparison against a plate material texture for Zr-2.5Nb seems appropriate.
Figure 46. $R$ predicted with ATXVBO for Zr-2.5Nb plate using AET, AIT and AIT, DSA identified in Figure 7, compared to test results for Zircaloy-4(Rx) plate (Wang & Murty, 1998).
Figure 47. $P$ predicted with ATXVBO for Zr-2.5Nb plate using AET, AIT and AIT, DSA identified in Figure 7, compared to test results for Zircaloy-4(Rx) plate (Wang & Murty, 1998).

$P$: Zr-2.5Nb, AET Sol 44: (0.67; 0.162; 0.168)
$P$: Zr-2.5Nb, AIT Sol 2: (0.67; 0.162; 0.168)
$P$: Zr-2.5Nb, AIT, DSA Sol 2: (0.67; 0.162; 0.168)

$P$ - Wang, Murty, 1998 Fig 4, Zircaloy-4 CWSR
As shown in Figure 46, Wang & Murty (1998)\textsuperscript{41} concluded that R is about 1.5 at all temperatures tested while, as seen in Figure 47, that P is about 2.8 from ambient temperature, decreasing when higher than 327\(^{\circ}\)C to eventually a value of 1 (isotropic).

The following observations are made in Figure 46 and Figure 47:

1. The predictions with AET show a continuous increasing dependency of R and P for temperatures up to 500\(^{\circ}\)C, whereas AIT and AIT, DSA based predictions for Zr-2.5Nb are reflecting slope changes observed experimentally with the other Zr-alloys, even consistent above 300\(^{\circ}\)C. However, the predictions of R and P for Zr-2.5Nb at lower temperatures are not consistent with the experimental values.

2. R and P as reported by Wang & Murty (1998) are quite different at lower temperatures, while the predictions obtained for R and P with ATXVBO are quite similar. This inconsistency may be attributed to differences in texture: The predictions used \(f_T = 0.162\) and \(f_L = 0.168\) of plate material. While the texture for the

\textsuperscript{41} There are some potential inconsistencies between the two references used here which rules out an exact comparison between these published results for Zr-alloys and Zr-2.5Nb predictions of R and P with ATXVBO:

1) The result for R of 1.5 obtained by Wang & Murty (1998) for the Zircaloy-4(Rx) plate material in Figure 46 (at room temperature) is significantly less than the 3.18\(\pm\)0.28 for Zircaloy-4 (Rx) reported by Murty, Jallepalli & Mahmood (1994) in Figure 44. The value of \(f_T-f_R\) for plate metal in Figure 46 is not provided by Wang & Murty (1998), but it is expected to be low as \(f_R\) is large.

2) It is also observed that P for Zircaloy-4 obtained by Wang & Murty (1998) in Figure 47 is about 3 while Murty, Jallepalli and Mahmood reported 9.53\(\pm\)0.31 (Figure 45). The value of P of 9.53\(\pm\)0.31 reported in Table 3 of Murty, Jallepalli, & Mahmood (1994) for Zircaloy-4 (CWSR) seems to be much higher than the values reported for the other alloys considered there. Considering the texture and heat treatment similarities with Alloy 3 shown in the same figure, a value of around 4 would have been expected. There might be a typographical error in their Table 3. Murty, Jallepalli, & Mahmood (1994) Table 3 reported that the value for P for recrystallized Zircaloy-4 is 3.76\(\pm\)3.76: This also appears to be a typographical error in the error value presented. These apparent typographical errors are evident in Figure 43.
published experimental values is not known, it is speculated that the texture for this Zircaloy-4 CWSR material might be the same as that reported by Murty, Jallepalli, & Mahmood (1994) for the same material, $f_T = 0.172$ and $f_L = 0.1$, as shown in Figure 40.

### 7.2.3 Conclusions from investigation into Poisson contraction

The conclusion in Section 7.1.6 regarding the need to include strain rate sensitivity in $H$ with Equation (13) at higher temperatures only, appears to be confirmed by the observations made in Sections 7.2.1 and 7.2.2, where results of $R$ and $P$ predicted for Zr-2.5Nb with ATXVBO at $250^\circ$C show consistent trends with those obtained by measurements for Zr-alloys, but not at $100^\circ$C.

### 7.3 Loading not applied in material preferred directions and yield loci

ATXVBO has the ability to predict the response to loads that are not applied in the material preferred directions without having to perform tensorial transformations first, as explained in Appendix A\(^{42}\) and Appendix B. This ability is demonstrated in this section.

The strains applied to the uniaxial plate specimens in Figure 3 (sample tested at $100^\circ$C) was taken as starting point for this biaxial evaluation. The direction of deformation was changed incrementally in a series of bi-axial runs, each time from the undeformed state, while the strain magnitude was maintained as a constant, as shown in Figure 48.

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\(^{42}\) Section A.2
Three texture states were considered, the plate texture similar to that used for optimization as part of Dataset G11 (Table 4), the capsule texture for MPT73 (F) from Dataset G4 (Table 4) as well as the isotropic case. Runs were performed with the AET, AIT as well as AIT, DSA ATXVBO analysis approaches (Section 4.3.3) using constants optimized with Dataset G11. Stress states were captured at increasing effective inelastic strain (\( p \)) intervals for the plate material for the results shown in Figure 49 for a 100\(^\circ\)C and in Figure 51 for a 250\(^\circ\)C evaluation temperature. Yield loci constructed for all three texture states, obtained at an effective strain of 0.2%, are compared in Figure 50 for 100\(^\circ\)C and Figure 52 for 250\(^\circ\)C. Figure 53 shows the response with the constants
obtained after optimization with the AET and AIT analysis approaches if optimized with Dataset G4.
(a) Strategy AET Sol 44 at 100°C.

(b) Strategy AIT Sol 2 at 100°C.
Figure 49. Yield loci at different effective inelastic strain intervals for Zr-2.5Nb plate material at 100°C for different ATXVBO strategies, using constants obtained by optimising Dataset G11 in Table 4.
(a) Strategies AET Sol 44 and AIT Sol 2 at 100°C.
Figure 50. Yield loci at 0.002 effective inelastic strain for Zr-2.5Nb material with different textures at 100°C for different ATXVBO strategies, using constants obtained by optimising Dataset G11 in Table 4.

(b) Strategies AET Sol 44 and AIT, DSA Sol 2 at 100°C.
(a) Strategy AET Sol 44 at 250°C.

(b) Strategy AIT Sol 2 at 250°C.
Figure 51. Yield loci at different effective inelastic strain intervals for Zr-2.5Nb plate material at 250°C for different ATXVBO strategies, using constants obtained by optimising Dataset G11 in Table 4.
(a) Strategies AET Sol 44 and AIT Sol 2 at 250°C.
Figure 52. Yield loci at p=0.002 effective inelastic strain for Zr-2.5Nb material with different textures at 250°C for different ATXVBO strategies, using constants obtained by optimising Dataset G11 in Table 4.
Figure 53. Yield loci at 0.002 effective inelastic strain for Zr-2.5Nb material with different textures at 100°C for AET Sol 77 and AIT Sol 2, using constants obtained by optimising Dataset G4 in Table 4.

It is concluded from Figure 49 to Figure 53 that ATXVBO is capturing the elliptical yield locus shape very well.

An evaluation of the assumption of slip predominantly parallel to the HCP basal planes in Zr alloys (Section 3.4) shows the expected behaviour in Figure 52(a), Figure 52(b) and Figure 53: Considering transverse stress only, a smaller $f_T$ is expected to
results in higher tangential strain and lower tangential stresses. That is captured correctly, with the exception of AIT, DSA Sol 2 in Figure 50(b) at 100°C, where the transverse stress appears to be under-predicted for a higher \( f_T \). For longitudinal stress only, a smaller \( f_L \) is expected to result in higher axial strain and lower axial stresses. That is captured correctly.

These figures echo the conclusion made in earlier sections regarding the inability to properly capture the effect of temperature: Crimping of the yield locus is expected as the evaluation temperature increases, which is not observed from a comparison between Figure 50(b) and Figure 52(b).

### 7.3.1 Conclusions from investigation into loading in non-preferred directions

The elliptical yield locus is predicted consistently, despite the fact that no yield locus is defined in the theory. This is not unexpected given the fact that normality holds with VBO as both the equilibrium stress and kinematic stress are in the same direction as the inelastic strain rate in the asymptotic state (Kreml E., 1996). Relative changes of the yield loci with changes in texture support the theory of slip parallel to basal planes, with a few noted discrepancies: All three approaches AET, AIT and AIT, DSA fail to predict the behaviour meaningfully below 300°C and that the equations used to capture DSA need to be explored further (Recommendation 3)).
CHAPTER 8. CONCLUSIONS

8.1 Summary of conclusions

1) Texture can be incorporated reliably as input variable to describe small deformation of Zr alloys in a phenomenological deformation model by describing the elastic and inelastic material polycrystal tensor properties as functions of single crystal properties and the Kearns factors. This study introduces the concept of describing the inelastic polycrystal properties analogously to the published methods for elastic polycrystal properties.

2) ATXVBO does not rely on a yield surface but still predicts the transition from elastic to inelastic behaviour on a consistent basis. The elliptical yield locus is predicted consistently, despite the fact that no yield locus shape is defined in the theory. This goes a long way to validate the theory and the use of a genetic algorithm for this application.

3) The experimental data from literature that describes the small tensile deformation of Zr alloys with recorded complete texture information supports the theory that slip occurs parallel to the crystal basal planes for the temperatures considered.

4) Experimental data without specific information of the texture and manufacturing history of the samples cannot be used for optimization or validation purposes of this anisotropic deformation model.

5) The effect of dynamic strain aging cannot be described with the correlations as defined in this study. Different DSA correlations need to be considered in different temperature ranges.
6) Assuming equal elastic and inelastic strain component ratios to reduce the number of constants in ATXVBO cannot be used for Zr-2.5Nb.

7) Material from different manufacturing routes should not be combined for optimization purposes.

8.2 Validation of assumptions

The following key assumptions were made (with cross references to the proof of validation):

1) The Zr HCP crystals undergo predominant slip parallel to basal planes and not twinning when the material is subjected to tensile strains. Validation is provided in Section 3.4 for small deformation at temperatures of interest.

2) Anisotropic material properties can be expressed as a function of texture only. Validation is provided in Section 3.2. Note from Section 7.1.6 that optimization is required for every manufacturing route, but that predicting deformation variation as a result of sample to sample texture variation is captured by ATXVBO.

3) Material properties vary linearly or as a second order polynomial with temperature for H in the equilibrium stress rate: Validation from an evaluation of experimental data is provided in Section 4.1.2. However, it is observed in Section 7.2.3 that the values of R and P calculated for Zr-2.5Nb with ATXVBO are different than the values obtained experimentally with Zr alloys, especially at temperatures below 300°C. This leads to Conclusion 5) that this assumption cannot be validated with the formulations of temperature dependency used in ATXVBO considered in this study. This assumption is related to Assumption 8).
4) Use a small deformation model as in-reactor strain values eventually targeted for prediction with ATXVBO are relatively small. The justification for this assumption is presented in Section 3.3.3.

5) The texture does not evolve during small tensile deformation: An argument to justify this assumption is presented in Section 3.3.3.

6) Texture is not a function of temperature: Validation is provided in Section 3.3.3.

7) Anomalous behaviour of Zr-2.5Nb material during thermal creep testing observed by Christodoulou et al. (2002) and attributed to DSA by them could be explained by texture variation instead (Section 3.3.4.2): This assumption cannot be validated unless repeat tests are performed at 250 and 300°C\[^{43}\], with texture uniquely identified for each sample. However, it is demonstrated in Section 7.1.1 that ATXVBO is able to capture the observed textural sensitivity of the material and that the differences observed by Christodoulou et al. (2002) may indeed have been the result of sample-to-sample texture variation instead. Independent tests by Li (2009) did not predict differences in creep response, where the testing was done at a higher 350°C.

8) ATXVBO can predict DSA effects exhibited by Zr alloys, where the adjusted isotropic stress \((\Lambda + H\Gamma)\) used in the equilibrium stress rate Equation (11) is intended to capture DSA effects. \(H\) is either expressed as a function of overstress by Equation (12) for the AET and AIT strategies or also as a function of the inelastic strain rate by Equation (13) for the AIT, DSA strategy. These strategies did not pass

\[^{43}\] Temperatures where anomalies were observed, Figure G-22.
the validation tests at temperatures other than the optimization temperatures, especially below 300°C resulting in Recommendation 3).

8.3 Meeting objectives - Positive attributes of ATXVBO

This summary explains how the objectives identified in Chapter 2 are being met:

Objective 1) – The anisotropic unified model should not have a yield surface.

It is shown in Section 4.1 that the anisotropic unified models used for predicting Zr alloy behaviour in literature all rely on a yield surface, while AVBO not.

Objective 2) – Demonstrate that material anisotropy can be characterised by texture only.

It is shown in Section 3.3.2 from literature how texture correlates with material grain size, extrusion temperature and extrusion ratio for double melted Zr-2.5Nb. The correlations are proven to hold for quadruple melted material as well.

Objective 3) – Show that small tensile deformation of Zr-2.5Nb can be described by one predominant mechanism in support of the choice of a phenomenological approach.

It is shown in Section 3.4 that the experimental Zr-2.5Nb results of Li (2009) also follow the trend exhibited by other Zr alloys to undergo predominant slip parallel to basal planes at the temperatures of interest when subjected to tensile strains. It is also summarized in Sections 3.4 and 4.3.3 how compressive inelastic strain behaviour of Zr alloys experience twinning and different strain hardening/softening characteristics. Potential avenues to also include compressive and cyclic inelastic behaviour in ATXVBO are suggested in Recommendation 5), Chapter 9.

Objective 4) - Introduce the capability to predict inelastic deformation at any constant temperature and non-evolving texture into AVBO.
It is shown in Section 4.3 how AVBO is expanded into ATXVBO which allows temperature and texture as non-evolving input parameters.

**Objective 5) – Use a unified theory that can be expanded to include irradiation effects.**

It is known from literature (Section A.2.6) that isotropic stress equation could be used to introduce irradiation effects.

**Objective 6) – Limit the number of constants.**

It is shown in Sections 4.3.4 and 4.3.5 how the number of constants required was substantially reduced with the introduction of the single crystal based anisotropy tensors. It is shown in Section 5.5.2.4 that a further reduction, assuming equal elastic and inelastic strain component ratios, cannot be used for Zr-2.5Nb.

**Objective 7) – Derive constants from limited test data.**

Section 5.1 describes how in principle, as a result of the introduction of single crystal information, only one uniaxial dataset for plastic deformation and one dataset for thermal creep is required to determine the constants through optimization.

**Objective 8) – Investigate whether the model can handle material manufacturing variability.**

Sections 6.1.1 and 6.2.7 conclude that biases are present in the results obtained with ATXVBO when constants optimized with data for another manufacturing approach are used for predictions. It is also demonstrated in Section 7.1.5 that the results cannot be adjusted with a strain bias corrector or by adjusting one of the viscosity function parameters and that re-optimization is required.
8.4 Potential limitations of ATXVBO

1) The assumptions regarding temperature dependency in Section 4.1.2 and Section 4.3.1.1 require further attention given the inconsistent predictions at different temperatures (Section 8.1, Conclusion 5)).

2) Material from different manufacturing routes cannot be combined for optimization purposes (Section 5.5.3.4).

3) Applying the theory under different conditions than used in this study will require re-evaluation of the supporting arguments for choosing this phenomenological model that does not distinguish between different slip mechanisms and does not include twinning, as observed during the compressive plastic straining of Zircaloy (Section 3.3.3).
CHAPTER 9. RECOMMENDATIONS

1) Repeat plastic deformation tests with sample specific knowledge of specimen texture at different temperatures.

2) Perform thermal creep tests with sample specific knowledge of specimen texture at temperatures below 350°C.

3) Perform numerical experiments with Equations (11) to (13) or variants to establish which correlations provide the best prediction for the deformation of Zr-2.5Nb for different temperatures ranges. It will also be informative if non-linear, for instance Arrhenius-type, relations would better describe the material property temperature dependencies\(^ {44} \).

4) Evaluate ATXVBO as tool to predict irradiation creep and growth by introduction of test based dependencies in the isotropic stress definition.

5) To capture texture evolution while the material is undergoing plastic compressive straining, introduce the capability to account for twinning of HCP crystals. This could be achieved by postulating that a twinned texture is present in a fraction of the overall volume of the material. This will require the introduction of inelastic strain dependent evolution functions for two of the three Kearns factors.

\(^ {44} \) Miller (1987) accounted for dislocation movement phenomena in formulating MATMOD using Arrhenius-like temperature dependent equations. Delobelle et al. (1996) demonstrated that only some of the constants in their theory are temperature-dependent.
CHAPTER 10. REFERENCES


TABLES

Table 1  Comparison between elastic and equivalent inelastic single crystal tensors.

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<th>Elastic strain rate</th>
<th>$c^{sc}[T]$</th>
<th>$s^{sc}[T] = c^{sc}[T]^{-1}$</th>
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<td>Equivalent single crystal inelastic properties</td>
<td>$d^{sc}_e [T]$</td>
<td>$b^{sc}_e [T] = d^{sc}_e [T]^{-1}$</td>
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<td>$d^{sc}_g [T]$</td>
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<td>$d^{sc}_f [T]$</td>
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Table 2  Comparison between elastic and inelastic polycrystal tensors.

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<th>Elastic strain rate</th>
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<th>$S = C[c^{sc}[T], f_R, f_T]^{-1}$</th>
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<tr>
<td>Equivalent single crystal inelastic properties</td>
<td>$D^e[b^{sc}_e [T], f_R, f_T]$</td>
<td>$B^e = D^e[d^{sc}_e [T], f_R, f_T]^{-1}$</td>
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<td>$D^g[b^{sc}_g [T], f_R, f_T]$</td>
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<tr>
<td></td>
<td>$D^f[b^{sc}_f [T], f_R, f_T]$</td>
<td>$B^f = D^f[d^{sc}_f [T], f_R, f_T]^{-1}$</td>
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Table 3  Comparison of number of constants.
(See Section 4.3.5)

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<th>Temp. an input?</th>
<th>Texture an input?</th>
<th>VBO/AVBO variant</th>
<th>Number of constants</th>
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<tr>
<td>Isotropic</td>
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<td>VBO: with DSA, Equation (13) (Ho &amp; Krempl, 2000)</td>
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<td>Anisotropic</td>
<td>Yes</td>
<td>No</td>
<td>AVBO (AIT, Section 4.3.4)</td>
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<td>AVBO, with temp as input variable, Assume inelastic anisotropy tensor ratios equal to the isotropy ratios (AET, Section 4.3.3)</td>
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<td>ATXVBO (AET) (Assume inelastic anisotropy ratios equal the isotropy ratios)</td>
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Table 4  Optimization datasets.

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<th>G9</th>
<th>G4</th>
<th>G11(3)</th>
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<td>Plastic deformation</td>
<td>“Chr 2000 Fig 6a, 250°C, 0.001 1/s, Axial, Plate, $f_R=0.67$, $f_T=0.162$, $f_L=0.168$”</td>
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<td>X</td>
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<td>(From Dataset A2,</td>
<td>(See Table G-5 for manufacturing details.)</td>
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<tr>
<td>Figure G-18.)</td>
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<td>“Chr 2000 Fig 6b, 100°C, 0.001 1/s, Trans, Plate, $f_R=0.67$, $f_T=0.162$, $f_L=0.168$”</td>
<td>X</td>
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<td>(See Table G-5 for manufacturing details.)</td>
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<td>“Chr 2000 Fig 6b, 150°C, 0.001 1/s, Trans, Plate, $f_R=0.67$, $f_T=0.162$, $f_L=0.168$”</td>
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<td>(See Table G-4 for manufacturing details. Texture not uniquely identified for tube samples, as discussed in Section G.2. Texture of Tube A is arbitrarily selected.)</td>
<td>X</td>
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<td>“MPT66-05(F)(S), $f_R=0.359$, $f_T=0.554$, $f_L=0.087$”, both $\varepsilon_L$ and $\varepsilon_T$</td>
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<td>X</td>
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<td>(From Dataset F9, Figure G-27, $\sigma_T=300$MPa, $\sigma_A/\sigma_T=0.476$, 350°C)</td>
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<tr>
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<td>(Extruded at 815°C, See Table G-8 for manufacturing details.)</td>
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<td>Thermal creep</td>
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Table 5. Creep tests performed at 350°C (Li W., 2009): Filtered combinations.

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<tr>
<th>Dataset</th>
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Table 6. Summary of uniaxial plastic deformation and biaxial creep optimization and validation evaluations with ATXVBO.

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Stress-strain: Datasets G11 and G9: Figure G-18
Strain-time: Datasets G11 and G9: Figure G-27
## Predictions:

(Legend at bottom of table)

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Legend for Table 6 and 6:
P: Plastic deformation at constant strain rate  
MOO: Multi-Objective Optimization,  
C: Creep deformation  
V: Validation,  
S: Sensitivity evaluation,  
β: β-quenched billet,  
CW: Cold Work post extrusion  
U: Unknown
Table 7. Summary of uniaxial plastic deformation and biaxial creep sensitivity evaluations with ATXVBO.

This table is referenced in 6.2.7. Its legend is provided on the first page of this appendix.

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Table 8 Constant values optimized with ATXVBO.

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APPENDIX A. OVERVIEW OF VBO AND AVBO

This is a literature overview of VBO and AVBO. It summarizes the background covered in a number of publications and assists in understanding the generalization from VBO to AVBO. It includes several equations\(^{45}\) for reference purposes only.

A.1. VBO

A.1.1. Uniaxial VBO

Based on experimental observations, Krempl, McMahon, & Yao (1986) defined a model to describe inelastic strain rate as a function of overstress \(\sigma - g\). Their uniaxial flow law is captured in Equation (A-1):

\[
\dot{\varepsilon} = \dot{\varepsilon}^{\text{el}} + \dot{\varepsilon}^{\text{in}} = \frac{\dot{\sigma}}{E} + \frac{\sigma - g}{E \kappa[\sigma - g]} \tag{A-1}
\]

\(\sigma\) is the stress achieved at a fast strain rate. \(g\) is the equilibrium stress, the stress achieved at a very slow strain rate. \(E\) is Young’s modulus and \(\kappa\) is the viscosity function that represents a relaxation time, a decreasing function of overstress.

Krempl (1995) later demonstrated that the equation can also be obtained by a generalization of the standard linear system (SLS), as depicted in Figure A-1\(^{45}\): For an SLS, the viscoelastic response as shown in Figure A-1(a), is described by:

\[
\dot{\varepsilon} = \frac{\dot{\sigma}}{E_1} + \frac{\sigma - aE_2 \varepsilon}{a\zeta} = \dot{\varepsilon}^{\text{el}} + \dot{\varepsilon}^{\text{in}}, \quad a = \frac{E_1}{E_1 + E_2} \tag{A-2}
\]

\(^{45}\) Some of the symbols used here are only applicable to this discussion and are not listed in the List of Abbreviations, Symbols and Definitions.
By changing the Voigt element (Figure A-1(b), with a strike through its modified components) to denote non-linear response with strain, and allowing the dashpot to be governed by overstress, the non-linear viscoplastic response is described by Equation Error! Reference source not found.). Viscoplastic behaviour of the equilibrium stress $g[\varepsilon]$ is modeled by a still rate–independent growth law, no longer a straight line.

Krempl, McMahon, & Yao (1986) defined the equilibrium stress as

$$
\dot{g} = \psi[\sigma - g]\dot{\varepsilon} - \frac{g - f}{b[\sigma - g]}|\dot{\varepsilon}|. 
$$

(A-3)

$\psi$, coined the shape function, also postulated to be overstress dependent, is a Vocé shape function that describes the transition from elastic to inelastic behaviour with $1 < \psi[\sigma - g] < E_t$. To obtain the appropriate asymptotic value $\{g\}$, $b$ was defined as:

$$
b[\sigma - g] = \frac{A}{\psi[\sigma - g] - E_t}. 
$$

(A-4)

The kinematic stress

$$
f = E_t\varepsilon
$$

(A-5)
captures the residual stress: It was coined the kinematic stress as it models the Bauschinger effect. $A$ was labeled the isotropic stress, as it predicts cyclic neutral behaviour, but with an evolution law, it can predict cyclic hardening/softening.

For $t \to 0$, Equations (A-2) and (A-4) predict elastic behaviour. For $t \to \infty$, Equation (A-2) shows that $\{\dot{\sigma}\} = \{\dot{g}\}$ and Equation (A-4) shows that $\{\dot{g}\} = \{\dot{f}\}$. It is also evident that $\left\{\frac{d\sigma}{d\varepsilon}\right\} = \left\{\frac{dg}{d\varepsilon}\right\} = \left\{\frac{df}{d\varepsilon}\right\} = E_t$. The evolution of the various stress terms are depicted in Figure A-1(b).
A.1.2. **Total stress (VBO)**

\[
\sigma = (\sigma - g) + (g - f) + f
\]  
(A-6)

Multi-axial formulations express the viscosity and shape functions as functions of the effective overstress \( \Gamma \) (A-72) instead of the overstress. The multi-axial small deformation isotropic version of VBO (Krempl E., 1996) as used by Majors (1993) is expressed through the following set of nonlinear first-order differential equations and supporting definitions:

A.1.3. **Total strain rate (VBO)**

\[
\dot{\varepsilon} = \dot{\varepsilon}^{\text{el}} + \dot{\varepsilon}^{\text{in}} \quad \text{or} \quad \dot{\varepsilon} = \dot{\varepsilon}^{\text{el}} + \dot{\varepsilon}^{\text{in}}
\]  
(A-7)

A.1.4. **Linear elastic strain rate (VBO)**

From the linear elastic stress-strain relation

\[
\varepsilon_{ij}^{\text{el}} = \frac{1 + \nu}{E}\sigma_{ij} - \frac{\nu}{E}\delta_{ij}\sigma_{kk}, \ m, n, k = 1 \to 3 \quad \dot{\varepsilon}^{\text{el}} = \frac{1 + \nu}{E}\dot{\sigma} - \frac{\nu}{E}\delta_{ij}\text{tr}(\dot{\sigma})I
\]  
(A-8)

it follows that

\[
\dot{\varepsilon}_{kk}^{\text{el}} = \frac{1 + \nu}{E}\dot{\sigma}_{kk} - \frac{\nu}{E}3\dot{\sigma}_{kk} = \frac{1 - 2\nu}{E}\dot{\sigma}_{kk} \quad \text{tr}(\dot{\varepsilon}^{\text{el}}) = \frac{1 - 2\nu}{E}\text{tr}(\dot{\sigma})
\]  
(A-9)

so that equation (A-7) can be described in terms of the deviatoric components as

\[
\left(\dot{\varepsilon}_{ij}^{\text{el}} + \frac{1}{3}\delta_{ij}\dot{\varepsilon}_{kk}^{\text{el}}\right) = \frac{1 + \nu}{E}\left(\dot{\sigma}_{ij}^{d} + \frac{1}{3}\delta_{ij}\dot{\sigma}_{kk}^{d}\right) - \frac{\nu}{E}\delta_{ij}\dot{\sigma}_{kk}^{d}
\]  
(A-10)

which leads to

\[
\dot{\varepsilon}_{ij}^{\text{el}} = \frac{1 + \nu}{E}\dot{\sigma}_{ij}^{d}
\]  
(A-11)

Or, strain rate is often expressed as:
\[ \varepsilon_{ij}^{el} = \frac{1 + \nu^{el}}{E} \left( \sigma_{ij}^{d} + \frac{1}{3} \delta_{ij} \sigma_{kk}^{d} \right) - \frac{\nu^{el}}{E} \delta_{ij} \sigma_{kk}^{d} \]

\[ \varepsilon_{ij}^{el} = \frac{1 + \nu^{el}}{E} \sigma_{ij}^{d} + 1 - \frac{2\nu^{el}}{3E} \delta_{ij} \sigma_{kk}^{d} + \frac{1 - 2\nu^{el}}{3E} \delta_{ij} \text{tr}(\sigma)I \]  

(A-12)

### A.1.5. Inelastic strain rate (VBO)

From Equation Error! Reference source not found., the inelastic strain rate is defined as

\[ \varepsilon^{in} = \frac{(1 + \nu^{in})}{k[\Gamma]} \sigma^{d} = \frac{(1 + \nu^{in})}{E k[\Gamma]} (\sigma^{d} - g^{d}) \]  

(A-13)

where the deviatoric overstress \( \sigma^{d} \) is defined as

\[ \sigma^{d} = \sigma^{d} - g^{d} \]  

(A-14)

With \( \nu^{in} = 0.5 \), it follows that

\[ \varepsilon^{in} = \frac{3}{2} \frac{(\sigma^{d} - g^{d})}{k[\Gamma]} = \frac{3}{2} \frac{(\sigma^{d} - g^{d})}{E k[\Gamma]} \]  

(A-15)

as most often stated in literature.

The viscosity function, characterizing the overstress, is usually expressed as

\[ k[\Gamma] = k_{1} \left( 1 + \frac{\Gamma}{k_{2}} \right)^{-k_{3}} \]  

(A-16)

\( k_{1}, k_{2} \) and \( k_{3} \) are constants. Majors introduced an enhancement by substituting \( k_{3} \) with \( k_{3\nu} \) to allow a better fit of overstress amplitudes at high rates, where \( k \) had been found to over-predict the overstress. He let

\[ k_{3\nu}[\Gamma] = k_{3} (1 + \exp(k_{5}(\Gamma - k_{4}))) \]  

(A-17)

so that
A.1.6. Equilibrium stress rate (VBO)

There are two definitions of the equilibrium stress, the Yao, Equation (A-34), and Lee, Equation (A-49), versions. The difference between the two equations is in the dynamic recovery term (see Section A.1.6.6) as compared by Krempl and Gleason (1996). Both the Yao and Lee versions are discussed below, as it is required in section A.2.4 to clearly document the origin of the equilibrium stress rate used for AVBO.

The following two relations, from Equations (A-11) and (A-13), are used for the conversion between stress and strain based formulations:

\[
\frac{\dot{e}^{el}}{1 + \nu^{el}} = \frac{\sigma^d}{E}
\]  
(A-21)

\[
k[\Gamma] = k_1 \left(1 + \frac{\Gamma}{k_2}\right)^{-k_3(1+\exp (k_5(\Gamma-k_4)))}. 
\]  
(A-18)

Since \(k[\Gamma] = \frac{k[\Gamma]}{E}\) it follows that \(k_1 = \frac{k_1}{E}\). Therefore,

\[
\tilde{k}[\Gamma] = \frac{k_1}{E} \left(1 + \frac{\Gamma}{k_2}\right)^{-k_3(1+\exp (k_5(\Gamma-k_4)))}. 
\]  
(A-19)

Tachibana & Krempl (1995) did not apply a viscosity function in the following variation of the inelastic strain rate flow law for high homologous temperatures. They opted to write it in the form of a power law creep equation (only provided for reference purposes):

\[
\dot{\varepsilon}^{in} = \frac{3B}{2} \left(\frac{1}{\sigma}\right)^m \left(\frac{\sigma^d - g^d}{\Gamma}\right)
\]  
(A-20)
\[
\dot{\mathbf{e}}^{\text{in}} \frac{1}{1 + \nu^{\text{in}}} = \left( \sigma^{d} - \mathbf{g}^{d} \right) \frac{1}{E \bar{k}[\Gamma]}
\]  
(A-22)

A.1.6.1. Equilibrium stress rate with Yao’s dynamic recovery definition

Equation (A-3) is restated as

\[
\dot{\mathbf{g}}^{d} = \psi[\Gamma] \left( \frac{\mathbf{e}^{\text{el}}}{1 + \nu^{\text{el}}} + \frac{\dot{\mathbf{e}}^{\text{in}}}{1 + \nu^{\text{in}}} \right) - \frac{\mathbf{g}^{d} - \mathbf{f}^{d}}{b[\Gamma]} \dot{\mathbf{p}},
\]  
(A-23)

where \( \dot{\mathbf{p}} \) is the effective inelastic strain rate, as defined in Equation (A-30). Since

\[b[\Gamma] = \frac{A_{Y}}{\psi[\Gamma] - E_{t}},\]  
(A-24)

with \( A_{Y} \) the isotropic stress considered to be a constant by Yao, \( \dot{\mathbf{g}}^{d} \) becomes

\[
\dot{\mathbf{g}}^{d} = \psi[\Gamma] \left( \frac{\mathbf{e}^{\text{el}}}{1 + \nu^{\text{el}}} + \frac{\dot{\mathbf{e}}^{\text{in}}}{1 + \nu^{\text{in}}} \right) - (\psi[\Gamma] - E_{t}) \left( \frac{\mathbf{g}^{d} - \mathbf{f}^{d}}{A_{Y}} \right) \dot{\mathbf{p}}
\]  
(A-25)

The factor \( \frac{\mathbf{g}^{d} - \mathbf{f}^{d}}{A_{Y}} \) approaches 1 at large strain. \( \psi[\Gamma] \), the shape function, is described as a Voce function and varies between \( \sim 0.99 E \) and \( E_{t} \) for \( 0 \leq \Gamma \leq \infty \). The normalized shape function \( \overline{\psi}[\Gamma] \) is expressed as

\[\overline{\psi}[\Gamma] \] is sometimes expressed in terms of overall quantities (Krempl & Gleason, 1996).

\[b[\Gamma] = \frac{A^{*}}{\psi[\Gamma] - E_{t}^{*}}\]

with

\[A^{*} = \frac{A}{1 + \frac{E_{t}}{E}}\]

and the overall tangent modulus (Krempl, Creep-Plasticity Interaction, 1999)

\[E_{t}^{*} = \frac{E_{t}}{1 + \frac{E_{t}}{E}} \] or \[1 + \frac{1}{E_{t}^{*}} = \frac{1}{E} + \frac{1}{E_{t}}\]

To avoid confusion, the equilibrium stress is not expressed in terms of \( b[\Gamma] \) in this summary.
\[ \bar{\psi}[\Gamma] = \frac{\psi[\Gamma]}{E} = \frac{\psi_1 + (\psi_2 - \psi_1)e^{(-\psi_3 \Gamma)}}{E} \]  

(A-26)

where \( \psi_1, \psi_2 \) and \( \psi_3 \) are constants. The value of \( \bar{\psi}_2 = \psi_2/E \) is about 0.95 to model quasi-elastic behaviour. The normalized shape function was adapted for 9Cr-1Mo steel by Majors (1993) to include dependency on a decreasing value of \( A \):

\[ \bar{\psi}[\Gamma] = \frac{\psi_1}{E} + \frac{\psi_2^* [A] - \psi_1}{E} e^{(-\psi_3 \Gamma)} \]  

(A-27)

with

\[ \psi_2^* [A] = \frac{A_0 \left( \frac{1}{\psi_2^0 - 1} \right)}{A_0 \left( \psi_2^0 (A - A_0) \right) + 1} \]  

(A-28)

\( \psi_2^* = \psi_2^0 \) when \( A = A_0 \). Substituting Equations (A-21) and (A-22) into (A-25) results in

\[ \dot{\mathbf{g}}^d = \psi[\Gamma] \left( \frac{\sigma^d}{E} + \frac{(\sigma^d - g^d)}{E k[\Gamma]} \right) - (\psi[\Gamma] - E_c) \frac{(g^d - f^d)}{A} \dot{p}. \]  

(A-29)

\( \dot{p} \) is defined in terms of strain as

\[ \dot{p} = \sqrt{\frac{\dot{e}_{\text{in}} \cdot \dot{e}_{\text{in}}}{1 + \nu_{\text{in}}}} = \sqrt{\frac{\dot{e}_{ij} \dot{e}_{ij}}{1 + \nu_{\text{in}}}} \quad i, j = 1 \text{ to } 3 \]

(A-30)

Therefore, using Equation (A-13),

\[ \dot{p} = \frac{1}{E k[\Gamma]} \sqrt{(1 + \nu_{\text{in}})(\sigma^d - g^d) \cdot (\sigma^d - g^d)}. \]

(A-31)

Then, the relation between the effective overstress \( \Gamma \), defined later in Equation (A-72) and effective inelastic strain rate \( \dot{p} \) is described by the flow rule
\[ \dot{\mathbf{g}}^d = \frac{\dot{\mathbf{v}}}{E} + \frac{\dot{\mathbf{v}}}{E + \frac{1}{E k[\Gamma]}} \left( \sigma^d - \mathbf{g}^d \right) - \left( \mathbf{g}^d - f^d \right) \frac{\mathbf{K}}{E k[\Gamma]} \]  
(A-32)

Using Equations (A-32), Equation (A-29) becomes

\[ \dot{\mathbf{g}}^d = \psi[\Gamma] \left( \frac{\dot{\mathbf{v}}}{E} + \frac{\dot{\mathbf{v}}}{E k[\Gamma]} \right) - \left( \mathbf{g}^d - f^d \right) \frac{\mathbf{K}}{E k[\Gamma]} - \left( \psi[\Gamma] - E_t \right) \left( \mathbf{g}^d - f^d \right) \frac{\mathbf{K}}{E k[\Gamma]} \]  
(A-33)

Therefore, expressed in terms of stress components, the Yao version of the equilibrium stress is

\[ \dot{\mathbf{g}}^d = \frac{\dot{\mathbf{v}}}{E} + \frac{\dot{\mathbf{v}}}{E k[\Gamma]} \left( \sigma^d - \mathbf{g}^d \right) \]  
(A-34)

Substituting Equations (A-21), (A-22) and (A-32) into (A-34) expresses the Yao version of equilibrium stress in terms of strain:

\[ \dot{\mathbf{g}}^d = \psi[\Gamma] \left( \frac{\dot{\mathbf{v}}}{E} + \frac{\dot{\mathbf{v}}}{E k[\Gamma]} \right) - \left( \mathbf{g}^d - f^d \right) \frac{\mathbf{K}}{E k[\Gamma]} \]  
(A-35)

The last term in the Yao Equations (A-34) and (A-35), \( E_t \frac{\mathbf{g}^d - f^d}{A} \), was modified by M.R. Eggleston (Majors, 1993) to be reliant on the deviatoric kinematic strain rate \( \mathbf{f}^d (1 - \psi[\Gamma]) \) instead.

\[ \dot{\mathbf{g}}^d = \psi[\Gamma] \mathbf{g}^d + \frac{\dot{\mathbf{v}}}{E} + \frac{\dot{\mathbf{v}}}{E k[\Gamma]} \left( \sigma^d - \mathbf{g}^d \right) \]  
(A-36)

and

\[ \dot{\mathbf{g}}^d = E \psi[\Gamma] \left( \frac{\dot{\mathbf{v}}}{E} + \frac{\dot{\mathbf{v}}}{E k[\Gamma]} \right) - \left( \mathbf{g}^d - f^d \right) \frac{\mathbf{K}}{E k[\Gamma]} \]  
(A-37)
Note that, since \( f^d = \frac{E_t}{E} \left( \sigma^d - g^d \right) \) (Equation (A-62), the Eggleston version of the last term can be expressed as

\[
\dot{f}^d (1 - \bar{\Psi} [\Gamma]) = \frac{E_t}{E} \frac{\sigma^d - g^d}{k[\Gamma]} (1 - \bar{\Psi} [\Gamma])
\]  

(A-38)

Therefore:

\[
\frac{E_t}{E} \frac{\sigma^d - g^d}{k[\Gamma]} (1 - \bar{\Psi} [\Gamma]) \equiv E_t \frac{\left( g^d - f^d \right)}{A} \Gamma
\]  

(A-39)

\[
(\sigma^d - g^d)(1 - \bar{\Psi} [\Gamma]) \equiv (g^d - f^d) \frac{\Gamma}{A}
\]  

(A-40)

The Eggleston version of the equilibrium stress, now expressed in terms of the deviatoric overstress, then is

\[
g^d = \bar{\Psi} [\Gamma] \sigma^d + \bar{\Psi} [\Gamma] \left( \frac{\sigma^d - g^d}{k[\Gamma]} - \frac{(\sigma^d - g^d)(1 - \bar{\Psi} [\Gamma])}{k[\Gamma]} \right)
\]  

(A-41)

\[
+ \frac{E_t}{E} \frac{\sigma^d - g^d}{k[\Gamma]} (1 - \bar{\Psi} [\Gamma]) + \frac{E_t}{E} \sigma^d (1 - \bar{\Psi} [\Gamma])
\]  

(A-42)

and

\[
= E \bar{\Psi} [\Gamma] \frac{\dot{\epsilon}^{\text{el}}}{1 + \nu} + (E \bar{\Psi} [\Gamma]^2 - E_t \bar{\Psi} [\Gamma] + E_t) \frac{\dot{\epsilon}^{\text{in}}}{1 + \nu / \nu^{\text{in}}}
\]  

(A-43)

Note that the Eggleston version lost its dependency on \( A \).

Majors introduced the constant \( c \) instead of \( E \), with a value close to \( E \), enabling additional control over “yielding” behaviour. He furthermore introduced an additional term \( R[g_{\text{eff}}] g^d \) to account for recovery. Functions similar to this recovery function were
being investigated by Cernocky and Krempl (1978). Majors’ version of $\dot{g}^d$, based on Yao and Eggleston’s formulation of dynamic recovery therefore reads as follows, expressed in terms of deviatoric stress and strain, respectively, with $R[g_{\text{eff}}]g^d$ defined in Equation (A-59):

$$
\dot{g}^d = \bar{\psi}[\Gamma] \dot{\sigma}^d + c \bar{\psi}[\Gamma] \left( \frac{\sigma^d - g^d}{E k[\Gamma]} - \frac{g^d - f^d}{A} \frac{\Gamma}{E k[\Gamma]} \right) + \tilde{f}^d (1 - \bar{\psi}[\Gamma]) - R[g_{\text{eff}}]g^d \quad (A-44)
$$

and

$$
\dot{g}^d = E \bar{\psi}[\Gamma] \frac{\dot{e}^{el}}{1 + \nu^{el}} + c \bar{\psi}[\Gamma] \left( \frac{\dot{e}^{in}}{1 + \nu^{in}} - \frac{g^d - f^d}{A} \frac{\rho}{E} \right) + \tilde{f}^d (1 - \bar{\psi}[\Gamma]) - R[g_{\text{eff}}]g^d \quad (A-45)
$$

A.1.6.2. **Equilibrium stress rate with Sütçü’s dynamic recovery definition**

Another growth law was proposed by Sütçü (1985) for his anisotropic theory. This approach uses a different definition of dynamic recovery,

$$
\frac{\sigma^d - g^d}{A} \frac{\Theta}{E k[\Gamma]} \text{ instead of } \frac{g^d - f^d}{A} \frac{\Gamma}{E k[\Gamma]}.
$$

When this substitution is made in Equation (A-34), somewhat re-arranged,

$$
\dot{g}^d = \bar{\psi}[\Gamma] \dot{\sigma}^d + \bar{\psi}[\Gamma] \left( \frac{\sigma^d - g^d}{k[\Gamma]} - E \frac{g^d - f^d}{A} \frac{\Gamma}{E k[\Gamma]} \right) + \frac{g^d - f^d}{A} \frac{\Gamma}{E k[\Gamma]} E_t \quad (A-46)
$$

it yields

$$
\dot{g}^d = \bar{\psi}[\Gamma] \dot{\sigma}^d + \bar{\psi}[\Gamma] \left( \frac{\sigma^d - g^d}{k[\Gamma]} - E \frac{\sigma^d - g^d}{A} \frac{\Theta}{E k[\Gamma]} \right) + \frac{\sigma^d - g^d}{A} \frac{\Theta}{E k[\Gamma]} E_t \quad (A-46)
$$

$$
= \bar{\psi}[\Gamma] \dot{\sigma}^d + \bar{\psi}[\Gamma] \frac{\sigma^d - g^d}{k[\Gamma]} \left( 1 - \frac{\Theta}{A} + \frac{E_t}{A E \bar{\psi}[\Gamma]} \right)
$$
\[
\dot{g}^d = \ddot{\psi}[\Gamma] \sigma^d + \ddot{\psi}[\Gamma] \frac{\sigma^d - g^d}{k[\Gamma]} \left( 1 - \frac{\Theta}{A} \left( 1 - \frac{E_t}{E\dot{\psi}[\Gamma]} \right) \right)
\] (A-47)

Krempl & Gleason (1996) indicated that the alternative equilibrium growth law was proposed by Sütçü and Krempl, yet proposed it be called the Lee formulation – note that Lee and Krempl (1991) did credit Sütçü for introducing the dynamic equivalency. Using Equations (A-21) and (A-22) in Equation (A-47) results in

\[
\dot{g}^d = E\ddot{\psi}[\Gamma] \left( \frac{\dot{e}^{el}}{1 + \nu^{el}} + \frac{\dot{e}^{in}}{1 + \nu^{in}} - \frac{\Theta}{A} \left( 1 - \frac{E_t}{E\dot{\psi}[\Gamma]} \right) \frac{\dot{e}^{in}}{1 + \nu^{in}} \right).
\] (A-48)

Equation (A-48) is used in Section A.2.4, Equation (A-92) to demonstrate the suspected origin of the equilibrium stress formulation used by Sütçü (1985).

A.1.6.3. **Equilibrium stress rate with Lee’s dynamic recovery definition**

A different approach was proposed by Lee (1989) to express the dynamic recovery term in terms of the overstress. His version was derived utilizing an interpolation strategy. Equation A14 of Lee & Krempl (1991) describes the deviatoric equilibrium stress rate as follows, with \( \Theta \) defined in Equation (A-75):

\[
\dot{g}^d = E\ddot{\psi}[\Gamma] \left( \frac{\dot{e}^{el}}{1 + \nu^{el}} + \frac{\dot{e}^{in}}{1 + \nu^{in}} - \frac{\Theta}{A} \left( E\ddot{\psi}[\Gamma] \left( 1 + \frac{E_t}{E} \right) - E_t \right) \frac{\dot{e}^{in}}{1 + \nu^{in}} \right)
\]

which can be restated as

\[
\dot{g}^d = E\ddot{\psi}[\Gamma] \left( \frac{\dot{e}^{el}}{1 + \nu^{el}} + \frac{\dot{e}^{in}}{1 + \nu^{in}} - \frac{\Theta}{A} \left( 1 - \frac{E_t}{E\dot{\psi}[\Gamma]} \left( 1 - \ddot{\psi}[\Gamma] \right) \right) \frac{\dot{e}^{in}}{1 + \nu^{in}} \right)
\] (A-49)

It is only provided for reference purposes.
A.1.6.4. Equilibrium stress rate adjusted for modeling DSA

DSA is applicable to Zr-alloys (Section 3.3.4.2). Provision has been made in VBO to address this strain rate related phenomenon: Ho and Krempl (2000) added an overstress dependent function to the isotropic stress, using the Yao formulation of equilibrium stress rate of Majors (omitting the recovery term $R[g_{eff}]^d$ and letting $c = E$, Equations (A-44) and (A-45). Omitting the recovery term potentially removes the capability of modeling secondary and tertiary creep effects (section A.1.6.6). However, Ho and Krempl (2002) showed that dynamic recovery and secondary and tertiary creep effects are captured with their modified formulation of $\dot{g}^d$:

$$\dot{g}^d = \ddot{\psi}[\Gamma] g^d + \ddot{\psi}[\Gamma] \left( \frac{\sigma^d - g^d}{k[\Gamma]} - \frac{g^d - f^d}{A + H\Gamma [\Gamma]} \right) + \dot{f}^d (1 - \ddot{\psi}[\Gamma])$$  \hspace{1cm} (A-50)

$$\dot{g}^d = E \ddot{\psi}[\Gamma] \frac{\dot{\epsilon}^{el}}{1 + \nu^{el}} + E \ddot{\psi}[\Gamma] \left( \frac{\dot{\epsilon}^{in}}{1 + \nu^{in}} - \frac{g^d - f^d}{A + H\Gamma \dot{p}} \right) + \dot{f}^d (1 - \ddot{\psi}[\Gamma])$$  \hspace{1cm} (A-51)

Strain rate sensitivity was introduced as functions of either the accumulated effective strain and/or the accumulated effective strain rate:

$$H[p] = H_1 e^{-H_2 p} + H_3$$  \hspace{1cm} (A-52)

$$H[\dot{p}] = H_3 \frac{1}{H_1 \sqrt{2\pi}} e^{-\frac{(\ln \dot{p} - H_2)^2}{2(H_1)^2}}$$  \hspace{1cm} (A-53)

$$H[p, \dot{p}] = (H_3 e^{-H_4 p} + H_5) \frac{1}{H_1 \sqrt{2\pi}} e^{-\frac{(\ln \dot{p} - H_2)^2}{2(H_1)^2}}$$  \hspace{1cm} (A-54)

Equation (A-53) is a normal distribution of $\ln \dot{p}$, with $H_2$ the mean and $H_1$ the standard deviation. This equation was selected for implementation in ATXVBO, with the assumption that DSA is a strain rate dependent phenomenon for Zr alloys.

A-12
For this work, another version of $H$ was explored, by setting it as a constant,

$$H = H_3$$ \hfill (A-55)\]

making the adjustment of $A$ in Equations (A-50) and (A-51) a function of overstress only. This was done to inspect for the effect of strain rate only. Results obtained with this version, Equation (A-55), is identified as AIT, while results obtained with Equation (A-53) is labelled as AIT, DSA. These concepts are discussed in Section 4.3.3.

If the same Ho based approach were to be followed using the modified Yao Equations (A-47) and (A-48) of Sütçü (1985), the deviatoric strain rate is expressed as:

$$
\dot{\varepsilon}^d = \bar{\Psi}^{[\Gamma]} \dot{\varepsilon}^d + \bar{\Psi}^{[\Gamma]} \frac{\sigma^d - \mathbf{g}^d}{k^{[\Gamma]}} \left( 1 - \frac{\Theta}{A + \lambda H} \left( 1 - \frac{E_t}{E \bar{\Psi}^{[\Gamma]}} \right) \right) \hfill (A-56)
$$

$$
\dot{\varepsilon}^d = E \bar{\Psi}^{[\Gamma]} \left( \frac{\dot{e}^{el}}{1 + \nu^{el}} + \frac{\dot{e}^{in}}{1 + \nu^{in}} - \frac{\Theta}{A + \lambda H} \left( 1 - \frac{E_t}{E \bar{\Psi}^{[\Gamma]}} \right) \frac{\dot{e}^{in}}{1 + \nu^{in}} \right) \hfill (A-57)
$$

As stated in Section 4.3.2, this equation has been adopted for implementation in ATXVBO. The decision is based on observations made following a comparison of Equation (A-48) with Equation (A-92) for AVBO, also introducing DSA modelling capability.

**A.1.6.5. Equilibrium stress at high homologous temperatures (VBO)**

The Tachibana and Krempl version (1995) does not include the kinematic hardening state variable $\mathbf{f}^d$, as it was argued that work hardening is negligible at high temperature.

$$
\dot{\mathbf{g}}^d = \bar{\Psi}^{[\Gamma]} \dot{\mathbf{g}}^d + c \bar{\Psi}^{[\Gamma]} \left( B \left( \frac{\Gamma^m}{\sigma} \right)^m \left( \frac{\sigma^d - \mathbf{g}^d}{\Gamma} \right) - \frac{\mathbf{g}^d}{A \dot{p}} \right) - R[g_{eff}] \mathbf{g}^d \hfill (A-58)
$$
B, $\bar{\sigma}$, and m are temperature dependent constants (Tachibana & Krempl, 1995). This formulation is only provided for reference purposes.

### A.1.6.6. Summary of definitions as applicable to equilibrium stress

In the various forms of the equilibrium stress above, the various terms / components serve the following purposes:

\[ \psi[\Gamma] \sigma^d \]  
Elastic contribution

\[ \psi[\Gamma] \frac{\sigma^d - g^d}{k[\Gamma]} \]  
Inelastic contribution

\[ \psi[\Gamma] \frac{g^d - f^d}{A} \frac{\Gamma}{k[\Gamma]} \]  
Dynamic recovery using Yao version.

\[ \psi[\Gamma] \frac{\sigma^d - g^d}{A} \frac{\Theta}{k[\Gamma]} \]  
Dynamic recovery using Lee version (Krempl E. , 1996)

\[ (g^d - f^d) \frac{E_t}{A} \frac{\Gamma}{E k[\Gamma]} \]  
Kinematic hardening

\[ \hat{f}^d (1 - \psi[\Gamma]) \]  
Kinematic hardening using the Eggleston approach (Majors, 1993). The equilibrium stress approaches the tangent modulus without the growth term $\hat{f}^d (1 - \psi)$.

\[ A \]  
Isotropic stress.

\[ R[g_{eff}] g^d \]  
Recovery function (Majors, 1993) that allows primary, secondary and tertiary creep in the quasi-elastic range. Without it, only primary creep can be described. Secondary and tertiary creep are alternatively described by replacing $A$ with $A + \Delta \Gamma$ (Ho & Krempl, 2000).

The recovery function is expressed as (with the effective stress $g_{eff}$ defined in Equation (A-77)):

\[ R[g_{eff}] = \frac{1}{2} RG_3 (\tanh(UG) + \tanh(VG)) \]  
(A-59)

A-14
\[ UG = -3 + 6 \frac{g_{\text{eff}} - RG_1}{RG_2 - RG_1} \quad VG = 3 + 6 \frac{g_{\text{eff}} + RG_1}{RG_2 - RG_1} \]  

(A-60)

### A.1.7. Kinematic stress rate (VBO)

The deviatoric kinematic stress growth law, from Equation (A-5), is:

\[ \dot{\sigma}^d = \frac{2}{3} E_t \bar{e}^{in} = \frac{1}{(1 + v^{in})} E_t \bar{e}^{in} \]  

(A-61)

Using Equation (A-13), it is

\[ \dot{\sigma}^d = \frac{E_t}{E k[\Gamma]} (\sigma^d - g^d). \]  

(A-62)

Majors (1993) introduced isotropic stress sensitivity to force the slope of the kinematic stress versus inelastic strain curve to approach zero as \( A \) approaches its minimum, to be used with the rate insensitive isotropic stress definition, Equation (A-65):

\[ \dot{\sigma}^d = \frac{2}{3} E_t \bar{e}^{in} \frac{A - B_0}{A_0 - B_0} \]  

(A-63)

\[ \dot{\sigma}^d = \frac{E_t}{k[\Gamma] A_0 - B_0} (\sigma^d - g^d) \]  

(A-64)

\( A_0 \) and \( B_0 \) are constants\(^{45}\), with \( B_0 < A_0 \). As earlier, Majors’ equations are provided for reference purposes. Note that Tachibana and Krempl (1995) did not include kinematic stress evolution in their high homologous temperature application of VBO.

### A.1.8. Isotropic stress and stress rate (VBO)

The isotropic stress is a scalar that affects the transition between initial quasi-elastic and full inelastic behaviour. Time independence is ensured with no dependence on the viscosity function \( \bar{k}[\Gamma] \).
Yao & Kreml (1985) considered the isotropic stress to be a constant $A_Y$. Equation (A-63) used by Majors (1993) to account for hardening at higher temperatures used the following definition of a variable isotropic stress:

$$A = B_0 + \frac{A_o - B_0}{1 + G_1^* \lambda}$$

(A-65)

$$A = B_0 + \frac{A_o - B_0}{1 + G_1^*(hp - \eta)}$$

$\lambda = hp - \eta$ allows history dependent softening. $G_1^*$ and $h$ are constants. $\eta$ is the deformation history modified accumulated inelastic strain and $p$ is the accumulated inelastic strain (Equation (A-30). $\eta$ evolves as

$$\dot{\eta} = h\dot{p} - R_1[\eta] \eta,$$  \hspace{1cm} (A-66)

where $R_1[\eta]$ is of the same form as $R[g_{eff}]$, provided as Equation (A-69). Note that Tachibana and Kreml (1995) used a somewhat different version $\dot{\eta} = \dot{p} - R_1[\eta]$. Cyclic neutral behaviour is modeled when the isotropic stress $A$ takes on a constant value.

Majors (1993) suggested, but did not implement the following form

$$\dot{A} = -\frac{G_1^* R_1[\eta] \eta(A_o - B_0)}{(1 + G_1^* \lambda)^2} + \text{hardening term.} \hspace{1cm} (A-67)$$

Another form was used by Tachibana & Kreml (1995):

$$\dot{A} = -\beta \left(\frac{A - A_2}{A_2}\right) R_1[\eta] = -\beta \left(\frac{A - A_2}{A_2}\right) \lambda$$  \hspace{1cm} (A-68)

The second recovery function, $R_1[\eta]$, is:

$$R_1[\eta] = \frac{1}{2} RA_3\left(\tanh(UA) + \tanh(VA)\right)$$  \hspace{1cm} (A-69)
UA = \(-3 + 6 \frac{\eta - RA_1}{RA_2 - RA_1}\) \quad VA = \(3 + 6 \frac{\eta + RA_1}{RA_2 - RA_1}\)  

(A-70)

Ho and Krempl (2000) used a different definition for isotropic stress rate. Their simpler form was selected for generalization for the AVBO versions developed in section A.2.6:

\[
\hat{A} = A_c (A_f - A) \hat{\rho}
\]

(A-71)

(Ac (dimensionless) controls the speed at which the final solution Af (dimension of stress) is being approached. Both Ac and Af are constants.

A.1.9. Effective stress formulations

A.1.9.1. Effective overstress \(\Gamma\) (VBO)

From the definition of effective strain \(\dot{\rho}\) (Equations (A-30) and (A-32) it follows that

\[
\Gamma = E \bar{k} [\Gamma] \sqrt{\frac{2}{3} \dot{\epsilon}^{in} \cdot \epsilon^{in}}
\]

(A-72)

which results in

\[
\Gamma^2 = \frac{3}{2} (\sigma^d - g^d) \cdot (\sigma^d - g^d) = \frac{3}{2} ((\sigma^d_n - g^d_n)(\sigma^d_n - g^d_n))
\]

(A-73)

with the aid of Equation (A-22), and having set \(\nu^{in} = 0.5\). Without the last assumption, the more general expression for the effective overstress is

\[
\Gamma = \sqrt{(1 + \nu^{in})(\sigma^d - g^d) \cdot (\sigma^d - g^d)} = E \bar{k}[\Gamma] \sqrt{\frac{1}{1 + \nu^{in}} \dot{\epsilon}^{in} \cdot \epsilon^{in}}.
\]

(A-74)

A.1.9.2. Effective stress \(\Theta\) (VBO)

The effective stress based on \(g^d - f^d\), again with \(\nu^{in} = 0.5\), is
\[ \Theta^2 = \frac{3}{2} (g^d - f^d) \cdot (g^d - f^d), \quad (A-75) \]

while the more general version is

\[ \Theta^2 = (1 + \nu' n) (g^d - f^d) \cdot (g^d - f^d). \quad (A-76) \]

**A.1.9.3. Effective stress used in Majors’ recovery function**

The effective stress used by Majors (1993) is based on the deviatoric equilibrium stress, again provided for reference purposes only:

\[ g_{eff}^d = (1 + \nu' n)(g^d) \cdot (g^d) \quad (A-77) \]
A.2. **Small deformation orthotropic AVBO**

The orthotropic constitutive equations are provided as a reproduction of the derivation of the selected version of AVBO, to demonstrate its generalization from selected VBO equations in Section A.1. It relies on the Representation Theorem as summarized in Appendix B: That theorem provides a condensed alternative to carrying out tensor transformations to describe stress and strain components in a direction other than the material preferred directions. This alternative to performing transformations was selected for its conciseness and the fact that equations of the transformation version of AVBO (Lee K.-D., 1989) are not as readily comparable with the VBO equations. Lee’s version were adopted by others who modelled AVBO e.g. Chow (1993) and Colak (2001) and is the AVBO version quoted in two summaries of the method (Kreml E., 1996) (Kreml E., 1999).

A.2.1. **Total strain rate (AVBO)**

\[ \dot\varepsilon = \dot\varepsilon^\text{el} + \dot\varepsilon^\text{in} \text{ or } \dot\varepsilon = \dot\varepsilon^\text{el} + \dot\varepsilon^\text{in} \]  

(A-78)

A.2.2. **Elastic strain rate (AVBO)**

The linear elastic strain rate is expressed as

\[ \dot\varepsilon^\text{el} = S\dot\sigma. \]  

(A-79)

For an orthotopic material:
Applying the representation equation (B-2), the elastic strain rate

\[
\dot{e}^{el} = \dot{e}^{el}(\dot{\sigma}, M_1, M_2, M_3),
\]

is expressed as a function of one variable, the stress rate as

\[
\dot{e}^{el} = S_1 M_1 + S_2 M_2 + S_3 M_3 + S_4 (M_1 \dot{\sigma} + \sigma M_1) + S_5 (M_2 \dot{\sigma} + \sigma M_2) + S_6 (M_3 \dot{\sigma} + \sigma M_3).
\]  

(A-81)

Applying Equation (B-5) provides:

\[
S_1 = (S_1 - 2(S_8 + S_9 - S_7)) \dot{\sigma}_{11} + S_6 \dot{\sigma}_{22} + S_5 \dot{\sigma}_{33}
\]

\[
S_2 = S_6 \dot{\sigma}_{11} + (S_2 - 2(S_7 + S_9 - S_8)) \dot{\sigma}_{22} + S_4 \dot{\sigma}_{33}
\]

\[
S_3 = S_5 \dot{\sigma}_{11} + S_4 \dot{\sigma}_{22} + (S_3 - 2(S_7 + S_8 - S_9)) \dot{\sigma}_{33}
\]

\[
S_4 = S_8 + S_9 - S_7 \\
S_5 = S_7 + S_9 - S_8 \\
S_6 = S_7 + S_8 - S_9
\]

(A-82)

The compliance \( S \) can be expressed as a function of the nine components of the orthotropic compliance tensor or as a polycrystal approximation using the five single crystal compliance components and texture (Section 4.3.1.2).
A.2.3. Inelastic strain rate (AVBO)

The representation is equated to the following viscoplastic formulation, as a generalization of Equation (A-13):

\[
\dot{\epsilon}^{\text{in}} = \frac{B^\varepsilon (\sigma - g)}{k[\Gamma]} = \frac{B^\varepsilon (\sigma - g)}{E_1 k[\Gamma]} = \frac{S_1 B^\varepsilon (\sigma - g)}{k[\Gamma]}
\]

\[
\frac{\dot{\epsilon}^{\text{in}}}{1/E_1 k[\Gamma]} = B^\varepsilon o
\]

where,

\[
B^\varepsilon = \begin{bmatrix}
B_1^\varepsilon & B_6^\varepsilon & B_5^\varepsilon & 0 & 0 & 0 \\
B_6^\varepsilon & B_2^\varepsilon & B_4^\varepsilon & 0 & 0 & 0 \\
B_5^\varepsilon & B_4^\varepsilon & B_3^\varepsilon & 0 & 0 & 0 \\
0 & 0 & 0 & B_7^\varepsilon & 0 & 0 \\
0 & 0 & 0 & 0 & B_8^\varepsilon & 0 \\
0 & 0 & 0 & 0 & 0 & B_9^\varepsilon
\end{bmatrix}
\]

and, consistent with equation (A-14),

\[
o = \sigma - g.
\]

The proportionality assumed between the inelastic strain rate and the overstress, rather than the deviatoric overstress as with VBO, has also been adopted by others who have modeled AVBO (e.g. Chow (1993), Colak (2001) and Krempl (1996)). To account for any arbitrary load condition, not applied in the material preferred directions, the inelastic strain rate is expressed as a function of the overstress applying the representation equations (B-2):
The generator coefficient functions \( \mathbf{B}^e \) follow immediately from Equations (B-4):

\[
\begin{align*}
\mathbf{B}_1^e &= (B_1^e - 2(B_5^e + B_9^e - B_7^e))o_1 + B_6^e o_2 + B_8^e o_3 \\
\mathbf{B}_2^e &= B_5^e o_1 + (B_2^e - 2(B_7^e + B_5^e - B_9^e))o_2 + B_4^e o_3 \\
\mathbf{B}_3^e &= B_5^e o_1 + B_4^e o_2 + (B_3^e - 2(B_5^e + B_6^e - B_8^e))o_3 \\
\mathbf{B}_4^e &= B_6^e + B_9^e - B_7^e \\
\mathbf{B}_5^e &= B_7^e + B_5^e - B_6^e \\
\mathbf{B}_6^e &= B_7^e + B_6^e - B_5^e
\end{align*}
\]

In the above, the effective equilibrium overstress \( \Gamma \) is from equations (A-106). Sütçü (1985) normalized the components of \( \mathbf{B}^e \) by division with \( B_1^e \). He similarly normalized \( \mathbf{S} \) by \( S_1 \). This allowed him to equate the elastic and inelastic ratios to reduce the number of constants, as discussed in Section 4.3.3. Inelastic material property ratios have been used in the other AVBO models as well, (Lee K.-D., 1989), (Chow, 1993) (Colak, 2001), where the inelastic ratios were considered to be a constant or to evolve, as applied by Colak (2001) for large deformation.

### A.2.4. Equilibrium stress (AVBO)

#### A.2.4.1. Sütçü’s definition of equilibrium stress rate

Generalizing Majors’ version of the equilibrium stress, Equation (A-44), would have been the preference, given the extent to which he validated it against a Cr-Mo alloy. However, a representation of his equations with five argument tensors \( \mathbf{d}, \mathbf{d}, \mathbf{g}, \mathbf{f}, \mathbf{f} \) would not permit the elegant direct comparison against the Boehler
Equations (B-2) and (B-4) for a single argument tensor when applying the Representation Theorem. It would also result in a very large number of constants. Sütçü (1985) proposed the following growth law (not elaborating on its origin) for \( \mathbf{g} \) to reduce the number of argument tensors to one:

\[
\frac{\dot{\mathbf{g}}}{\Psi[\Gamma]} = \mathbf{D}^g \dot{\xi}
\]

(A-88)

where

\[
\dot{\xi} = \dot{\varepsilon} - \frac{\Theta}{A_f} (1 - q[\Gamma]) \varepsilon^{\text{in}} \quad \text{and}
\]

\[
q[\Gamma] = \frac{P_1}{\Psi[\Gamma]} = \frac{P_1}{E_1 \Psi[\Gamma]}.
\]

(A-89)

(A-90)

\( P_1 \) is a constant, the equivalent of \( E_t \) for VBO. \( \mathbf{D}^g \), dimensionless, is defined as

\[
\mathbf{D}^g = \begin{bmatrix}
D_1^g & D_2^g & D_3^g & 0 & 0 & 0 \\
D_4^g & D_5^g & D_6^g & 0 & 0 & 0 \\
D_7^g & D_8^g & D_9^g & 0 & 0 & 0 \\
0 & 0 & 0 & D_7^g & 0 & 0 \\
0 & 0 & 0 & 0 & D_8^g & 0 \\
0 & 0 & 0 & 0 & 0 & D_9^g
\end{bmatrix}
\]

(A-91)

With Equation (A-89) inserted into (A-88), the resulting Equation (A-92) resembles the Yao version of VBO of \( \dot{\mathbf{g}} \) as modified by Sütçü, Equation (A-48):

\[
\frac{\dot{\mathbf{g}}}{\Psi[\Gamma]} = \frac{\dot{\mathbf{g}}}{E_1 \Psi[\Gamma]} = \mathbf{D}^g \left( \dot{\varepsilon} - \frac{\Theta}{A_f} (1 - q[\Gamma]) \varepsilon^{\text{in}} \right)
\]

(A-92)

\[
= \mathbf{D}^g \left( \dot{\varepsilon} - \frac{\Theta}{A_f} \left( 1 - \frac{P_1}{E_1 \Psi[\Gamma]} \right) \varepsilon^{\text{in}} \right)
\]

A-23
Sütçü only accounted for a constant asymptotic isotropic stress $A_f$. He initially assumed a squared $\frac{\Theta}{A_f}$ dependency (Sütçü M., 1985), but subsequently reduced it to a linear relationship (Sütçü & Kremp, 1990). Also, the fact that isotropic stress rate is included in this study (Section A.2.6) and other versions of VBO, supports the following substitution of $A$ for $A_f$ in Equations (A-92) and (A-89):

$$\frac{\dot{g}}{\psi[\Gamma]} = \frac{\dot{g}}{E_1 \psi[\Gamma]} = D^g \dot{\xi} = D^g \left( \frac{\dot{\varepsilon}}{E_1 \psi[\Gamma]} - \frac{P}{1 - A} \right) \dot{\varepsilon}^{in}$$

(A-93)

where

$$\dot{\xi} = \dot{\varepsilon} - \frac{\Theta}{A} (1 - \varphi[\Gamma]) \dot{\varepsilon}^{in}$$

(A-94)

To account for arbitrary force directions, the representation for $\frac{\dot{g}}{E_1 \psi[\Gamma]}$, using equation (B-2), is used to arrive at

$$\frac{\dot{g}[\dot{\xi}, M_1, M_2, M_3]}{E_1 \psi[\Gamma]} = D^g_1 M_1 + D^g_2 M_2 + D^g_3 M_3$$

$$+ D^g_4 (M_1 \dot{\xi} + \dot{\xi} M_1) + D^g_5 (M_2 \dot{\xi} + \dot{\xi} M_2) + D^g_6 (M_3 \dot{\xi} + \dot{\xi} M_3).$$

(A-95)

This approach does not assume proportionality between $\dot{\varepsilon}$ and $\dot{\varepsilon}^{in}$ through $\dot{\xi}$, as both $\dot{\varepsilon}^{el}$ and $\dot{\varepsilon}^{in}$ have their own transformation relations, Equations (A-81) and (A-83), respectively. The generator coefficient functions for Equation (A-95) follow by again applying Equations (B-4):
\[ D_1^G = \left( D_1^g - 2(D_8^g + D_9^g - D_7^g) \right) \dot{\varepsilon} + D_6^g \dot{\varepsilon}_2 + D_5^g \dot{\varepsilon}_3 \]

\[ D_2^G = D_6^g \dot{\varepsilon}_1 + \left( D_1^g - 2(D_7^g + D_9^g - D_8^g) \right) \dot{\varepsilon}_2 + D_4^g \dot{\varepsilon}_3 \]

\[ D_3^G = D_5^g \dot{\varepsilon}_1 + D_4^g \dot{\varepsilon}_2 + \left( D_3^g - 2(D_7^g + D_8^g - D_9^g) \right) \dot{\varepsilon}_3 \]

\[ D_4^G = D_8^g + D_9^g - D_7^g \]

\[ D_5^G = D_7^g + D_9^g - D_8^g \]

\[ D_6^G = D_7^g + D_8^g - D_9^g \]

### A.2.4.2. Accounting for DSA in the equilibrium stress rate

To account for DSA, the isotropic strain in Equation (A-93) is enhanced, following the same principles followed with Equation (A-57), to provide

\[
\frac{\dot{g}}{E_1 \tilde{\psi} [\Gamma]} = D^g \left( \dot{\varepsilon} - \frac{\Theta}{A + H \Gamma} (1 - \varphi [\Gamma]) \dot{\varepsilon}^{in} \right) \tag{A-97}
\]

\[
= D^g \left( \dot{\varepsilon} - \frac{\Theta}{A + H \Gamma} \left( 1 - \frac{P_1}{E_1 \tilde{\psi} [\Gamma]} \right) \dot{\varepsilon}^{in} \right)
\]

where \( H \) is defined in Section A.1.6.4. Therefore, \( \dot{\xi} \) is stated as follows for the DSA formulation of \( \dot{\xi} \):

\[
\dot{\xi} = \dot{\varepsilon} - \frac{\Theta}{A + H \Gamma} (1 - \varphi [\Gamma]) \dot{\varepsilon}^{in} \tag{A-98}
\]

### A.2.5. Kinematic stress (AVBO)

#### A.2.5.1. Sütçü definitions of kinematic stress

Sütçü (1985) did not employ a growth law for kinematic stress. He let

\[
f = P_1 D^g \varepsilon \tag{A-99}
\]
P₁ is a constant, also employed in Section A.2.4. Since Zr alloys exhibit a significant Bauschinger effect, a growth law should be included for this application, as proposed in the next section.

A.2.5.2. Growth law for kinematic stress

The proposed equation follows from a generalization of Equation (A-61), which assumes proportionality between kinematic stress rate and inelastic strain rate:

$$ \mathbf{\dot{f}} = P_1 \mathbf{D}^f \mathbf{\dot{\epsilon}}^{\text{in}} \quad (A-100) $$

D^f is a dimensionless tensor. Unlike Sütçü (1985), no relation is assumed between D^f and D^g, Equation (A-99). For any arbitrary stress state, it is again expressed as a representation employing (B-2):

$$ \frac{\mathbf{f}[\mathbf{\dot{\epsilon}}^{\text{in}}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3]}{P_1} = \mathcal{D}_1^f \mathbf{M}_1 + \mathcal{D}_2^f \mathbf{M}_2 + \mathcal{D}_3^f \mathbf{M}_3 $$

$$ + \mathcal{D}_4^f (\mathbf{M}_1 \mathbf{\dot{\epsilon}}^{\text{in}} + \mathbf{\dot{\epsilon}}^{\text{in}} \mathbf{M}_1) + \mathcal{D}_5^f (\mathbf{M}_2 \mathbf{\dot{\epsilon}}^{\text{in}} + \mathbf{\dot{\epsilon}}^{\text{in}} \mathbf{M}_2) + \mathcal{D}_6^f (\mathbf{M}_3 \mathbf{\dot{\epsilon}}^{\text{in}} + \mathbf{\dot{\epsilon}}^{\text{in}} \mathbf{M}_3) $$

The generator coefficient functions, from Equation (B-4) are:

$$ \mathcal{D}_1^f = \left( \mathcal{D}_1^f - 2(\mathcal{D}_8^f + \mathcal{D}_9^f - \mathcal{D}_7^f) \right) \mathbf{\dot{\epsilon}}^{\text{in}}_1 + \mathcal{D}_6^f \mathbf{\dot{\epsilon}}^{\text{in}}_2 + \mathcal{D}_5^f \mathbf{\dot{\epsilon}}^{\text{in}}_3 $$

$$ \mathcal{D}_2^f = \mathcal{D}_6^f \mathbf{\dot{\epsilon}}^{\text{in}}_1 + \left( \mathcal{D}_2^f - 2(\mathcal{D}_7^f + \mathcal{D}_9^f - \mathcal{D}_8^f) \right) \mathbf{\dot{\epsilon}}^{\text{in}}_2 + \mathcal{D}_4^f \mathbf{\dot{\epsilon}}^{\text{in}}_3 $$

$$ \mathcal{D}_3^f = \mathcal{D}_5^f \mathbf{\dot{\epsilon}}^{\text{in}}_1 + \mathcal{D}_4^f \mathbf{\dot{\epsilon}}^{\text{in}}_2 + \left( \mathcal{D}_3^f - 2(\mathcal{D}_7^f + \mathcal{D}_9^f - \mathcal{D}_8^f) \right) \mathbf{\dot{\epsilon}}^{\text{in}}_3 $$

$$ \mathcal{D}_4^f = \mathcal{D}_8^f + \mathcal{D}_9^f - \mathcal{D}_7^f \quad \mathcal{D}_5^f = \mathcal{D}_7^f + \mathcal{D}_9^f - \mathcal{D}_8^f \quad \mathcal{D}_6^f = \mathcal{D}_7^f + \mathcal{D}_8^f - \mathcal{D}_9^f $$

D^f is defined as:
A.2.6. **Isotropic stress and stress rate (AVBO)**

Sütçü (1985) considered the isotropic stress to be constant, i.e. isotropic stress $A_f$ only in Equation (A-105), and incorporated it into the equilibrium stress rate ODE through his definition of the effective stress $\Gamma_{\text{Sütçü}}$ Equation (A-104).

$$\Gamma_{\text{Sütçü}} = \frac{\Theta}{A_f}.$$  \hspace{1cm} (A-104)

Lee (1989) did not include isotropic stress in his multi-dimensional transformation version of AVBO either. The exclusion of an isotropic stress or its rate is limiting the possible applications of the theory. For instance, it may very well be required for the introduction of irradiation hardening as done for MATMOD (described in Section 4.1) by Miller (1987). The isotropic stress rate for VBO Equation (A-71) will be used. $\Lambda_c$ is a scalar constant and $A_f$, the asymptote of $A$, approaches the overstress $\Theta$ (Krempl & Gleason, 1996).

$$\dot{A} = \Lambda_c (A_f - A) \dot{p}$$  \hspace{1cm} (A-105)

A.2.7. **Effective overstress $\Gamma$ (AVBO)**

Consistent with Sütçü (1985), apart from not normalizing $B^e$ by $B^e_1$, the effective overstress is defined as
\[ \Gamma^2 = (B^e \cdot (\sigma - g)) \cdot (B^e \cdot (\sigma - g)). \]  
(A-106)

A.2.8. Effective stress \( \Theta \) (AVBO)

The effective stress is similarly defined as

\[ \Theta^2 = (B^e \cdot (g - f)) \cdot (B^e \cdot (g - f)). \]  
(A-107)
A.3. Figures Appendix A

(a) Viscoelastic response of SLS

Very slow response:
Equilibrium stress = \( \sigma_f \)

Very fast response:
Equilibrium stress = \( aE_2\epsilon \)

(b) Viscoplastic response of modified SLS used in conjunction with an equilibrium growth law (Krempl E., 1995)

Very slow response:
Equilibrium stress

\[ \sigma - g \]

\[ g - f = A \]

Figure A-1  SLS as a basis for the uniaxial VBO flow law.
APPENDIX B. REPRESENTATION THEOREM

A representation theorem describes stress components in a direction other than the material preferred directions, as applied by Sütçü (1985)(1992) for AVBO. It provides a condensed alternative to carrying out tensor transformations to achieve the same objective. This is a summary of the version adopted from Boehler (1979)(1987).

Consider the response $T = F(A_1, A_2, \ldots, A_c, v_1, v_2, v_3)$ of the $3 \times 3$ tensors $A_1, A_2, \ldots, A_c$, and the orthonormal basis vectors $v_1$ to $v_3$ that describe the material preferred directions. The objective of the representation theorem is to find an invariant function $F$ that satisfies

$$T = F(Q A_1 Q^T, Q A_2 Q^T, \ldots, Q A_c Q^T, \ldots, Q v_1, Q v_2, Q v_3)$$

for any coordinate transformation $Q$, thus making $T$ insensitive to a transformation. Boehler (1979)(1987) defined a set of non-polynomial representations for orthotropic functions with only one argument tensor $A_1$ and generator coefficient functions $\alpha_i$ as

$$T(A_1, M_1, M_2, M_3) = \alpha_1 M_1 + \alpha_2 M_2 + \alpha_3 M_3 +$$

$$\alpha_4 (M_1 A_1 + A_1 M_1) + \alpha_5 (M_2 A_1 + A_1 M_2) + \alpha_6 (M_3 A_1 + A_1 M_3)$$

(B-2)

with $M_1 = v_i \otimes v_i$, no sum:

$$M_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad M_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad M_3 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

(B-3)

Most of the symbols used here are only applicable to this discussion and are not listed in the List of Abbreviations, Symbols and Definitions.
It is possible to compare Eq. (B-2) with a physically based known linear relation of the form

\[
T = \begin{bmatrix}
a & f & e & 0 & 0 & 0 \\
f & b & d & 0 & 0 & 0 \\
e & d & c & 0 & 0 & 0 \\
0 & 0 & 0 & g & 0 & 0 \\
0 & 0 & 0 & 0 & h & 0 \\
0 & 0 & 0 & 0 & 0 & i \\
\end{bmatrix} A_1. \quad (B-4)
\]

Assuming that the generator coefficient functions \( \alpha_i \) are linear, Boehler showed that these functions are then described by Equations (B-5) after equations (B-2) and (B-4) were equated.

\[
\begin{align*}
\alpha_1 &= (a - 2(h + i - g)) \text{tr}M_1A_1 + (f) \text{tr}M_2A_1 + (e) \text{tr}M_3A_1 \\
\alpha_2 &= (f) \text{tr}M_1A_1 + (b - 2(g + i - h)) \text{tr}M_2A_1 + (d) \text{tr}M_3A_1 \\
\alpha_3 &= (e) \text{tr}M_1A_1 + (d) \text{tr}M_2A_1 + (c - 2(g + h - i)) \text{tr}M_3A_1 \\
\alpha_4 &= h + i - g, \quad \alpha_5 = g + i - h, \quad \alpha_6 = g + h - i
\end{align*}
\]

This representation is used for various linearised sets of differential equations in Section A.2 to align principal and material preferred directions without performing tensor transformations.
APPENDIX C. PREDICTION OF ELASTIC COMPLIANCE AND STIFFNESS TENSORS USING ODCs AND KEARNS FACTORS

This summary\textsuperscript{48} describes from literature how elastic material properties are obtained from single crystal material properties and texture utilizing Kearns factors derived from diffraction intensities. Proof of verification of correct implementation of the equations is shown. Parallels are drawn to these equations in Appendix D to derive equations to describe inelastic material properties.

C.1. Texture definition of HCP materials with pole figures, orientation distribution functions and Kearns factors

The orientation $\mathbf{g}$ describes the transformation from the $(x, y, z)$ coordinate systems of a single crystal to the $(X, Y, Z)$ coordinate system of a polycrystal sample. The orientation is described by the three spherical coordinate Euler angles $\Psi$, $\theta$ and $\phi$\textsuperscript{49}. $\Psi$ describes the rotation from the meridian, $\theta$ the latitude distance from the north pole and $\phi$ the rotation around the c-axis of the single crystal, in the case of an HCP crystal.

A pole figure captures the intensity distribution of one orientation as an area representation. This, the preferred direction, associated with a Bragg condition in the case of X-ray diffraction, is for instance the normal to the (0001) basal plane or to the $\{10\overline{1}0\}$ prismatic planes for HCP materials. The pole figure shows crystal orientation on

\textsuperscript{48} Section C.1 is a standalone description for background purposes and the List of Abbreviations, Symbols and Definitions do not apply.

\textsuperscript{49} Symbol convention of Kocks, Tomé, & Wenk (1988, see Chapter 2, Fig. 11).
a sample plane, in terms of two of the three Euler angles ($\Psi$ and $\theta$). An inverse pole figure shows the sample orientation on a crystal plane, showing the orientation of $\theta$ and $\phi$.

Since a pole figure does not show the $\phi$ distribution of the orientation distribution (OD) of the sample, mathematical effort is required to describe the orientation distribution function (ODF), $f(g)$, from the pole figure intensity values. The crystal basal plane pole density $p_{(0001)}$ at a location on the pole figure is related to the ODF through

$$p_{(0001)}(\alpha, \beta) = \frac{1}{2\pi} \int_0^{2\pi} F(\Psi, \theta, \phi) d\phi,$$  \hspace{1cm} (C-1)

where $(\alpha, \beta)$ defines the position of the pole on the surface of the northern half of the unit sphere (see Figure C-1), and therefore the position of the pole on the pole figure surface - $\alpha$ is the polar angle and $\beta$ the azimuthal angle. The pole density is related to the measured normalized intensity $I$ through

$$p_{(0001)}(\alpha, \beta) = \frac{I(\cos \alpha, \beta)}{\int_0^{2\pi} \int_{-1}^{1} I(\cos \alpha, \beta) \, d\alpha \, d\beta}.$$  \hspace{1cm} (C-2)

With the ODF available, the texture can be presented for any value of $\phi$ with Equation (C-2), presented as a series of crystal orientation distributions (CODs) for incremental values of $\phi$. The ODF is described through harmonic or direct methods (Kocks, Tomé, & Wenk, 1988). With the harmonic method, the ODF is described by a series of generalized spherical harmonics

$$F(\Psi, \Theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} W_{lmn} z_{lmn}(\cos \Theta) e^{-im\Psi} e^{-in\phi}.$$  \hspace{1cm} (C-3)
where $W_{lmn}$ are the orientation distribution coefficients (ODCs), and $Z_{lmn}$ are Jacobi polynomials (Roe, 1965). The ODCs are determined through solving a set of linear simultaneous equations generated with Equations (C-1) and (C-3) for a number of pole figures obtained for different poles (i.e. for different incident X-ray angles). The volumetric identity of the sample, the OD is thus approximated from the planar information available through a number of pole figures. The pole density $p_{(0001)}$ can also be described as a spherical harmonic,

$$p_{(0001)}(\alpha, \beta) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Q_{lm} P_l^m (\cos \alpha) \exp^{-im\beta} \ \ \ \ (C-4)$$

where $Q_{lm}$ are pole figure expansion coefficients and $P_l^m$ are normalized associated Legendre functions. With Equations (C-1), (C-3) and (C-4) it can be shown that the $W_{lmn}$ and $P_l^m$ coefficients are related by Equation (C-5), from Roe (1965).

$$Q_{lm} = 2\pi \sqrt{\frac{2}{2l+1}} \sum_{n=-1}^{l} W_{lmn} P_l^n (\cos \Theta) \exp^{-in\phi} \ \ \ \ (C-5)$$

Since $\Theta = 0$ for a basal pole figure, only ODCs with $n = 0$ will not be zero (Anderson, Thompson, & Cook, 1999). As a consequence they were able to reduce Equation (C-5) to

$$Q_{lm} = \pi W_{lm0} \ \ \ \ (C-6)$$

The ODF of HCP materials are completely described by ODCs up to the 4th order, resulting in only the six coefficients $W_{000}$, $W_{200}$, $W_{220}$, $W_{400}$, $W_{420}$ and $W_{440}$.

Kearns (1965) defined a parameter that describes the effective fraction of crystals with the basal normal direction parallel to a reference direction of the sample.
normal (or radial R for tube) direction it is designated as \( f_R \), as \( f_T \) in the tangential and \( f_L \) in the longitudinal directions. The respective factors are described in terms of their own polar \((\alpha_R, \alpha_T, \alpha_L)\) and azimuth \((\beta_R, \beta_T, \beta_L)\) angles, as defined in Figure C-1. The three factors are:

\[
f_R = \frac{1}{V} \int_0^{\pi/2} \int_0^{2\pi} I(\alpha_R, \beta_R) \sin \alpha_R \cos^2 \alpha_R \, d \beta_R \, d \alpha_R
\]

\( (C-7) \)

\[
f_T = \frac{1}{V} \int_0^{\pi/2} \int_0^{2\pi} I(\alpha_T, \beta_T) \sin \alpha_T \cos^2 \alpha_T \, d \beta_T \, d \alpha_T
\]

\( (C-8) \)

\[
f_L = \frac{1}{V} \int_0^{\pi/2} \int_0^{2\pi} I(\alpha_L, \beta_L) \sin \alpha_L \cos^2 \alpha_L \, d \beta_L \, d \alpha_L
\]

\( (C-9) \)

\( I(\alpha_R, \beta_R) = I(\alpha_T, \beta_T) = I(\alpha_L, \beta_L) \) is the normalized diffracted intensity at the pole, with the normalization obtained with \( V \) (Anderson, Thompson, & Cook, 1999):

\[
V = \int_0^{\pi/2} \int_0^{2\pi} I(\alpha_R, \beta_R) \sin \alpha_R \, d \beta_R \, d \alpha_R
\]

\( (C-10) \)

Either \((\alpha_R, \beta_R), (\alpha_T, \beta_T)\) or \((\alpha_L, \beta_L)\) could have been used. With \( \alpha = \alpha_R \) and \( \beta = \beta_R \), the relations have been described as follows by Nakatsuka (1981) and Anderson, Thompson, & Cook (1999): Nakatsuka employed a right hand and Anderson et al. a left hand RTL coordinate system, also rotated relative to Nakatsuka’s; \( f_T \) and \( f_L \) are therefore reversed when comparing to their results. The coordinate systems are compared in Figure C-2. This study utilizes a right hand system. Therefore, Equations (C-7) to (C-10) become:
The Kearns factors therefore effectively describe the polycrystal texture from the contribution of three fictitious single crystals aligned with the sample directions. Also, since \( f_R + f_T + f_L = 1 \), the texture can be described by two of the three factors.

Anderson et al. (1999) showed how the Kearns factors relate to the ODCs. Equating equations (C-2) and (C-4), substituting the resultant \( Q_{lm} \) into (C-5) and subsequent substitution into (C-7) to eliminate \( Q_{lm} \), lead to (C-15). Note that only the 0\(^{th}\) and 2\(^{nd}\) order ODCs were utilized, as 4\(^{th}\) coefficients had to be ignored in order to carry out the manipulation. Note that these equations are based on their coordinate system as shown in Figure C-2 (\( f_T \) and \( f_L \) reversed).

\[
f_R = \frac{1}{V} \int_{0}^{\pi/2} \int_{0}^{2\pi} I(\alpha, \beta) \sin \alpha \cos^2 \alpha \, d\beta \, d\alpha \quad \text{(C-11)}
\]

\[
f_T = \frac{1}{V} \int_{0}^{\pi/2} \int_{0}^{2\pi} I(\alpha, \beta) \sin \alpha \cos^2 \beta \, d\beta \, d\alpha \quad \text{(C-12)}
\]

\[
f_L = \frac{1}{V} \int_{0}^{\pi/2} \int_{0}^{2\pi} I(\alpha, \beta) \sin \alpha \sin^2 \beta \, d\beta \, d\alpha \quad \text{(C-13)}
\]

with

\[
V = \int_{0}^{\pi/2} \int_{0}^{2\pi} I(\alpha, \beta) \sin \alpha \, d\beta \, d\alpha. \quad \text{(C-14)}
\]

The Kearns factors therefore effectively describe the polycrystal texture from the contribution of three fictitious single crystals aligned with the sample directions. Also, since \( f_R + f_T + f_L = 1 \), the texture can be described by two of the three factors.

Anderson et al. (1999) showed how the Kearns factors relate to the ODCs. Equating equations (C-2) and (C-4), substituting the resultant \( Q_{lm} \) into (C-5) and subsequent substitution into (C-7) to eliminate \( Q_{lm} \), lead to (C-15). Note that only the 0\(^{th}\) and 2\(^{nd}\) order ODCs were utilized, as 4\(^{th}\) coefficients had to be ignored in order to carry out the manipulation. Note that these equations are based on their coordinate system as shown in Figure C-2 (\( f_T \) and \( f_L \) reversed).

\[
f_R = \frac{4\pi^2\sqrt{2}}{3} W_{000} + \frac{8\pi^2\sqrt{10}}{15} W_{200} \quad \text{(C-15)}
\]

\[
f_T = \frac{4\pi^2\sqrt{2}}{3} W_{000} - \frac{4\pi^2\sqrt{10}}{15} W_{200} - \frac{8\pi^2\sqrt{15}}{15} W_{220}
\]
f_L = \frac{4\pi^2\sqrt{2}}{3} W_{000} - \frac{4\pi^2\sqrt{10}}{15} W_{200} + \frac{8\pi^2\sqrt{15}}{15} W_{220}

When inverted, the ODCs are expressed as follows in terms of the Kearns factors (Gruber, Brown, & Lucadamo, 2011), with \( W_{000} \), \( W_{200} \) and \( W_{220} \).

\[
W_{000} = \frac{1}{4\pi^2\sqrt{2}} \quad W_{200} = \frac{\sqrt{10}}{16\pi^2} (3f_L - 1) \quad W_{220} = \frac{\sqrt{15}}{16\pi^2} (f_R - f_T)
\]  \quad (C-16)

### C.2. Single crystal elastic compliance and stiffness properties

Fisher and Renken (1964) determined single alpha zirconium crystal stiffness properties experimentally at temperatures from 4K to 1156K. The inverse single crystal compliance tensor was derived by Rosenbaum and Lewis (1977). The single crystal properties (Equation (C-17)) are described by five components tensors, given the symmetry of the transversely isotropic HCP crystals (Nye, 1985).

\[
\begin{pmatrix}
    s_{11} & s_{12} & s_{13} & 0 & 0 & 0 \\
    s_{12} & s_{11} & s_{13} & 0 & 0 & 0 \\
    s_{13} & s_{13} & s_{33} & 0 & 0 & 0 \\
    0 & 0 & 0 & s_{44} & 0 & 0 \\
    0 & 0 & 0 & 0 & s_{44} & 0 \\
    0 & 0 & 0 & 0 & 0 & 2(s_{11} - s_{12})
\end{pmatrix}
= \begin{pmatrix}
    c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\
    c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\
    c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\
    0 & 0 & 0 & c_{44} & 0 & 0 \\
    0 & 0 & 0 & 0 & c_{44} & 0 \\
    0 & 0 & 0 & 0 & 0 & \frac{c_{11} - c_{12}}{2}
\end{pmatrix}^{-1}
\]  \quad (C-17)

It uses contracted notation (11→1, 22→2, 33→3, 23→4, 13→5, 12→6, i.e. \( c_{1122} \equiv c_{12} \)).

Turner et al. (1995) introduced temperature dependency by deriving polynomial approximations of the elastic single crystal properties, as provided in Sections C.2.1 and C.2.2.
C.2.1. **Single crystal stiffness tensor approximation**

\[
c_{ij}^{sc}[T_K] = c_{ij}^{sc(0)} + c_{ij}^{sc(1)} T_K + c_{ij}^{sc(2)} T_K^2 + c_{ij}^{sc(3)} T_K^3
\]  

(C-18)

<table>
<thead>
<tr>
<th>(c_{ij}^{sc(0)} \times 10^0)</th>
<th>(c_{ij}^{sc(1)} \times 10^3)</th>
<th>(c_{ij}^{sc(2)} \times 10^6)</th>
<th>(c_{ij}^{sc(3)} \times 10^9)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(c_{11}^{sc}[T_K])</td>
<td>159.43</td>
<td>-58.133</td>
<td>14.470</td>
</tr>
<tr>
<td>(c_{12}^{sc}[T_K])</td>
<td>61.357</td>
<td>49.009</td>
<td>-41.198</td>
</tr>
<tr>
<td>(c_{13}^{sc}[T_K])</td>
<td>64.912</td>
<td>0.018</td>
<td>4.483</td>
</tr>
<tr>
<td>(c_{33}^{sc}[T_K])</td>
<td>174.080</td>
<td>-30.996</td>
<td>-1.375</td>
</tr>
<tr>
<td>(c_{44}^{sc}[T_K])</td>
<td>37.290</td>
<td>-20.790</td>
<td>11.433</td>
</tr>
</tbody>
</table>

Note: Stiffness in GPa, temperature \(T_K\) in K.

If linear regression is carried out instead, the coefficients are as follows:

\[
c_{ij}^{sc}[T] = c_{ij}^{sc(0)} + c_{ij}^{sc(1)} T
\]  

(C-19)

<table>
<thead>
<tr>
<th>(c_{ij}^{sc(0)} \times 10^0)</th>
<th>(c_{ij}^{sc(1)} \times 10^3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(c_{11}^{sc}[T])</td>
<td>144.03913</td>
</tr>
<tr>
<td>(c_{12}^{sc}[T])</td>
<td>73.19312</td>
</tr>
<tr>
<td>(c_{13}^{sc}[T])</td>
<td>65.39794</td>
</tr>
<tr>
<td>(c_{33}^{sc}[T])</td>
<td>165.64619</td>
</tr>
<tr>
<td>(c_{44}^{sc}[T])</td>
<td>32.18668</td>
</tr>
</tbody>
</table>

Note: Stiffness in GPa, temperature in °C.

The two approximations are compared to the experimental values in Figure C-3 and Section C.4.1.1 – Equation (C-19) is selected for implementation.
C.2.2. Single crystal compliance tensor approximation

The single crystal compliance tensor in the crystal directions are (Li & Thompson, 1990), with the c-axis in the 33 direction.

\[ \mathbf{s}^{sc}[T] = \mathbf{c}^{sc}[T]^{-1} \]

\[
\begin{bmatrix}
    s_{11}^{sc}[T] & s_{12}^{sc}[T] & s_{13}^{sc}[T] & 0 & 0 & 0 \\
    s_{12}^{sc}[T] & s_{11}^{sc}[T] & s_{13}^{sc}[T] & 0 & 0 & 0 \\
    s_{13}^{sc}[T] & s_{13}^{sc}[T] & s_{33}^{sc}[T] & 0 & 0 & 0 \\
    0 & 0 & 0 & s_{44}^{sc}[T] & 0 & 0 \\
    0 & 0 & 0 & 0 & s_{44}^{sc}[T] & 0 \\
    0 & 0 & 0 & 0 & 0 & 2(s_{11}^{sc}[T] - s_{12}^{sc}[T])
\end{bmatrix}
\]  (C-20)

The inverse relationships are (Li & Thompson, 1990)

<table>
<thead>
<tr>
<th>( s_{11}^{sc}[T] )</th>
<th>( \frac{1}{2} \left( \frac{c_{33}^{sc}[T]}{c_0[T]} + \frac{1}{c_{11}^{sc}[T] - c_{12}^{sc}[T]} \right) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( s_{12}^{sc}[T] )</td>
<td>( \frac{1}{2} \left( \frac{c_{33}^{sc}[T]}{c_0[T]} - \frac{1}{c_{11}^{sc}[T] - c_{12}^{sc}[T]} \right) )</td>
</tr>
<tr>
<td>( s_{13}^{sc}[T] )</td>
<td>( -\frac{c_{13}^{sc}[T]}{c_0[T]} )  (C-21)</td>
</tr>
<tr>
<td>( s_{33}^{sc}[T] )</td>
<td>( \frac{c_{11}^{sc}[T] + c_{12}^{sc}[T]}{c_0[T]} )</td>
</tr>
<tr>
<td>( s_{44}^{sc}[T] )</td>
<td>( \frac{1}{c_{44}^{sc}[T]} )</td>
</tr>
<tr>
<td>( c_0[T] )</td>
<td>( c_{33}^{sc}[T](c_{11}^{sc}[T] + c_{12}^{sc}[T]) - 2c_{13}^{sc}[T]^2 )</td>
</tr>
</tbody>
</table>
C.3. Polycrystal elastic compliance and stiffness tensor calculations using crystal properties

C.3.1. Properties obtained from diffraction data

Upper bound compliance tensors are predicted by assuming compatibility (equal strain) of the single and polycrystals following the Voigt approach, while lower bound compliance tensors are predicted by assuming equilibrium (equal stress) of the single and polycrystals with the Reuss approach. (Kocks, Tomé, & Wenk, 1988). The upper bound and lower bound stiffness ($C=C_{ijkl}$), compliance ($S=S_{ijkl}$) tensors are summarized as,

<table>
<thead>
<tr>
<th>Voigt</th>
<th>Reuss</th>
<th>Hill</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upper bound</td>
<td>$C^V = \langle c^{sc'} \rangle$</td>
<td>$C^R = (S^R)^{-1}$</td>
<td>$C^H = C^{Hill} = \frac{1}{2} (C^V + C^R)$</td>
</tr>
<tr>
<td>Lower bound</td>
<td>$S^V = (C^V)^{-1}$</td>
<td>$S^R = \langle s^{sc'} \rangle = \langle (c^{sc'})^{-1} \rangle$</td>
<td>$S^{Hill} = \frac{1}{2} (S^V + S^R)$</td>
</tr>
</tbody>
</table>

where $c^{sc'}$ and $s^{sc'}$ are the crystal stiffness and compliance tensors in the polycrystal directions. Note that $C^H = C^{Hill} \neq S^{Hill^{-1}}$. For consistent numeric predictions, $S^H$ is used here instead of $S^{Hill}$ since the latter does not meet the Hill compliance definition. A

---

50 The volume average quantities are obtained for a tensor $Z$ from

$$\langle Z \rangle = \frac{1}{V} \int_{0}^{\pi/2} \int_{0}^{2\pi} Z_{ij}(\alpha, \beta) \cdot I(\alpha, \beta) \, \sin \alpha \, d\beta \, d\alpha$$

51 They used a LH coordinate system (Figure C-2(c)). Their derivation does not indicate if it is based on engineering or true strain. It was concluded from a comparison of results that they have used engineering strain. Consequently their definitions for $S_{44}$, $S_{55}$ and $S_{66}$ have been halved.
more cumbersome approach, employing the geometric mean (Tomé, 1998) does not suffer from this inconsistency. When transformed to the polycrystal axes, the transformed crystal compliance is (Nakatsuka, 1981):

\[
\mathbf{s}^{sc'} [T, \alpha, \beta] = \begin{bmatrix}
  s_{11}^{sc'} & s_{12}^{sc'} & s_{13}^{sc'} & 0 & 0 & 0 \\
  s_{12}^{sc'} & s_{11}^{sc'} & s_{23}^{sc'} & 0 & 0 & 0 \\
  s_{13}^{sc'} & s_{12}^{sc'} & s_{23}^{sc'} & 0 & 0 & 0 \\
  0 & 0 & 0 & s_{44}^{sc'} & 0 & 0 \\
  0 & 0 & 0 & 0 & s_{55}^{sc'} & 0 \\
  0 & 0 & 0 & 0 & 0 & s_{66}^{sc'}
\end{bmatrix}.
\]  

(C-25)

\[
s_{11}^{sc'} [T, \alpha, \beta] = s_{11}^{sc [T]} \sin^4 \alpha + s_{33}^{sc [T]} \cos^4 \alpha + (2s_{13}^{sc [T]} + s_{44}^{sc [T]}) \sin^2 \alpha \cos^2 \alpha
\]

\[
s_{12}^{sc'} [T, \alpha, \beta] = A^{sc} \cos^2 \alpha \sin^2 \alpha \cos^2 \beta + B^{sc} (\cos^2 \alpha + \sin^2 \alpha \cos^2 \beta) + s_{12}^{sc [T]}
\]

\[
s_{13}^{sc'} [T, \alpha, \beta] = A^{sc} \cos^2 \alpha \sin^2 \alpha \sin^2 \beta + B^{sc} (\cos^2 \alpha + \sin^2 \alpha \sin^2 \beta) + s_{12}^{sc [T]}
\]

\[
s_{23}^{sc'} [T, \alpha, \beta] = A^{sc} \sin^4 \alpha \cos^2 \alpha \sin^2 \beta + B^{sc} \sin^2 \alpha \cos^2 \alpha + s_{12}^{sc [T]}
\]

\[
s_{22}^{sc'} [T, \alpha, \beta] = A^{sc} \sin^4 \alpha \cos^4 \beta + (2s_{13}^{sc [T]} + s_{44}^{sc [T]} - 2s_{11}^{sc [T]}) \sin^2 \alpha \cos^2 \beta + s_{11}^{sc [T]}
\]

\[
s_{33}^{sc'} [T, \alpha, \beta] = A^{sc} \sin^4 \alpha \sin^4 \beta + (2s_{13}^{sc [T]} + s_{44}^{sc [T]} - 2s_{11}^{sc [T]}) \sin^2 \alpha \sin^2 \beta + s_{11}^{sc [T]}
\]

\[
s_{44}^{sc'} [T, \alpha, \beta] = 4A^{sc} \sin^4 \alpha \sin^2 \beta \cos^2 \beta + (s_{44}^{sc [T]} - s_{44}^{sc [T]}) \cos^2 \alpha + s_{44}^{sc [T]} \sin^2 \alpha
\]

\[
s_{55}^{sc'} [T, \alpha, \beta] = 4A^{sc} \cos^2 \alpha \sin^2 \alpha \sin^2 \beta + (2s_{11}^{sc [T]} - 2s_{12}^{sc [T]} - s_{44}^{sc [T]}) \sin^2 \alpha \cos^2 \beta
\]

\[
+ s_{44}^{sc [T]}
\]

\[
s_{66}^{sc'} [T, \alpha, \beta] = 4A^{sc} \cos^2 \alpha \sin^2 \alpha \cos^2 \beta + (2s_{11}^{sc [T]} - 2s_{12}^{sc [T]} - s_{44}^{sc [T]}) \sin^2 \alpha \sin^2 \beta
\]

\[
+ s_{44}^{sc [T]}
\]

where:

\[
A^{sc} = s_{11}^{sc [T]} - 2s_{13}^{sc [T]} + s_{33}^{sc [T]} - s_{44}^{sc [T]}
\]

\[
B^{sc} = s_{13}^{sc [T]} - s_{12}^{sc [T]}
\]
The polycrystal volume averages can now be determined, e.g. the Reuss compliance is expressed as

\[
S_{ij}^{R}[T] = \langle s_{ij}^{sc'}[T, \alpha, \beta] \rangle = \frac{1}{V} \int_0^{\pi/2} \int_0^{2\pi} s_{ij}^{sc'}[T, \alpha, \beta] \cdot I(\alpha, \beta) \sin \alpha \, d\beta \, d\alpha.
\] (C-26)

Therefore, the polycrystal elastic moduli can be determined from Equation (C-26), only knowing the diffraction intensities and crystal properties (Rosenbaum & Lewis, 1977). As a result of the assumption that the compliance of the polycrystal is the space average of the single crystal values, Rosenbaum & Lewis recognized the limitation that material grain boundary effects and inter-crystalline interaction are not captured in the volume averaged calculation of material properties. The limitations also apply to the Kearns factors, equations (C-11) to (C-13).

C.3.2. Elastic properties obtained from the ODCs and Kearns factors

The similarities between the derivation of the polycrystal compliance tensor and the Kearns factors allow the development of relationships between them. The different approaches followed by Nakatsuka (1981) and Anderson et al. (1999) were considered for implementation and that evaluation is documented here.

C.3.2.1. Nakatsuka approach to obtain elastic polycrystal properties from Kearns factors and single crystal properties

Nakatsuka (1981) assumed that the polycrystal compliance can be expressed as a function of the Kearns factors. He assumed that the single crystal compliance in the pole
direction can be described as the following assumed function of the single crystal compliances in the sample directions:

\[ s_{ij}^{sc'}[T,\alpha,\beta] = s_{ij}^{sc'}[T]\bigg|_R \cos^2 \alpha + s_{ij}^{sc'}[T]\bigg|_T \sin^2 \alpha \cos^2 \beta \\
+ s_{ij}^{sc'}[T]\bigg|_L \sin^2 \alpha \sin^2 \beta. \]  

(C-27)

\[ s_{ij}^{sc'}[T]\bigg|_R, \ s_{ij}^{sc'}[T]\bigg|_T \text{ and } s_{ij}^{sc'}[T]\bigg|_L \text{ are the single crystal compliances with the c-axis along the } R, T \text{ and } L \text{ directions. To obtain the polycrystal compliance, Equation (C-27) is substituted into equation (C-26):} \]

\[ S_{ij}^{R}[T] = \frac{1}{V} \int_0^{2\pi} \int_0^{\pi/2} \left( s_{ij}^{sc'}[T]\bigg|_R \cos^2 \alpha + s_{ij}^{sc'}[T]\bigg|_T \sin^2 \alpha \cos^2 \beta \\
+ s_{ij}^{sc'}[T]\bigg|_L \sin^2 \alpha \sin^2 \beta \right) \cdot I(\alpha,\beta) \sin \alpha \sin \alpha d\beta d\alpha \\
+ s_{ij}^{sc'}[T]\bigg|_T \cdot \frac{1}{V} \int_0^{2\pi} \int_0^{\pi/2} I(\alpha,\beta) \cdot \sin^3 \alpha \cos^2 \beta d\beta d\alpha \\
+ s_{ij}^{sc'}[T]\bigg|_L \cdot \frac{1}{V} \int_0^{2\pi} \int_0^{\pi/2} I(\alpha,\beta) \cdot \sin^3 \alpha \sin^2 \beta d\beta d\alpha \\
\]

Therefore, using (C-11) to (C-13), the Reuss compliance can be expressed as

\[ S_{ij}^{R}[T]_{Nakatsuka} = s_{ij}^{sc'}[T]\bigg|_R f_R + s_{ij}^{sc'}[T]\bigg|_T f_T + s_{ij}^{sc'}[T]\bigg|_L f_L \]  

(C-29)
By substituting the transformed crystal compliances (in the R, T and L directions) with $s_{ij}^{\text{sc}}[T]$, the compliance components in the crystal directions, Nakatsuka simplified this equation to

$$
S_{ij}^{R}[T]_{\text{Nakatsuka}} = \begin{bmatrix}
F(f_{R}, T) & H(f_{L}, T) & H(f_{T}, T) & 0 & 0 & 0 \\
H(f_{L}, T) & F(f_{T}, T) & H(f_{R}, T) & 0 & 0 & 0 \\
H(f_{T}, T) & H(f_{R}, T) & F(f_{L}, T) & 0 & 0 & 0 \\
0 & 0 & 0 & G(f_{R}, T) & 0 & 0 \\
0 & 0 & 0 & 0 & G(f_{T}, T) & 0 \\
0 & 0 & 0 & 0 & 0 & G(f_{L}, T)
\end{bmatrix}
$$

(C-30)

where

$$
F(x, T) = x(s_{33}^{\text{sc}}[T] - s_{11}^{\text{sc}}[T]) + s_{11}^{\text{sc}}[T]
$$

$$
G(x, T) = x(s_{12}^{\text{sc}}[T] - s_{15}^{\text{sc}}[T]) + s_{15}^{\text{sc}}[T]
$$

$$
H(x, T) = x(2s_{11}^{\text{sc}}[T] - 2s_{12}^{\text{sc}}[T] - s_{44}^{\text{sc}}[T]) + s_{44}^{\text{sc}}[T]
$$

(C-31)

and

$$
x = f_{R} \text{ or } f_{T} \text{ or } f_{L}.
$$

These equations apply for a right hand crystal coordinate system with the 3-axis and HCP c-axis coinciding.

**C.3.2.2. Polycrystal properties from Kearns factors derived from ODCs (Li and then Anderson)**

Li & Thompson (1990) expressed the upper and lower bound compliances in terms of the six ODCs $W_{000}$, $W_{200}$, $W_{220}$, $W_{400}$, $W_{420}$ and $W_{440}$ used in the series expansion to fully describe an HCP material ODF. They followed the methodology of Sayers (1987) (1986). These expressions used in conjunction with (C-16), ignoring the fourth order ODCs allow an approximation of the upper and lower bound compliance tensors. The
derivations by Li & Thompson (1990) are based on the assumption\textsuperscript{51} that the upper and lower bound compliance and stiffness tensors can be expressed as

\[
\begin{align*}
C_{ij}^{R}|_{Li} &= C_{ij}^{0}|^{R} + \Delta C_{ij} = \left( S_{ij}^{0}|^{R} \right)^{-1} + \Delta C_{ij} \\
C_{ij}^{V}|_{Li} &= C_{ij}^{0}|^{V} + \Delta C_{ij} \\
C^{R}|_{Li} &= C^{0}|^{R} + \Delta C = (S^{0}|^{R})^{-1} + \Delta C^{R} \\
C^{V}|_{Li} &= C^{0}|^{V} + \Delta C^{V} \\
S^{R}|_{Li} &= (C^{R}|_{Li})^{-1} \\
S^{V}|_{Li} &= C^{V}|_{Li}^{-1}
\end{align*}
\]

and the averaged Hill tensors as\textsuperscript{52}

\[
\begin{align*}
C^{H}|_{Li} &= \frac{1}{2} \left( C^{R}|_{Li} + C^{V}|_{Li} \right) = \frac{1}{2} \left( C^{0}|^{R} + \Delta C^{R} + C^{0}|^{V} + \Delta C^{V} \right) \\
S^{H}|_{Li} &= C^{H}|_{Li}^{-1}
\end{align*}
\]

where $S_{ij}^{0}$ and $C_{ij}^{0}$ are isotropic (texture free) and $\Delta C_{ij}$ differences as a result of the presence of texture, respectively. The isotropic components are functions of the untransformed single crystal compliance (or stiffness) components. The anisotropic differences are functions of the single crystal compliance (or stiffness) components as well as the six ODCs.

\textsuperscript{51} They used a LH coordinate system (Figure C-2(c)). Their derivation does not indicate if it is based on engineering or true strain. It was concluded from a comparison of results that they have used engineering strain. Consequently their definitions for $S_{44}$, $S_{55}$ and $S_{66}$ have been halved.

\textsuperscript{52} Note that $S^{H}|_{Li} = \frac{1}{2} \left( S^{R}|_{Li} + S^{V}|_{Li} \right)$ is not used here (see motivation in section C.3.1 of this appendix).
### Stiffness tensor components (Voigt or Reuss)

<table>
<thead>
<tr>
<th>Component</th>
<th>Isotropic term</th>
<th>Anisotropic term containing $53$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}\mid L_i = C_{11}^{\text{I}}$</td>
<td>$C_{11}^{\text{I}} = C_{11}^0$</td>
<td>$\Delta C_{11}^{(2)} = 16\pi^2 V_1 Y_1$</td>
</tr>
<tr>
<td>$C_{22}\mid L_i = C_{22}^{\text{I}}$</td>
<td>$C_{22}^{\text{I}} = C_{22}^0 + \Delta C_{22}^{(4)}$</td>
<td>$\Delta C_{22}^{(4)} = 16\pi^2 W_2 \kappa_2$</td>
</tr>
<tr>
<td>$C_{33}\mid L_i = C_{33}^{\text{I}}$</td>
<td>$C_{33}^{\text{I}} = C_{33}^0 + \Delta C_{33}^{(4)}$</td>
<td>$\Delta C_{33}^{(4)} = 16\pi^2 W_3 \kappa_3$</td>
</tr>
<tr>
<td>$C_{23}\mid L_i = C_{23}^{\text{I}}$</td>
<td>$C_{23}^{\text{I}} = C_{12}^0 + \Delta C_{23}^{(4)}$</td>
<td>$\Delta C_{23}^{(2)} = 8\pi^2 V_2 Y_1$</td>
</tr>
<tr>
<td>$C_{13}\mid L_i = C_{13}^{\text{I}}$</td>
<td>$C_{13}^{\text{I}} = C_{13}^0 + \Delta C_{13}^{(4)}$</td>
<td>$\Delta C_{13}^{(4)} = 16\pi^2 W_5 \kappa_5$</td>
</tr>
<tr>
<td>$C_{12}\mid L_i = C_{12}^{\text{I}}$</td>
<td>$C_{12}^{\text{I}} = C_{12}^0 + \Delta C_{12}^{(4)}$</td>
<td>$\Delta C_{12}^{(2)} = 8\pi^2 V_2 Y_2$</td>
</tr>
<tr>
<td>$C_{44}\mid L_i = C_{44}^{\text{I}}$</td>
<td>$C_{44}^{\text{I}} = C_{44}^0 + \Delta C_{44}^{(4)}$</td>
<td>$\Delta C_{44}^{(4)} = 16\pi^2 W_4 \kappa_4$</td>
</tr>
<tr>
<td>$C_{55}\mid L_i = C_{55}^{\text{I}}$</td>
<td>$C_{55}^{\text{I}} = C_{55}^0 + \Delta C_{55}^{(4)}$</td>
<td>$\Delta C_{55}^{(2)} = 4\pi^2 V_3 Y_1$</td>
</tr>
<tr>
<td>$C_{66}\mid L_i = C_{66}^{\text{I}}$</td>
<td>$C_{66}^{\text{I}} = C_{66}^0 + \Delta C_{66}^{(4)}$</td>
<td>$\Delta C_{66}^{(4)} = 16\pi^2 W_6 \kappa_6$</td>
</tr>
</tbody>
</table>

53 The anisotropic term is the same for Voigt or Reuss
The isotropic compliance and stiffness components are\(^5\)

<table>
<thead>
<tr>
<th>Voigt</th>
<th>(C_{11}^0 \mid^V = \frac{1}{15} (8c_{11}^{sc} + 3c_{33}^{sc} + 4c_{13}^{sc} + 8c_{44}^{sc}))</th>
<th>(C-36)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(C_{12}^0 \mid^V = \frac{1}{15} (c_{11}^{sc} + 5c_{12}^{sc} + c_{33}^{sc} + 8c_{13}^{sc} - 4c_{44}^{sc}))</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(C_{44}^0 \mid^V = \frac{1}{30} (7c_{11}^{sc} - 5c_{12}^{sc} + 2c_{33}^{sc} - 4c_{13}^{sc} + 12c_{44}^{sc}))</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Reuss</th>
<th>(S_{11}^0 \mid^R = \frac{1}{15} (8s_{11}^{sc} + 3s_{33}^{sc} + 4s_{13}^{sc} + 2s_{44}^{sc}))</th>
<th>(C-37)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(S_{12}^0 \mid^R = \frac{1}{15} (s_{11}^{sc} + 5s_{12}^{sc} + s_{33}^{sc} + 8s_{13}^{sc} - s_{44}^{sc}))</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(S_{44}^0 \mid^R = \frac{2}{15} (7s_{11}^{sc} - 5s_{12}^{sc} + 2s_{33}^{sc} - 4s_{13}^{sc} + 3s_{44}^{sc}))</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(C_{11}^0 \mid^R = \frac{s_{11}^{0} + s_{12}^{0}}{(s_{11}^{0} - s_{12}^{0})(s_{11}^{0} + 2s_{12}^{0})})</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(C_{12}^0 \mid^R = -\frac{s_{12}^{0}}{(s_{11}^{0} - s_{12}^{0})(s_{11}^{0} + 2s_{12}^{0})})</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(C_{44}^0 \mid^R = \frac{1}{s_{44}^{0}})</td>
<td></td>
</tr>
</tbody>
</table>

The second order anisotropic term factors are

<table>
<thead>
<tr>
<th></th>
<th>(\gamma_1 = \frac{1}{210} (\sqrt{10}W_{200} - 2\sqrt{15}W_{220}))</th>
<th>(C-38)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(\gamma_2 = \frac{1}{210} (\sqrt{10}W_{200} + 2\sqrt{15}W_{220}))</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\gamma_3 = -\frac{1}{105} \sqrt{10}W_{200})</td>
<td></td>
</tr>
</tbody>
</table>

\(^5\) Note that the single crystal tensors are not transformed here, unlike in Section C.3.1
The fourth order anisotropic term factors (not utilised) are:

\[
\begin{align*}
\kappa_1 &= \frac{1}{105}(3\sqrt{2}W_{400} - 4\sqrt{5}W_{420} + 2\sqrt{35}W_{440}) \\
\kappa_2 &= \frac{1}{105}(3\sqrt{2}W_{400} + 4\sqrt{5}W_{420} + 2\sqrt{35}W_{440}) \\
\kappa_3 &= \frac{8}{105}\sqrt{2}W_{400} \\
\kappa_4 &= -\frac{4}{105}(\sqrt{2}W_{400} + \sqrt{5}W_{420}) \\
\kappa_5 &= -\frac{4}{105}(\sqrt{2}W_{400} - \sqrt{5}W_{420}) \\
\kappa_6 &= \frac{4}{105}(\sqrt{2}W_{400} - 2\sqrt{35}W_{440})
\end{align*}
\]

The coefficients for the anisotropic terms are\(^{55}\)

<table>
<thead>
<tr>
<th></th>
<th>Voigt</th>
<th>Reuss</th>
</tr>
</thead>
<tbody>
<tr>
<td>(V_1^{el})</td>
<td>(a_2^{el})</td>
<td>(-4C_{44}^0a_2 - 14C_{12}^0C_{44}^0a_1)</td>
</tr>
<tr>
<td>(V_2^{el})</td>
<td>(a_3^{el})</td>
<td>(-4C_{44}^0a_3 + 14C_{12}^0C_{44}^0a_1)</td>
</tr>
<tr>
<td>(V_3^{el})</td>
<td>(a_4^{el})</td>
<td>(-4C_{44}^0a_4)</td>
</tr>
<tr>
<td>(W^{el})</td>
<td>(a_5^{el})</td>
<td>(-4C_{44}^0a_5)</td>
</tr>
</tbody>
</table>

\(^{55}\) The superscript \(el\) is used to distinguish from the inelastic values determined in Equation (D-13).
with

<table>
<thead>
<tr>
<th></th>
<th>Voigt</th>
<th>Reuss</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_1^{el}$</td>
<td>-</td>
<td>$s_{11}^{sc} + s_{12}^{sc} - s_{23}^{sc} - s_{13}^{sc}$</td>
</tr>
<tr>
<td>$a_2^{el}$</td>
<td>$4c_{11}^{sc} - 3c_{33}^{sc} - c_{13}^{sc} - 2c_{44}^{sc}$</td>
<td>$4s_{11}^{sc} - 3s_{33}^{sc} - s_{13}^{sc} - \frac{1}{2}s_{44}^{sc}$</td>
</tr>
<tr>
<td>$a_3^{el}$</td>
<td>$c_{11}^{sc} - 7c_{12}^{sc} + c_{33}^{sc} + 5c_{13}^{sc} - 4c_{44}^{sc}$</td>
<td>$s_{11}^{sc} - 7s_{12}^{sc} + s_{33}^{sc} + 5s_{13}^{sc} - s_{44}^{sc}$</td>
</tr>
<tr>
<td>$a_4^{el}$</td>
<td>$-5c_{11}^{sc} + 7c_{12}^{sc} + 2c_{33}^{sc} - 4c_{13}^{sc}$ + $6c_{44}^{sc}$</td>
<td>$-5s_{11}^{sc} + 7s_{12}^{sc} + 2s_{33}^{sc} - 4s_{13}^{sc}$ + $\frac{3}{2}s_{44}^{sc}$</td>
</tr>
<tr>
<td>$a_5^{el}$</td>
<td>$c_{11}^{sc} + c_{33}^{sc} - 2c_{13}^{sc} - 4c_{44}^{sc}$</td>
<td>$s_{11}^{sc} + s_{33}^{sc} - 2s_{13}^{sc} - s_{44}^{sc}$</td>
</tr>
</tbody>
</table>

Substitution of Equations (C-16) into Equations (C-38) and (C-39) permits one to express the stiffness tensor (C-36) in terms of the Kearns factors.

### C.4. Comparison of elastic properties obtained from diffraction data and ODFs

The various approximations described in Section C.3.2 are compared and validated in this section.

#### C.4.1.1. Single crystal stiffness temperature dependency

It is demonstrated in Figure C-3 that both the third order polynomial (Fisher & Renken, 1964) and linear approach equations described in Section C.2.1 provide good approximations of the experimental data. Therefore, the linear approach has been selected for the polycrystal calculations.
C.4.1.2. Polycrystal stiffness texture and temperature dependency

Predictions for Zircaloy using the two approaches investigated in Section C.3.2 are compared in Figure C-4. Predictions identified with “f” utilize the equations proposed by Nakatsuka (1981) (Section C.3.2.1) predictions identified with “Wf” rely on the equations of (Li & Thompson, 1990) and (Anderson, Thompson, & Cook, 1999) as combined in Section C.3.2.2. Both predictions are compared with stiffness values derived from diffraction intensity, Equations (C-25), identified with “∫Intens”. Best agreement is obtained with the “Wf” predictions, despite ignoring fourth order ODCs.
C.5. Figures Appendix C

Figure C-1 Unit sphere with orientation angles

![Unit sphere with orientation angles](image)

**Figure C-1** Unit sphere with orientation angles

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Right hand RTL system, used in this report.</td>
<td>Rotated left hand RTL system.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(a)</th>
<th>(b)</th>
<th>(c)</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Diagram" /></td>
<td><img src="image" alt="Diagram" /></td>
<td><img src="image" alt="Diagram" /></td>
</tr>
</tbody>
</table>

**Figure C-2** Comparison of coordinate systems
Figure C-3 Comparison of single crystal experimental stiffness and approximation values.

See Sections C.2.1, C.2.2 and C.4.1.1.

Experimental results: Fisher and Renken (1964)

Third order polynomial: Turner et al. (1995)

Linear approximation: This study
Figure C-4  Stiffness tensor components for Zircaloy 2 as a function of texture and temperature.
APPENDIX D. PREDICTION OF ANISOTROPIC INELASTIC PROPERTY TENSORS USING ODCs AND KEARNS FACTORS

It is postulated that inelastic single crystal tensors exist than can be used with the Kearns factors to calculate inelastic polycrystal tensors, following the methods for elastic material property tensors provided in Appendix C.

D.1. Inelastic material equivalent single crystal property temperature dependent relationships

The equivalent single crystal behaviour is described by polynomial functions of temperature, consistent with the elastic relationships described in Section C.2. The linear version is shown in Equation (D-1) and the 2nd order version in Equation (D-2). The form is consistent for inelastic strain, equilibrium stress and kinematic stress, and the equations and coefficients to describe each of the phenomena are compared in Table 1.

\[ d_{ij}^{sc}[T] = d_{ij}^{sc(0)} + d_{ij}^{sc(1)}T \]  \hspace{1cm} (D-1)

\[ d_{ij}^{sc}[T] = d_{ij}^{sc(0)} + d_{ij}^{sc(1)}T + d_{ij}^{sc(2)}T^2 \]  \hspace{1cm} (D-2)

D.2. Equivalent single crystal tensor and inverse relationship

Equivalent to Equation (C-20), the single crystal inelastic stiffness are expressed as Equation (D-3) and the inelastic compliance as Equation (D-4):
\[
\mathbf{d}^{sc}[T] = \begin{bmatrix}
    d^{sc}_{11}[T] & d^{sc}_{12}[T] & d^{sc}_{13}[T] & 0 & 0 & 0 \\
    d^{sc}_{12}[T] & d^{sc}_{11}[T] & d^{sc}_{13}[T] & 0 & 0 & 0 \\
    d^{sc}_{13}[T] & d^{sc}_{13}[T] & d^{sc}_{33}[T] & 0 & 0 & 0 \\
    0 & 0 & 0 & d^{sc}_{44}[T] & 0 & 0 \\
    0 & 0 & 0 & 0 & d^{sc}_{44}[T] & 0 \\
    0 & 0 & 0 & 0 & 0 & 2(d^{sc}_{11}[T] - d^{sc}_{12}[T])
\end{bmatrix}, \quad (D-3)
\]

\[
\mathbf{b}^{sc}[T] = \mathbf{d}^{sc}[T]^{-1} = \begin{bmatrix}
    b^{sc}_{11}[T] & b^{sc}_{12}[T] & b^{sc}_{13}[T] & 0 & 0 & 0 \\
    b^{sc}_{12}[T] & b^{sc}_{12}[T] & b^{sc}_{13}[T] & 0 & 0 & 0 \\
    b^{sc}_{13}[T] & b^{sc}_{13}[T] & b^{sc}_{33}[T] & 0 & 0 & 0 \\
    0 & 0 & 0 & b^{sc}_{44}[T] & 0 & 0 \\
    0 & 0 & 0 & 0 & b^{sc}_{44}[T] & 0 \\
    0 & 0 & 0 & 0 & 0 & \frac{1}{2}(b^{sc}_{11}[T] - b^{sc}_{12}[T])
\end{bmatrix}, \quad (D-4)
\]

The components of these tensors are, equivalent to Equations (C-21):

\[
\begin{align*}
    b^{sc}_{11}[T] &= \frac{1}{2} \left( \frac{d^{sc}_{33}[T]}{d_0[T]} + \frac{1}{d^{sc}_{11}[T] - d^{sc}_{12}[T]} \right) \\
    b^{sc}_{12}[T] &= \frac{1}{2} \left( \frac{d^{sc}_{33}[T]}{d_0[T]} - \frac{1}{d^{sc}_{11}[T] - d^{sc}_{12}[T]} \right) \\
    b^{sc}_{13}[T] &= -\frac{d^{sc}_{13}[T]}{d_0[T]} \\
    b^{sc}_{33}[T] &= \frac{d^{sc}_{11}[T] + d^{sc}_{12}[T]}{d_0[T]} \\
    b^{sc}_{44}[T] &= \frac{1}{d^{sc}_{44}[T]} \\
    d_0[T] &= d^{sc}_{55}[T](d^{sc}_{11}[T] + d^{sc}_{12}[T]) - 2d^{sc}_{55}[T]^2.
\end{align*}
\]
D.3. Equivalent polycrystal properties

The combined routine proposed in Section C.3.2, combining methodologies of Li et al. (1990) and Anderson et al. (1999) to determine elastic properties is now employed to determine the inelastic properties. Equivalencies are summarized in Table 1, Table 2, Figure D-2 and Figure D-1. Equation (D-6) is the equivalent of Equation (C-32). The averaged Hill tensors are defined as

\[
D_{ij}^{R} = D_{ij}^{0} + \Delta D_{ij} = \left( B_{ij}^{0} \right)^{-1} + \Delta D_{ij} \\
D_{ij}^{V} = D_{ij}^{0} + \Delta D_{ij}
\]

(Equation D-6)

\[
D^{R}_{11} = D^{0}_{11} + \Delta D^{R}_{11} = \left( B^{0}_{11} \right)^{-1} + \Delta D^{R}_{11} \\
D^{V}_{11} = D^{0}_{11} + \Delta D^{V}_{11}
\]

(Equation D-7)

\[
B^{H}_{11} = D^{H}_{11}^{-1}
\]

(Equation D-8)

As with Equation (C-35), the isotropic components are functions of the single crystal components and the anisotropic differences are functions of the single crystal components as well as the six ODCs, as summarized in Equation (D-9).

<table>
<thead>
<tr>
<th>Stiffness tensor components (Voigt or Reuss)</th>
<th>Isotropic term</th>
<th>Anisotropic term containing 2nd order ODCs⁵⁷</th>
</tr>
</thead>
<tbody>
<tr>
<td>D₁₁</td>
<td>Li = D₁₁</td>
<td>Li = D₀₁₁ + ΔD^{(2)}₁₁</td>
</tr>
<tr>
<td>ΔD^{(2)}₁₁</td>
<td>16π²V₁Y₁</td>
<td></td>
</tr>
</tbody>
</table>

⁵⁶ \( B^{H}_{11} = \frac{1}{2} \left( B^{R}_{11} + B^{V}_{11} \right) \) consistent with the approach followed in Footnote 52, p. 17.

⁵⁷ The anisotropic term is the same for Voigt or Reuss
Similar to Equation (C-38), the second order factors are

\[
\gamma_1 = \frac{1}{210} \left( \sqrt{10} W_{200} - 2 \sqrt{15} W_{220} \right)
\]

\[
\gamma_2 = \frac{1}{210} \left( \sqrt{10} W_{200} + 2 \sqrt{15} W_{220} \right)
\]

\[
\gamma_3 = -\frac{1}{105} \sqrt{10} W_{200}
\]

Similar to Equations (C-36) and (C-37), the isotropic components are provided as Equations (D-11) and (D-12).
The coefficients for the anisotropic terms, equivalent to Equations (C-40) are as follows –

Since the fourth order ODCs are not used, the equivalent of $W^{el}$ is not required.

![Table](D-13)
The equivalents of Equations (C-41) are:

<table>
<thead>
<tr>
<th>Voigt</th>
<th>Reuss</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_1^{in}$</td>
<td>-</td>
</tr>
<tr>
<td>$a_2^{in}$</td>
<td>$4d_{11}^{sc} - 3d_{33}^{sc} - d_{13}^{sc} - 2d_{44}^{sc}$</td>
</tr>
<tr>
<td>$a_3^{in}$</td>
<td>$d_{11}^{sc} - 7d_{12}^{sc} + d_{33}^{sc} + 5d_{13}^{sc} - 4d_{44}^{sc}$</td>
</tr>
<tr>
<td>$a_4^{in}$</td>
<td>$-5d_{11}^{sc} + 7d_{12}^{sc} + 2d_{33}^{sc} - 4d_{13}^{sc} + 6d_{44}^{sc}$</td>
</tr>
<tr>
<td>$a_5^{in}$</td>
<td>$d_{11}^{sc} + d_{33}^{sc} - 2d_{13}^{sc} - 4d_{44}^{sc}$</td>
</tr>
</tbody>
</table>
D.4. Figures Appendix D
Figure D-1     Comparison of computed material properties required for the ATXVBO ODEs.
Figure D-2  Sequence for computing the elastic and inelastic polycrystal property tensors.
APPENDIX E. SUMMARY OF EQUATIONS FOR ATXVBO

\[ x = 1 \text{ to } 2 \quad y = 1 \text{ to } 3 \quad u = 1 \text{ to } 5 \quad j = 1 \text{ to } 6 \quad i = 1 \text{ to } 9 \]

E.1. ATXVBO ODEs:

| Elastic strain | \[ \dot{\varepsilon}^{el} = S_y M_y + S_{y+3} (M_y \dot{\sigma} + \sigma M_y) \] (E-1) |
| Inelastic strain | \[ \dot{\varepsilon}^{in} = \frac{1}{E_1 K} \left( B_y^\varepsilon M_y + B_{y+3}^\varepsilon (M_y (\sigma - g) + (\sigma - g) M_y) \right) \] (E-2) |
| Equilibrium stress | \[ \dot{\varepsilon} = E_1 \psi \left( D_y^\varphi M_y + D_{y+3}^\varphi (M_y \dot{\xi} + \dot{\xi} M_y) \right) \]
\[ \dot{\xi} = \dot{\varepsilon} - \frac{\Theta}{A^H + H^T} (1 - \varphi) \dot{\varepsilon}^{in} \] (E-3) |
| Kinematic stress | \[ \dot{\varepsilon} = P_1 \left( D_y^f M_y + D_{y+3}^f (M_y \dot{\varepsilon}^{in} + \dot{\varepsilon}^{in} M_y) \right) \] (E-4) |
| Isotropic stress | \[ \dot{A} = A_c (A_f - A) \dot{p} \]
\[ A_c = \left( A_c^{r(1)} + A_c^{r(2)} T \right) ((1 - f_R - f_T) + C_R f_R + C_T f_T) \]
\[ A_f = \Theta \] (E-5) |
\[ \dot{p} = \frac{\dot{\varepsilon}^{in} \cdot \dot{\varepsilon}^{in}}{\sqrt{1 + \psi^{in}}} \] (E-6) |

E.2. Other equations used in ATXVBO\textsuperscript{eq}:

| Representation directional matrices | \[ M_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad M_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad M_3 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \] (E-7) |
Strain rate sensitivity coefficient for describing DSA

\[ H = H_3 \frac{1}{H_1 \sqrt{2\pi}} e^{-\frac{(\ln \dot{\phi} - H_3)^2}{2(H_1)^2}} \]

\[ H_y^{(2)} = (H_y^{(1)} + H_y^{(2)} + H_y^{(3)}T^2)((1 - f_R - f_T) + C_R f_R + C_T f_T) \]  

(E-8)

Viscosity function

\[ \tilde{k} = \frac{k_1}{E_1} \left(1 + \frac{\Gamma}{k_2}\right)^{-k_3} \]

\[ k_x = (k_x^{(1)} + k_x^{(2)}T)((1 - f_R - f_T) + C_R f_R + C_T f_T) \]  

(E-9)

Shape function

\[ \bar{\psi} = \frac{\psi_1}{E_1} + \frac{\psi_2 - \psi_1}{E_1} e^{-\psi_3 \Gamma} \]

\[ \psi_x = (\psi_x^{(1)} + \psi_x^{(2)}T)((1 - f_R - f_T) + C_R f_R + C_T f_T) \]  

(E-10)

Kinematic stress coefficient

\[ P_1 = (P_1^{(1)} + P_1^{(2)}T)((1 - f_R - f_T) + C_R f_R + C_T f_T) \]  

(E-11)

Normalised shape function

\[ \varphi = \frac{P_1}{E_1 \psi} \]  

(E-12)

Effective overstress based on \( \sigma - g \)

\[ \Gamma = \sqrt{(\mathbf{B}^\varepsilon \cdot (\sigma - g)) \cdot (\mathbf{B}^\varepsilon \cdot (\sigma - g))} \]  

(E-13)

Effective stress based on \( g - f \)

\[ \Theta = \sqrt{(\mathbf{B}^\varepsilon \cdot (g - f)) \cdot (\mathbf{B}^\varepsilon \cdot (g - f))} \]  

(E-14)
### E.3. Polycrystal properties from single crystal properties and texture

\[
\begin{align*}
S_1 &= (S_1 - 2(S_8 + S_9 - S_7))\hat{\sigma}_{11} + S_6\hat{\sigma}_{22} + S_5\hat{\sigma}_{33} \\
S_2 &= S_6\hat{\sigma}_{11} + (S_2 - 2(S_7 + S_9 - S_8))\hat{\sigma}_{22} + S_4\hat{\sigma}_{33} \\
S_3 &= S_5\hat{\sigma}_{11} + S_4\hat{\sigma}_{22} + (S_3 - 2(S_7 + S_8 - S_9))\hat{\sigma}_{33} \\
S_4 &= S_8 + S_9 - S_7 \\
S_5 &= S_7 + S_9 - S_8 \\
S_6 &= S_7 + S_8 - S_9
\end{align*}
\]

(E-15)

\[
\begin{align*}
\mathcal{D}^g_1 &= \left(D^g_1 - 2\left(D^g_8 + D^g_9 - D^g_7\right)\right)\dot{\xi}_1 + D^g_6\dot{\xi}_2 + D^g_5\dot{\xi}_3 \\
\mathcal{D}^g_2 &= D^g_6\dot{\xi}_1 + \left(D^g_2 - 2\left(D^g_7 + D^g_9 - D^g_8\right)\right)\dot{\xi}_2 + D^g_4\dot{\xi}_3 \\
\mathcal{D}^g_3 &= D^g_5\dot{\xi}_1 + D^g_4\dot{\xi}_2 + \left(D^g_3 - 2\left(D^g_7 + D^g_8 - D^g_9\right)\right)\dot{\xi}_3 \\
\mathcal{D}^g_4 &= D^g_8 + D^g_9 - D^g_7 \\
\mathcal{D}^g_5 &= D^g_7 + D^g_9 - D^g_8 \\
\mathcal{D}^g_6 &= D^g_7 + D^g_8 - D^g_9
\end{align*}
\]

(E-16)

\[
\begin{align*}
\mathcal{D}^f_1 &= \left(D^f_1 - 2(D^f_8 + D^f_9 - D^f_7)\right)\dot{\varepsilon}_{1}^{\text{in}} + D^f_6\dot{\varepsilon}_{2}^{\text{in}} + D^f_5\dot{\varepsilon}_{3}^{\text{in}} \\
\mathcal{D}^f_2 &= D^f_6\dot{\varepsilon}_{1}^{\text{in}} + \left(D^f_2 - 2(D^f_7 + D^f_9 - D^f_8)\right)\dot{\varepsilon}_{2}^{\text{in}} + D^f_4\dot{\varepsilon}_{3}^{\text{in}} \\
\mathcal{D}^f_3 &= D^f_5\dot{\varepsilon}_{1}^{\text{in}} + D^f_4\dot{\varepsilon}_{2}^{\text{in}} + \left(D^f_3 - 2(D^f_7 + D^f_8 - D^f_9)\right)\dot{\varepsilon}_{3}^{\text{in}} \\
\mathcal{D}^f_4 &= D^f_8 + D^f_9 - D^f_7 \\
\mathcal{D}^f_5 &= D^f_7 + D^f_9 - D^f_8 \\
\mathcal{D}^f_6 &= D^f_7 + D^f_8 - D^f_9
\end{align*}
\]

(E-17)

\[
\begin{align*}
\mathcal{B}^g_1 &= \left(B^g_1 + 2(B^g_8 + B^g_9 - B^g_7)\right)\varepsilon_{10} + B^g_6\varepsilon_{02} + B^g_5\varepsilon_{03} \\
\mathcal{B}^g_2 &= B^g_6\varepsilon_{01} + \left(B^g_2 + 2(B^g_7 + B^g_9 - B^g_8)\right)\varepsilon_{02} + B^g_4\varepsilon_{03} \\
\mathcal{B}^g_3 &= B^g_5\varepsilon_{01} + B^g_4\varepsilon_{02} + \left(B^g_3 + 2(B^g_7 + B^g_8 - B^g_9)\right)\varepsilon_{03} \\
\mathcal{B}^g_4 &= B^g_8 + B^g_9 - B^g_7 \\
\mathcal{B}^g_5 &= B^g_7 + B^g_9 - B^g_8 \\
\mathcal{B}^g_6 &= B^g_7 + B^g_8 - B^g_9
\end{align*}
\]

(E-18)
APPENDIX F. SEQUENCE OF ODE IMPLEMENTATION, INITIAL AND BOUNDARY CONDITIONS

The sequence of operations when solving the ODEs is shown in Figure F-1 for plastic deformation at constant creep rate and relaxation conditions and in Figure F-2 for thermal creep. The left hand side shows VBO and the right hand side AVBO/ATXVBO. IV refers to initial values and BC to boundary conditions. The right hand side also includes cross reference to the equations in Appendix E.
F.1. Figures Appendix G

Figure F-1  Sequence of solution steps to solve constant strain rate and relaxation boundary condition cases for loads applied in the m direction.
Figure F-2  Sequence of solution steps to solve thermal creep boundary condition cases for loads applied in the m direction.
APPENDIX G.  DEPENDENCE OF Zr-2.5Nb EXPERIMENTAL TEXTURE AND DEFORMATION DATA ON MANUFACTURING ASPECTS

There is limited Zr-alloy plastic deformation and thermal creep data available with texture adequately captured for application with ATXVO. This is a summary of data available for Zr-2.5Nb for that purpose. Section G.1 explores correlations between material composition, ingot melting practice, grain size (determined by billet cooling), extrusion temperature, extrusion ratio and texture. Section G.2 evaluates the effect of material characteristics on plastic deformation of Zr-2.5Nb, while thermal creep is explored similarly in Section G.3. Table G-12 provides an overall summary of the findings.

G.1.  Correlations between material characteristics and manufacturing aspects

Holt and Aldridge (1985) documented trends between texture and key manufacturing aspects for various Zr-2.5Nb specimens produced from double melted ingots, demonstrating significant correlation. The specimens for the thermal creep tests of Li (2009) selected for the evaluation of ATXVBO (Section G.3) were produced from quadruple melted ingots. As a result, an evaluation is performed here to demonstrate that the trends observed by Holt and Aldridge on correlations between texture and

58 Section 3.1 provides an overview of the manufacturing of pressure tubes.
manufacturing aspects still hold true. Additional observations regarding texture trends are also made\(^{59}\).

**G.1.1. Effect of material composition and ingot melting practice on texture**

The fact that the practice with respect to re-melting the ingots are different (Section 3.1) is reflected in differences in the material composition: When the composition of the ingots used for the specimens examined by Holt and Aldridge (1985) are compared to those of Li (2009), Table G-9, it is seen that the Fe, C, H and Ta were higher for the double melted material. The data considered here do not permit a detailed comparison of the effect of composition and melting practice on texture, yet these manufacturing aspects are known to affect the behaviour of tubes in-reactor (Bickel & Griffiths, 2007) (Bickel & Griffiths, 2008).

**G.1.2. Effect of billet cooling and grain size on texture**

Holt and Aldridge (1985) observed that a change to the grain size did not affect \(f_T\) or \(f_T-f_R\). It can be concluded from Table G-3 that where there is sufficient data available that shows \(f_R\) to increase and both \(f_T\) and \(f_T-f_R\) to decrease with an increase in grain size. No trend is seen for \(f_L\). Significant differences are seen between the results of Holt and Aldridge and Li (2009).

---

\(^{59}\) These comparisons do not show measurement uncertainty with the exception of Figure G-1.
G.1.3. Effect of extrusion temperature texture

Holt and Aldridge (1985) observed that a higher extrusion temperature resulted in a higher $f_L$ and lower $f_R/f_T$ (i.e. increasing $f_T-f_R$). Their conclusions are echoed in Table G-1, where it is also shown that $f_R$ decreases with an increase in extrusion temperature. Significant differences are seen between the reported texture magnitudes of Holt and Aldridge and Li (2009).

G.1.4. Effect of extrusion ratio on texture

Holt and Aldridge (1985) observed that a higher extrusion ratio results in a decreasing $f_R/f_T$ (i.e. increasing $f_T-f_R$) and decreasing $f_L$. Their conclusions are echoed in Table G-2, where it is also shown that $f_R$ decreases and $f_T$ increases with an increase in extrusion ratio. Significant differences are seen between the reported texture magnitudes of Holt and Aldridge and Li (2009).

G.1.5. Effect of cold work amount

The material specimens considered in the comparisons all experienced between 25% and 30% cold work, with the exception of the fuel sheath material used by Li (2009). As observed in Figure G-8 and as concluded in Table G-1, the behaviour of the 70% cold worked FS material results in significantly different texture.

G.2. Plastic deformation at constant strain rate

The uniaxial plastic deformation experimental data for tube material (Christodoulou, Turner, Ho, Chow, & Resta Levi, 2000), summarized in Table G-4 and reproduced as part of Figure G-18, do not provide the texture for every curve provided uniquely, i.e. any test
stress-strain curve can be for any one of twenty-five tubes (1 × “Tube A”, 1 × “Tube B”, 1 × “Tube C” and 22 × “Tube D”). Test data for plate material from the same reference is summarized in Table G-5. A single texture value is given for all tests, suggesting that all samples were produced from the same piece of plate. Table G-6 summarize the biaxial test data obtained with mini tubes by the same authors, again only for a single reported texture state. As a result, there are some limitations with the data of Christodoulou et al. (2000) for the purposes of this study: The lack of specimen specific data prohibits conclusions on texture dependency on plastic strain of tube material. Also, as all the test specimens were extruded at 815°C with unknown extrusion ratio, the effect of extrusion variability on plastic deformation could not be investigated. It is also not known if the billets for these samples were slow cooled or β-quenched. However, based on the assumption that the texture variance between their plate samples is small, these results were still found to be useful for this study.

To inspect the test temperature dependency, the stress versus strain plots provided at different temperatures in Figure G-18 were recast as stress versus temperature in Figure G-19 at distinct strain levels. Significant linear dependency with temperature is observed, confirming the linear thermal dependency assumption for ATXVBO as discussed in Section 4.1.2 and summarized in Appendix E.2, but challenged by an evaluation of R and P in Section 7.2.3.

G.3. Thermal creep

Christodoulou et al. (2002) also only reported average texture data for their thermal creep tests on pressure tube and mini pressure tube material. Li (2009) reported
specimen-specific texture data for the thermal creep testing performed at somewhat higher temperatures on mini tubes. The tests specimens for both are compared in Table G-7. Christodoulou et al. (2002) reported anomalous behaviour during repeat tests, as pointed out in Figure G-22. The results for biaxial testing in Figure G-23, again with only a single texture provided, also show significantly different results despite the fact that the temperatures are not that dissimilar. It is believed that specimen-specific texture might have explained the observed differences, as hypothesized in Section 3.3.4.2.

In order to verify if similar discrepancies can be observed in the other creep test data considered or if differences in behaviour at similar test conditions could be attributed to texture, all the tabulated test data provided by Li (2009) were evaluated in detail. The test specimens are summarized in Table G-8 and all the results shown in Figure G-24. The various creep test cases are summarized in Table G-10. The objectives for the selection of the creep test cases were two-fold: Firstly, cases had to be identified to allow for a systematic optimization and evaluation of ATXVBO, to isolate cases where texture variation is the only variable. Secondly, it allowed observations on the repeatability of the tests, given the anomalous behaviour reported by Christodoulou et al. (2002) following their creep tests carried out at lower temperatures. The database compiled from the results of Li (2009) was filtered to investigate the effect of billet cooling, extrusion temperature as well as the extrusion ratio. Since the tests were all carried out with pressurized capsules, different biaxial stress states could be obtained by varying the additional axial tensile or compressive force applied: Both tangential and axial stress values ($\sigma_T$ and $\sigma_L$) are reported in Table G-10.
From a review of Figure G-25 to Figure G-33, a number of conclusions are drawn in Table G-11 about the material behaviour from a texture point of view. The expected trend with respect to texture, identified at the top of that table, is based on the dominance of slip parallel to basal planes in Zr alloys (Section 3.4). Since the relative axial deformation was small and more prone to measurement error than the diametral strain, conclusions regarding deviations from the expected longitudinal behaviour cannot be made with the same level of certainty. Longitudinal deformation is therefore excluded from the discussion on anomalies presented below.

It is concluded from the qualitative evaluation of the 350°C thermal creep test results that slip parallel to basal planes could explain the observed behaviour for Zr-2.5Nb material extruded at 815°C. Therefore the data from Li (2009) lends itself well for optimization and validation purposes.
### Table G-1. Correlation between texture and increase in extrusion temperature for Zr-2.5Nb pressure tube material.

<table>
<thead>
<tr>
<th>Holt et al. (1985)</th>
<th>Figure</th>
<th>Extrusion temp. (°C)</th>
<th>Extr. ratio</th>
<th>Grain size</th>
<th>Cold work (%)</th>
<th>Observed trend with &gt; extrusion temperature (S – Strong, W – Weak, N – None, I - Inconclusive)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt; f_L with &gt;T_{extr} &lt; f_R/f_T (&gt; f_T-f_R) with &gt;T_{extr}</td>
<td>Figure G-2</td>
<td>650 to 852</td>
<td>10:1</td>
<td>Coarse</td>
<td>25 to 30</td>
<td>f_R, f_T, f_L, f_T-f_R</td>
</tr>
<tr>
<td>Figure G-3</td>
<td>Figure G-4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Figure G-5</td>
<td>Figure G-6</td>
<td>Figure G-7</td>
<td>Fine</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Figure G-8</td>
<td>700 to 950</td>
<td>10:1 &amp; 12:1</td>
<td>25 to 30 and 70</td>
<td>f_R, f_T, f_L, f_T-f_R</td>
<td>&lt;W, &lt;S, &gt;S, &lt;S</td>
<td>If 70% CW data excluded</td>
</tr>
<tr>
<td>Figure G-9</td>
<td>Figure G-10</td>
<td>650 to 852</td>
<td>4:1</td>
<td>Coarse</td>
<td>25 to 30</td>
<td>f_R, f_T, f_L, f_T-f_R</td>
</tr>
</tbody>
</table>
Table G-2. Correlation between texture and increase in extrusion ratio for Zr-2.5Nb pressure tube material.

<table>
<thead>
<tr>
<th>Holt et al. (1985)</th>
<th>Figure</th>
<th>Extrusion temp. (°C)</th>
<th>Extr. ratio</th>
<th>Grain size</th>
<th>Cold work (%)</th>
<th>Observed trend with &gt; extrusion ratio (S – Strong, W – Weak, N – None, I - Inconclusive)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt; f_L with &gt; extr. ratio</td>
<td>Figure G-11</td>
<td>650-652</td>
<td>4:1 &amp; 10:1</td>
<td>Coarse</td>
<td>25 to 30</td>
<td>f_R &lt;S f_T &gt;S f_L &lt;W f_T-f_R &gt;S</td>
</tr>
<tr>
<td>&lt; f_R/f_T (&gt; f_T-f_R) with &gt;extr. ratio up to 20:1</td>
<td>Figure G-12</td>
<td></td>
<td>Fine</td>
<td></td>
<td></td>
<td>Distinct differences between data of Holt et al. (1985) and Li (2009)</td>
</tr>
<tr>
<td></td>
<td>Figure G-13</td>
<td>812 to 815</td>
<td>10:1 &amp; 20:1</td>
<td>Coarse</td>
<td></td>
<td>Good correlation between data of Holt et al. (1985) and Li (2009)</td>
</tr>
<tr>
<td></td>
<td>Figure G-14</td>
<td></td>
<td>10:1 &amp; 32:1</td>
<td>Fine</td>
<td></td>
<td>Good correlation between data of Holt et al. (1985) and Li (2009)</td>
</tr>
</tbody>
</table>
Table G-3. Correlation between texture and increase in grain size for Zr-2.5Nb pressure tube material.

<table>
<thead>
<tr>
<th>Holt et al. (1985)</th>
<th>Figure</th>
<th>Extrusion temp. (°C)</th>
<th>Extr. ratio</th>
<th>Grain size</th>
<th>Cold work (%)</th>
<th>Observed trend with &gt; grain size (S – Strong, W – Weak, N – None, I - Inconclusive)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No effect on f_T</td>
<td>Figure G-15</td>
<td>650 to 652</td>
<td>4:1</td>
<td>Coarse and fine</td>
<td>25 to 30</td>
<td>f_R &gt;S f_T &lt;S f_L &lt;S f_T-f_R &lt;S</td>
</tr>
<tr>
<td>No trend for f_T-f_R</td>
<td>Figure G-16</td>
<td></td>
<td>10:1</td>
<td></td>
<td></td>
<td>f_R &gt;S f_T &lt;S f_L &lt;S f_T-f_R &lt;S</td>
</tr>
<tr>
<td></td>
<td>Figure G-17</td>
<td>812 to 815</td>
<td></td>
<td></td>
<td></td>
<td>f_R I f_T I f_L I f_T-f_R I</td>
</tr>
</tbody>
</table>
Table G-4. Dataset “A2”: Experimental uniaxial plastic deformation of tube material at constant strain rate.

Christodoulou et al. (2000), Fig. 5(a) (axial direction) and Fig. 5(b) (transverse direction) (Reproduced in Figure G-18)

<table>
<thead>
<tr>
<th>Tube No.</th>
<th>Billet cooling</th>
<th>Extrusion conditions</th>
<th>Test conditions</th>
<th>Texture</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Temp. (°C)</td>
<td>Ratio</td>
<td>Temp. (°C)</td>
</tr>
<tr>
<td>Tube A</td>
<td>Unknown</td>
<td>815</td>
<td>Unknown</td>
<td>250 &amp; 300</td>
</tr>
<tr>
<td>Tube B</td>
<td>Unknown</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tube C</td>
<td>Unknown</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ave. Tubes A to C</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tube D (average for 22 pressure tubes)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table G-5. Experimental uniaxial plastic deformation of plate material at constant strain rate.

Christodoulou et al. (2000) Fig. 6(a) (axial direction) and Fig. 6(b) (transverse direction) (Reproduced in Figure G-18)

<table>
<thead>
<tr>
<th>Plate No.</th>
<th>Billet cooling</th>
<th>Rolling conditions</th>
<th>Test conditions</th>
<th>Texture</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Unknown</td>
<td>Unknown</td>
<td>100, 150, 200 &amp; 250</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.670</td>
<td>0.168</td>
</tr>
</tbody>
</table>

Table G-6. Experimental uniaxial plastic deformation of mini tubes at constant strain rate.

Christodoulou et al. (2000) Fig. 7 (Reproduced in Figure G-20)

<table>
<thead>
<tr>
<th>Mini tube No.</th>
<th>Billet cooling</th>
<th>Extrusion conditions</th>
<th>Test conditions</th>
<th>Texture</th>
</tr>
</thead>
<tbody>
<tr>
<td>-</td>
<td>Unknown</td>
<td>815</td>
<td>25, 250 &amp; 300</td>
<td>0.0008</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.385</td>
<td>0.574</td>
</tr>
<tr>
<td>Test description</td>
<td>Billet cooling</td>
<td>Extrusion conditions</td>
<td>Test conditions</td>
<td>Texture</td>
</tr>
<tr>
<td>------------------</td>
<td>----------------</td>
<td>---------------------</td>
<td>----------------</td>
<td>---------</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Temp. (°C)</td>
<td>Ratio</td>
<td>Temp. (°C)</td>
</tr>
<tr>
<td>Christodoulou et al. (2002) Fig. 4 (Figure G-22)</td>
<td>Unknown</td>
<td>Assumed 815°C based on Causey et al. (1994) &amp; (2000) as indicated by Christodoulou (2002)</td>
<td>100</td>
<td>350 &amp; 400</td>
</tr>
<tr>
<td>Christodoulou et al. (2002) Fig. 5(a) (b) (Figure G-22)</td>
<td>Unknown</td>
<td>Assumed 815°C based on Causey et al. (1994) &amp; (2000) as indicated by Christodoulou (2002)</td>
<td>200</td>
<td>200, 275 &amp; 350</td>
</tr>
<tr>
<td>Christodoulou et al. (2002) Fig. 6 (Figure G-22)</td>
<td>Unknown</td>
<td>Assumed 815°C based on Causey et al. (1994) &amp; (2000) as indicated by Christodoulou (2002)</td>
<td>250</td>
<td>400, 475 &amp; 500</td>
</tr>
<tr>
<td>Christodoulou et al. (2002) Fig. 11&amp;12 (Figure G-23)</td>
<td>815</td>
<td>10:1</td>
<td>310, 320, 323</td>
<td>337</td>
</tr>
<tr>
<td>Li (2009) Appendix IV (Figure G-24 to Figure G-33)</td>
<td>β &amp; SC</td>
<td>650, 700, 815 or 975</td>
<td>12:1, 10:1 or 4:1</td>
<td>300, 350 and 400</td>
</tr>
</tbody>
</table>

β: β-quenched  SC: Slow cooled  MPT: Mini pressure tube  FS: Fuel sheath
Table G-8. Capsule summary (Li W., 2009)

<table>
<thead>
<tr>
<th>Tube No.</th>
<th>Ingot cooling</th>
<th>Billet/Ingots</th>
<th>Grain size (μm) Front</th>
<th>Extr. temp. (°C)</th>
<th>Extr. ratio</th>
<th>f_R (F)</th>
<th>f_T (F)</th>
<th>f_L (F)</th>
<th>f_R (B)</th>
<th>f_T (B)</th>
<th>f_L (B)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPT62</td>
<td>Pressure tube</td>
<td>Ingot A</td>
<td>β</td>
<td>0.2 to 0.5</td>
<td>650</td>
<td>4:1</td>
<td>0.424</td>
<td>0.52</td>
<td>0.056</td>
<td>0.411</td>
<td>0.522</td>
</tr>
<tr>
<td>MPT63</td>
<td></td>
<td></td>
<td>β</td>
<td>0.2 to 0.3</td>
<td>815</td>
<td>10:1</td>
<td>0.374</td>
<td>0.569</td>
<td>0.057</td>
<td>0.385</td>
<td>0.566</td>
</tr>
<tr>
<td>MPT65</td>
<td></td>
<td></td>
<td></td>
<td>0.7 to 1.5</td>
<td>650</td>
<td>4:1</td>
<td>0.453</td>
<td>0.468</td>
<td>0.079</td>
<td>0.448</td>
<td>0.471</td>
</tr>
<tr>
<td>MPT66</td>
<td></td>
<td>Pressure tube</td>
<td>Ingot B</td>
<td>0.4 to 0.8</td>
<td>815</td>
<td>10:1</td>
<td>0.359</td>
<td>0.554</td>
<td>0.087</td>
<td>0.389</td>
<td>0.523</td>
</tr>
<tr>
<td>MPT72</td>
<td></td>
<td>Pressure tube</td>
<td>Ingot B</td>
<td>0.4 to 0.8</td>
<td>815</td>
<td>10:1</td>
<td>0.375</td>
<td>0.582</td>
<td>0.043</td>
<td>0.381</td>
<td>0.56</td>
</tr>
<tr>
<td>MPT73</td>
<td></td>
<td></td>
<td>SC</td>
<td>0.4 to 0.8</td>
<td>815</td>
<td>10:1</td>
<td>0.382</td>
<td>0.538</td>
<td>0.08</td>
<td>0.377</td>
<td>0.542</td>
</tr>
<tr>
<td>MPT74</td>
<td></td>
<td></td>
<td>SC</td>
<td>0.4 to 0.8</td>
<td>650</td>
<td>4:1</td>
<td>0.376</td>
<td>0.529</td>
<td>0.094</td>
<td>0.431</td>
<td>0.486</td>
</tr>
<tr>
<td>MPT76</td>
<td></td>
<td></td>
<td>SC</td>
<td>0.7 to 1.5</td>
<td>650</td>
<td>4:1</td>
<td>0.381</td>
<td>0.542</td>
<td>0.076</td>
<td>0.416</td>
<td>0.506</td>
</tr>
<tr>
<td>MPT77</td>
<td></td>
<td></td>
<td>SC</td>
<td>0.7 to 1.5</td>
<td>650</td>
<td>4:1</td>
<td>0.376</td>
<td>0.529</td>
<td>0.094</td>
<td>0.431</td>
<td>0.486</td>
</tr>
<tr>
<td>MPT79</td>
<td></td>
<td></td>
<td>SC</td>
<td>0.7 to 1.5</td>
<td>650</td>
<td>4:1</td>
<td>0.376</td>
<td>0.529</td>
<td>0.094</td>
<td>0.431</td>
<td>0.486</td>
</tr>
<tr>
<td>MPT81</td>
<td></td>
<td></td>
<td>SC</td>
<td>0.5</td>
<td>975</td>
<td>10:1</td>
<td>0.335</td>
<td>0.441</td>
<td>0.223</td>
<td>0.336</td>
<td>0.558</td>
</tr>
<tr>
<td>MPT82</td>
<td></td>
<td></td>
<td>SC</td>
<td>0.5</td>
<td>975</td>
<td>10:1</td>
<td>0.326</td>
<td>0.492</td>
<td>0.181</td>
<td>0.343</td>
<td>0.553</td>
</tr>
<tr>
<td>FS</td>
<td>WR1</td>
<td>β</td>
<td>Unknown</td>
<td>700</td>
<td>12:1</td>
<td>0.55</td>
<td>0.389</td>
<td>0.059</td>
<td>N/A</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

β: β-quenched  SC: Slow cooled  F: Front end  B: Back end  MPT: Mini pressure tube  FS: Fuel sheath
### Table G-9. Capsule composition

<table>
<thead>
<tr>
<th>Elements, wt%</th>
<th>Impurities (ppm, weight)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zr</td>
<td>Nb</td>
</tr>
<tr>
<td>(Holt &amp; Aldridge, 1985) Table 1</td>
<td>2.4 to 2.8</td>
</tr>
<tr>
<td>(Li W., 2009) MPT62, 63, 65 and 66</td>
<td>2.5 to 2.8</td>
</tr>
<tr>
<td>(Li W., 2009) MPT72, 73, 74, 76, 77, 79, 81 and 82</td>
<td>2.5 to 2.8</td>
</tr>
<tr>
<td>(Li W., 2009) FS</td>
<td>2.6 to 2.7</td>
</tr>
</tbody>
</table>
Table G-10. Creep tests performed at 350°C (Li W., 2009): Filtered combinations.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Billet cooling</th>
<th>Fig</th>
<th>Tubes used for test</th>
<th>Extr. temp. (°C)</th>
<th>Extr. ratio</th>
<th>$\sigma_T$ (MPa)</th>
<th>$\sigma_L$ applied (MPa)</th>
<th>f_R</th>
<th>f_T</th>
<th>f_L</th>
</tr>
</thead>
<tbody>
<tr>
<td>All data</td>
<td>β and SC</td>
<td>Figure G-24</td>
<td>All</td>
<td>650, 815 &amp; 975</td>
<td>4:1 &amp; 10:1</td>
<td>100 to 325</td>
<td>-900 to 900</td>
<td>0.326</td>
<td>0.389</td>
<td>0.043</td>
</tr>
<tr>
<td>F3</td>
<td>SC</td>
<td>Figure G-25</td>
<td>MPT65 76 77 79</td>
<td>650</td>
<td>4:1</td>
<td>300</td>
<td>0</td>
<td>0.376</td>
<td>0.468</td>
<td>0.069</td>
</tr>
<tr>
<td>F4</td>
<td>SC</td>
<td>Figure G-26(a)</td>
<td>MPT72 73 74</td>
<td>650</td>
<td>10:1</td>
<td>300</td>
<td>0</td>
<td>0.375</td>
<td>0.518</td>
<td>0.043</td>
</tr>
<tr>
<td>F9</td>
<td>SC</td>
<td>Figure G-27</td>
<td>MPT66</td>
<td>815</td>
<td>10:1</td>
<td>275 to 325</td>
<td>0</td>
<td>0.359</td>
<td>0.554</td>
<td>0.087</td>
</tr>
<tr>
<td>F5</td>
<td>SC</td>
<td>Figure G-28(a)</td>
<td>MPT81 82</td>
<td>975</td>
<td>10:1</td>
<td>300</td>
<td>0</td>
<td>0.326</td>
<td>0.441</td>
<td>0.103</td>
</tr>
<tr>
<td>F6</td>
<td>β</td>
<td>Figure G-29</td>
<td>MPT63</td>
<td>815</td>
<td>10:1</td>
<td>300</td>
<td>0</td>
<td>0.374</td>
<td>0.389</td>
<td>0.057</td>
</tr>
<tr>
<td>F6a</td>
<td>β</td>
<td>Figure G-30</td>
<td>MPT63</td>
<td>815</td>
<td>10:1</td>
<td>300</td>
<td>0</td>
<td>0.359</td>
<td>0.554</td>
<td>0.087</td>
</tr>
<tr>
<td>β vs. SC</td>
<td>β and SC</td>
<td>Figure G-32</td>
<td>MPT63 68</td>
<td>815</td>
<td>10:1</td>
<td>300</td>
<td>0</td>
<td>0.359</td>
<td>0.554</td>
<td>0.087</td>
</tr>
<tr>
<td>Extr. temp.</td>
<td>SC</td>
<td>Figure G-33</td>
<td>MPT66 72 73 82</td>
<td>650, 815 &amp; 975</td>
<td>10:1</td>
<td>300</td>
<td>0</td>
<td>0.343</td>
<td>0.538</td>
<td>0.043</td>
</tr>
<tr>
<td>Extr. ratio</td>
<td>SC</td>
<td>Figure G-34</td>
<td>MPT72 73 76 77</td>
<td>650</td>
<td>4:1 &amp; 10:1</td>
<td>300</td>
<td>0</td>
<td>0.343</td>
<td>0.529</td>
<td>0.043</td>
</tr>
</tbody>
</table>
Table G-11. Correlations between creep strain and texture from a review of Table G-10 and Figure G-25 to Figure G-33

| Dataset | Fig | Expected trend of strain and texture for the assumption of predominant slip parallel to basal planes.  
(N: No correlation; >: Increasing; <: Decreasing.) |
|---------|-----|-------------------------------------------------------------------------------------------------|
| F3      | Figure G-25  
Slow cooled 650°C, 4:1 | MPT65-01 and MPT79-02 do not follow the trend of a smaller $f_L$ resulting in larger axial strain. This could be attributed to measurement sensitivity. MPT65-01 and MPT79-02 both show a larger $\varepsilon_T$ with smaller $f_T$, relative to the other datasets, but they seem to be reversed. |
|         | F4  
Figure G-26(a)  
Slow cooled 650°C, 10:1 $\sigma_L$: 0MPa | Texture variation within the selection is relatively small. No significant trend with texture is observed in the longitudinal direction. The transverse strain shows a small increase with reduction in $f_T$, as expected. |
|         | F4  
Figure G-26(b)  
Slow cooled 650°C, 10:1 $\sigma_L$: -900MPa | There is observable difference in the axial and transverse directions, but not correlated with texture explained by slip parallel to basal planes. If MPT 72-01 were to be ignored, the key trends for $<$fL & $>$\varepsilon_{L}$ as well as $<$fT & $>$\varepsilon_{T}$ are observed. |

See Section Chapter 3 for Tenckhoff’s (1988) prediction on the expected deformation dependence on texture.

Note that the longitudinal strain values are quite small and more effected by measurement sensitivity.
Expected trend of strain and texture for the assumption of predominant slip parallel to basal planes. (N: No correlation; >: Increasing; <: Decreasing.)

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Fig</th>
<th>Description</th>
<th>&gt;\varepsilon_L</th>
<th>&gt;\varepsilon_T</th>
</tr>
</thead>
<tbody>
<tr>
<td>F9</td>
<td>Figure G-27</td>
<td>Slow cooled 815°C, 10:1</td>
<td>MPT66-02 @ 275MPa &lt; MPT66-05 @ 300MPa &lt; MPT66-04 @ 325MPa. The strain of MPT66-04 reduces at about 100h, bringing the longitudinal strain measurements into question.</td>
<td>N</td>
</tr>
<tr>
<td>F5</td>
<td>Figure G-28(a)</td>
<td>Slow cooled 975°C, 10:1 σ_L: 0MPa</td>
<td>MPT81-02, 81-01, 81-03, 82-03 and 82-05 all show a strong opposite trend in the transverse direction with respect to f_T. They all also show a strong correlation with f_L.</td>
<td>N</td>
</tr>
<tr>
<td></td>
<td>Figure G-28(b)</td>
<td>Slow cooled 975°C, 10:1 σ_L: ±900MPa</td>
<td>Unlike Figure G-28(a), with no applied axial load, MPT 81-01 and 82-02 with an applied tensile load, show the expected transverse strain trend with respect to f_T. This may show anomalous behaviour.</td>
<td>N</td>
</tr>
</tbody>
</table>

All texture reported to be the same. It is unknown to what extent the texture might have changed along the long length of tube from which the samples had been prepared.
Dataset | Fig | Expected trend of strain and texture for the assumption of predominant slip parallel to basal planes.\(^{661}\) (N: No correlation; >: Increasing; <: Decreasing.) | \(\varepsilon_L\) | \(\varepsilon_T\) |
<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>F6</td>
<td>Figure G-29</td>
<td>Differences in response for tests conducted at the same material and test conditions only for the longitudinal direction could be attributed to measurement sensitivity. Otherwise very consistent response.</td>
<td>N</td>
<td>&lt;</td>
</tr>
<tr>
<td>F6a</td>
<td>Figure G-30</td>
<td>MPT63-05 and MPT 63-07 were subjected to the highest and lowest axial test loads, respectively, and they are expected to straddle MPT63-03 and MPT63-08. This behaviour is reflected in the axial strain response, but not in the transverse direction. As expected, the variation in the transverse direction as a result of differences in axial load is small; however, the Poisson effect should result in a consistent straddling trend with respect to axial load. MPT63-05 appears to underestimate transverse strain.</td>
<td>All texture reported to be the same. It is unknown to what extend the texture might have changed along the long length of tube from which the samples had been prepared. The variation in transverse response to variation in axial load might be attributed to differences in texture.</td>
<td>N</td>
</tr>
<tr>
<td></td>
<td>Figure G-31</td>
<td>The axial load case strain responses reflect the respective axial loads. However, as in Figure G-30, the expected trend with respect to axial load is not reflected in the transverse strain.</td>
<td>All texture relatively similar. Significant more strain for the (\beta)-quenched material with smaller grains.</td>
<td></td>
</tr>
<tr>
<td>(\beta) vs. SC</td>
<td>Figure G-32</td>
<td>Distinct separation between (\beta) and SC results and good repeatability for the same billet cooled condition, with some variability with longitudinal strain possibly the result of measurement sensitivity.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dataset</td>
<td>Fig</td>
<td>Expected trend of strain and texture for the assumption of predominant slip parallel to basal planes, (6061) (N: No correlation; &gt;: Increasing; &lt;: Decreasing.)</td>
<td></td>
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<tr>
<td>---------</td>
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<td>------------------------------------------------------------------------------------------------</td>
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</tr>
<tr>
<td>Extr. temp.</td>
<td>Figure G-33 Slow cooled 650°, 815°C &amp; 975°C, 10:1</td>
<td>Distinct separation of the strain response for different extrusion temperatures. There is good repeatability in transverse strain for the 975°C specimens. The transverse strain of the two 650°C samples are surprisingly similar considering that (f_T) for MPT72-02 is 0.582 while it is 0.538 for MPT73-02.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Extr. ratio</td>
<td>Figure G-34 Slow cooled 650°C, 4:1 &amp; 10:1 (\sigma_L): 0MPa</td>
<td>The longitudinal strain response separate by extrusion ratio, with the higher ratio resulting in higher strain. The results vary relatively little with texture. The transverse strain does not separate out with extrusion ratio.</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>All textures relatively similar.</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Unfortunately there is not enough experimental data at 815°C to investigate the effect of the extrusion ratio.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table G-12. Summary of correlations observed from experimental data considered for optimization of ATXVBO

<table>
<thead>
<tr>
<th>Manufacturing aspects</th>
<th>Material characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(S – Strong, W – Weak, N – None, I - Inconclusive)</td>
</tr>
<tr>
<td>Composition and ingot melting</td>
<td>&gt; Extrusion temp.</td>
</tr>
<tr>
<td>Texture, Section G.1</td>
<td>Section G.1.1</td>
</tr>
<tr>
<td></td>
<td></td>
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<td></td>
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<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Thermal creep, Section G.3</td>
<td>Not enough data to establish trends.</td>
</tr>
</tbody>
</table>

Note: \( f_T - f_R \) represents the variation of the c-axes in the radial-transverse plane for extruded tube (see Footnote 5).
G.5. Figures Appendix G

The texture ranges are obtained from the graphs that depict a number of trends associated with the in-reactor performance of Zr-2.5Nb material. Sample sizes as high as 87 were reported. Only values of $f_R$ were provided as it showed the best or strongest correlation with in-reactor elongation. E through AA denote different series of tubes.

- **Bickel 07** by Bickel & Griffiths (2007)
- **Chr 2000** by Christodoulou et al. (1996)
- **Holt 85** by Holt et al. (1985)
- **Li** by Li (2009)

### Table of Texture Data

<table>
<thead>
<tr>
<th>Source</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bickel 07</td>
<td>The texture was provided for 25 regular tubes as well as a value for mini tubes and plate material. It is assumed that the texture reported for the plate and mini tubes are also average values for multiple specimens as reported for Tube D. AC and D in the legend denote the tubes.</td>
</tr>
<tr>
<td>Holt 85</td>
<td>Only texture data obtained for an extrusion temperature of 812°C were used in this comparison. The sample sizes are small.</td>
</tr>
<tr>
<td>Li</td>
<td>The cylinders for the creep capsules were cut from a number of mini tubes, either from the front or back. The texture of the front and back ends of the mini tubes were reported.</td>
</tr>
</tbody>
</table>

**β** - β-quenched billet  
**SC** - Slow cooled billet  
**Last digit** - Texture sample size

**Figure G-1.** Comparison of texture values of samples with billets that were either β-quenched or slow-cooled in the β-phase and extruded at 812 - 815°C at a ratio of 10:1.
Figure G-2. Average Kearns factors of samples from billets that were slow-cooled in the β-phase and extruded at different temperatures at a ratio of 10:1.
Figure G-3. Front (F) and back (B) Kearns factors of samples from billets that were slow-cooled in the β-phase and extruded at different temperatures at a ratio of 10:1.
Figure G-4. Variation of c-axes of samples from billets that were slow-cooled in the β-phase and extruded at different temperatures at a ratio of 10:1.
Figure G-5. Average Kearns factors of samples from billets that were β-quenched and extruded at different temperatures at a ratio of 10:1.
Figure G-6. Front (F) and back (B) Kearns factors of samples from billets that were $\beta$-quenched and extruded at different temperatures at a ratio of 10:1.
Figure G-7. Variation of c-axes of samples from billets that were β-quenched and extruded at different temperatures at a ratio of 10:1.
Figure G-8. Kearns factors, front and back, as well as variation of c-axes of samples from billets that were β-quenched and extruded at different temperatures and that received 25-30% CW (extrusion ratio of 10:1) and 70% CW (extrusion ratio of 12:1).
Figure G-9. Average Kearns factors as well as variation of c-axes of samples from billets that were slow-cooled in the β-phase and extruded at different temperatures at a ratio of 4:1.
Figure G-10. Average Kearns factors as well as variation of c-axes of samples from billets that were $\beta$-quenched and extruded at different temperatures at a ratio of 4:1.
Figure G-11. Average Kearns factors as well as variation of c-axes of samples from billets that were slow-cooled in the β-phase and extruded at 650-652°C at a ratio between 4:1 and 10:1.
Figure G-12. Average Kearns factors as well as variation of c-axes of samples from billets that were β-quenched and extruded at 650-652°C at a ratio between 4:1 and 10:1.
Figure G-13. Average Kearns factors as well as variation of c-axes of samples from billets that were slow-cooled in the β-phase and extruded at 812-815°C at a ratio between 10:1 and 20:1.
Figure G-14. Average Kearns factors as well as variation of c-axes of samples from billets that were \( \beta \)-quenched and extruded at 812-815°C at a ratio between 10:1 and 33:1.
Figure G-15. Average Kearns factors as well as variation of c-axes of samples from billets that were β-quenched (fine) or slow-cooled in the β-phase (coarse) and extruded at 650-652°C at a ratio of 4:1.
Figure G-16. Average Kearns factors as well as variation of c-axes of samples from billets that were $\beta$-quenched (fine) or slow-cooled in the $\beta$-phase (coarse) and extruded at 650-652°C at a ratio of 10:1.
Figure G-17. Average Kearns factors as well as variation of c-axes of samples from billets that were $\beta$-quenched (fine) or slow-cooled in the $\beta$-phase (coarse) and extruded at 812-815°C at a ratio of 10:1.
All data included in Dataset A2, Table G-4\textsuperscript{62}.
Underlined data are included in Dataset G9, Table 4.

**Bold data** are included in Datasets G11 and G4, Table 4.

Figure G-18. Dataset A2, engineering stress versus strain at different temperatures, textures and strain rates for Zr-2.5Nb tested in the axial and transverse directions (Christodoulou, Turner, Ho, Chow, & Resta Levi, 2000).

\textsuperscript{62} The apparent drop in true stress values is ascribed to uncertainty introduced with digitization of engineering stress and strain values from Christodoulou et al.
Figure G-19. Stress versus temperature in the axial and transverse directions for different strain levels for Zr-2.5Nb, derived from Christodoulou et al. (2000).
Figure G-20. Dataset A3, stress versus strain for torsion of mini tubes at different temperatures and textures (only average available), Zr-2.5Nb (Christodoulou, Turner, Ho, Chow, & Resta Levi, 2000).
Marker shape and orientation:

<table>
<thead>
<tr>
<th>f_R</th>
<th>Transverse stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>100</td>
</tr>
<tr>
<td>&lt;0.326</td>
<td>▲</td>
</tr>
<tr>
<td>[0.326 ; 0.336]</td>
<td>▲</td>
</tr>
<tr>
<td>[0.343 ; 0.382]</td>
<td>▲</td>
</tr>
<tr>
<td>[0.389 ; 0.410]</td>
<td>▲</td>
</tr>
<tr>
<td>[0.418 ; 0.453]</td>
<td>▲</td>
</tr>
<tr>
<td>≥0.55</td>
<td>▲</td>
</tr>
</tbody>
</table>

Marker fill:

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<tr>
<th>σA/σT</th>
<th>[0 ; 0.2)</th>
<th>[0.2 ; 0.3)</th>
<th>[0.3 ; 0.4)</th>
<th>[0.4 ; 0.5)</th>
<th>[0.5 ; 0.6)</th>
<th>[0.6 ; 0.7)</th>
<th>[0.7 ; 1]</th>
</tr>
</thead>
</table>

Line style:

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
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<th>200</th>
<th>250</th>
<th>300</th>
<th>310</th>
<th>320</th>
<th>323</th>
<th>350</th>
<th>400</th>
</tr>
</thead>
</table>

Figure G-21. Legend used for experimental thermal creep results provided in Figure G-22. Average axial and transverse stress versus time curves of Zr-2.5Nb uniaxial test specimens from tube material at different temperatures and applied loads Christodoulou N. et al., with only one reported texture.
Figure G-22. Average axial and transverse stress versus time curves of Zr-2.5Nb uniaxial test specimens from tube material at different temperatures and applied loads Christodoulou N. et al. (2002), with only one reported texture.
(b) Transverse strain results

Figure G-22. (Continued)
Figure G-23. Average axial and transverse stress versus time curves of pressurized mini tubes at different temperatures, Zr-2.5Nb Christodoulou N. et al. (2002).
Figure G-24. Average axial and transverse stress versus time curves of mini pressure tube material at different temperatures, textures, applied loads and biaxial load ratios, Zr-2.5Nb (Li W., 2009).
Figure G-25. Dataset F3, Billet prep., Slow cooled, Extr. temp. = 650°C, Extr. ratio = 4:1, $\sigma_T = 300\,\text{MPa}$, $\sigma_{L\text{, applied}} = 0\,\text{MPa}$, Temp = 350°C (Li W., 2009).
(a) $\sigma_{L_{\text{applied}}} = 0$MPa

Figure G-26. Dataset F4, Billet prep., Slow cooled, Extr. temp. = 650°C, Extr. ratio = 10:1, $\sigma_T = 300$MPa, Temp = 350°C (Li W., 2009).
\( \sigma_{L, \text{applied}} = -900 \text{MPa} \)

Figure G-26 (continued)
Figure G-27. Dataset F9, Billet prep., Slow cooled, Extr. temp. = 815°C, Extr. ratio = 10:1, σT =275MPa, 300MPa and 325MPa, Temp = 350°C (Li W., 2009).
(a) $\sigma_{L,\text{applied}} = 0 \text{MPa}$
Figure G-28. Dataset F5, Billet prep., Slow cooled, Extr. temp. = 975°C, Extr. ratio = 10:1, $\sigma_T = 300$MPa, Temp = 350°C (Li W., 2009).

(b) $\sigma_{L_{\text{applied}}} = -900$MPa and 900MPa
Figure G-29. F6, Billet prep., β-quenched, Extr. temp. = 815°C, Extr. ratio = 10:1, $\sigma_T = 300$MPa, $\sigma_{L,\text{applied}} = 0$MPa, Temp = 350°C (Li W., 2009).
Figure G-30. F6a, billet prep., β-quenched, Extr. temp. = 815°C, Extr. ratio = 10:1, Cold work = 27-30%, $\sigma_T = 300$ MPa, $\sigma_{L\_applied} = 0$ MPa, -900 MPa and 900 MPa, Temp = 350°C (Li W., 2009).
Figure G-31. F6a, billet prep., β-quenched, Extr. temp. = 700°C, Extr. ratio = 12:1, Cold work = 70%, \( \sigma_T = 300 \text{ MPa} \), \( \sigma_L_{\text{applied}} = 0 \text{ MPa} \), -900 MPa and 900 MPa, Temp = 350°C (Li W., 2009).
Figure G-32. Comparison of billet cooling strategies; β-quenched versus slow cooled, Extr. temp. = 815°C, Extr. ratio = 10:1, \(\sigma_T = 300\text{MPa}, \sigma_{L\_applied} = 0\text{MPa}, \text{Temp} = 350°C\) (Li W., 2009).
Figure G-33. Comparison of extrusion temperature strategies; 650°C versus 815°C versus 975°C, Slow cooled, Extr. ratio = 10:1, $\sigma_T = 300$MPa, $\sigma_L$ applied = 0MPa, Temp = 350°C, texture restricted to $f_R=[0.343;0.382]$, $f_T=[0.538;0.582]$ & $f_L=[0.043;0.103]$ (Li W., 2009).
Figure G-34. Comparison of extrusion ratio strategies; Extrusion temp.=650°C, Slow cooled, Extr. ratio = 10:1 or 4:1, $\sigma_T = 300$ MPa, $\sigma_{L\_applied} = 0$ MPa, Temp = 350°C, texture restricted to $f_R=[0.343;0.382]$, $f_T=[0.529;0.582]$ & $F_L=[0.043;0.094]$ (Li W., 2009).
APPENDIX H. STRATEGIES TO DETERMINE MATERIAL PROPERTY TENSOR COMPONENTS

The elastic and inelastic deformation constitutive equations used in this study, for which constants are to be established for an HCP material, rely on limited measurements obtained from elastic/plastic and thermal creep tests. In fact, it is desirable to limit the number of tests for economical and practical purposes as explained in Chapter 2, Objective 7). Section H.1 explains how the number of tests could be reduced. Section H.2 explains how the constants are to be determined utilizing experimental data with a generic algorithm, while Section H.3 explains the optimization strategy.

H.1. Elastic constants of orthotropic materials

Section H.1.1 shows what range of tests would be required if the tests were to be carried out in the material preferred directions. Section H.1.2 explains how the number of tests can be reduced if tests were to be carried out in material non-preferred directions instead. Section H.1.3 describes how the assumption to describe the properties of an HCP polycrystalline material in terms of its single crystal properties and texture drastically reduces the number of tests required, where it is concluded that a single uniaxial test is in principle sufficient to invoke all the material input parameters during an optimization routine.

H.1.1. Tests performed in the material preferred directions

If the principal stress directions coincide with the material preferred directions of an orthotropic material, the elastic strain is obtained from Equation (A-79). Test loads
applied in the material preferred directions (Table H-1) each yield a single element of the compliance tensor; two tensile and three shear tests in different directions are required as a minimum to describe all nine constants. The practicality of this approach is hampered by experimental and measurement challenges posed by material geometry, e.g. tensile testing through thickness of plate, where a plane strain approximation may be required. Applying through-thickness load to obtain $S_3$ is challenging. For instance, Catlin et al. (1977) only determined five polycrystal compliance components, $S_1$ and $S_2$ with a tensile gauge section and $S_4, S_5$ and $S_6$ with an hourglass tensile specimen. They did not carry out shear tests to obtain $S_7, S_8$ and $S_9$.

**H.1.2. Polycrystal Sütçü compliance properties if the stress component directions are offset in-plane from the material preferred directions**

If the principal and privileged directions do not coincide, a coordinate transformation of any of the two, the stress state or the material, is required. As an alternative to performing tensor transformations, the Representation Theorem is used in this study (Appendix B). The elastic strain is then expressed in terms of the stress state with Equation (A-81), while the generator coefficients $S$ are described by Equation (A-82). When expressed with fourth order tensor indices (Sütçü M., 1992) instead, Equation (A-79) is expressed as:

$$\varepsilon_{ij}^\text{el} = S_{ijpq}\sigma_{pq} \quad (H-1)$$

The generator coefficients are described in terms of the compliance tensor, Equation (A-80), as:
\[ S_{ijpq} = L_p L_q \left( S_1 L_i L_j + S_6 T_i T_j + S_5 R_i R_j \right) + T_p T_q \left( S_6 L_i L_j + S_2 T_i T_j + S_4 R_i R_j \right) \\
+ R_p R_q \left( S_5 L_i L_j + S_4 T_i T_j + S_3 R_i R_j \right) + \frac{S_7}{2} \left( T_i T_p R_j R_q + T_j T_p R_i R_q \right) \\
+ \frac{S_8}{2} \left( L_i L_p R_j R_q + L_j L_p R_i R_q \right) + \frac{S_9}{2} \left( T_i L_p T_j T_q + T_j L_p T_i T_q \right) \] (H-2)

The generator coefficients, Equation (H-2) are expanded in Table H-2. The direction cosines \( L_i, T_i \) and \( R_i \) between unit vectors \( \mathbf{L}, \mathbf{T} \) and \( \mathbf{R} \) (LTR preferred coordinate system for material) and \( \mathbf{i}, \mathbf{j} \) and \( \mathbf{k} \) (123 principal coordinate system) are defined in Figure H-1.

The fourth order compliance tensor with direction cosines enables this evaluation. The number of constants in the compliance tensor that are invoked by a single test is increased, as summarized in Table H-4, evident from the functional dependency of \( S_{ijpq} \) on the elastic moduli \( S_m \) is shown at the bottom of Table H-3, where square brackets denote “a function of”. Therefore a testing program with loads applied in non-preferred material directions can be designed to reduced the testing scope in support of an optimization strategy. For the specific case of in-plane rotation considered here, through thickness testing is still required to capture \( S_3 \).

**H.1.3. Polycrystal compliance properties employing single crystal properties**

If an inversion of the stiffness \( \mathbf{C} \) is made to obtain the compliance \( \mathbf{S} \) with Equation (C-34) and the terms of \( \mathbf{C} \), Equation (C-33), are inspected using Equations (C-35) to (C-38) and (C-40) it is found that each of the nine components of \( \mathbf{S} \) is a function of all five of the single crystal components \( s_{11}^{sc}, s_{12}^{sc}, s_{13}^{sc}, s_{33}^{sc} \) and \( s_{44}^{sc} \). It is shown in Table H-5 that all five single crystal properties and therefore all nine
polycrystal properties are invoked by any one test. This benefit is unique to HCP materials when employing material average property approximations. This approach may prove to be invaluable considering the limited amount of deformation data available for in-reactor components. This derivation includes the elastic strain rate equation only, and it is assumed that the principles demonstrated here apply to all VBO equations, given the similarities in methodology. In fact, the single crystal elastic properties are published for Zircaloy and need not be established.

H.2. Obtain material property tensor components employed in ATXVBO

A strategy is followed to obtain the constants associated with the single crystal based material properties, building on the conclusion of Section H.1.3, using as little as one test for plastic deformation and one test for thermal creep deformation. This approach does not require that the loads are to be applied in the non-preferred material directions as suggested from the conclusions in Section H.1.2. A genetic algorithm, as motivated in Section 5.1, is being used for determining constants that would minimize differences between test and predicted values in Chapter 5. Other data sets not included in the optimization runs are used to validate the optimized constants in Chapter 6.

H.3. Definitions of fitness and optimization strategies – Pareto Front

The fitness describes how well the model approximates the experimental results during the optimization. It is calculated as a root mean square value of stress differences (experimental versus calculated) for plastic deformation ($f_{pl}$) and a root mean square strain value (experimental versus calculated) when thermal creep is optimized ($f_{cr}$).
However, to be able to compare \( f_{pl} \) (stress-based) and \( f_{cr} \) (strain-based) values, the latter is multiplied by the modulus of elasticity, with \( E_1 \) chosen for anisotropic cases.

\[
\begin{align*}
    f_{pl} &= \sqrt{\frac{\sum_{i=1}^{n} (\sigma_{calc_i} - \sigma_{exp_i})^2}{n}} \\
    f_{cr} &= E \sqrt{\frac{\sum_{i=1}^{n} (\epsilon_{calc_i} - \epsilon_{exp_i})^2}{n}}
\end{align*}
\]

(H-3)

To obtain an overall fitness, the fitness values are combined to obtain the overall fitness \( f_{tot} \) (Haupt & Haupt, 2004), which can be expressed as follows if the two functions were found to be correlated:

\[
f_{tot} = w_t f_{pl} + (1 - w_t) f_{cr}
\]

(H-4)

Stress values are shown by \( \sigma \), strain values by \( \epsilon \), and the subscripts “calc” and “exp” refer to predicted and experimental values, respectively, while \( w_t \) is a weight value.

However, the two fitness functions \( f_{pl} \) and \( f_{cr} \) were proven to be uncorrelated, and there cannot be one optimum overall fitness solution only. All possible optimized solutions form the Pareto front, which compares the two fitness values \( f_{pl} \) and \( f_{cr} \) in graphical form. The Pareto front is developed through the Multi-Objective Optimization (MOO) route. Feasible points on the Pareto front are inspected to find the most attractive solution, as identified in Figure 7 for three different MOO attempts using the same experimental Dataset G11.
### H.4. Tables Appendix H

Table H-1 Constants invoked by choices of experiment for orthotropic material – load applied in material preferred direction

<table>
<thead>
<tr>
<th>Measure</th>
<th>$S_1$</th>
<th>$S_2$</th>
<th>$S_3$</th>
<th>$S_4$</th>
<th>$S_5$</th>
<th>$S_6$</th>
<th>$S_7$</th>
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</thead>
<tbody>
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<tr>
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<td>$\varepsilon_3$</td>
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<td>$\varepsilon_1$</td>
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<tr>
<td></td>
<td>$\varepsilon_3$</td>
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<tr>
<td>$\sigma_6 \neq 0$</td>
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<td>X</td>
</tr>
</tbody>
</table>

---

63 Load is zero in directions not mentioned
64 Refer to Equation (A-79)
Table H-2 Fourth order compliance generator coefficients for Sütçü’s elastic constitutive equation

\[
S_{1111} = S_1 = L_1 L_1 (S_1 L_1 L_1 + S_6 T_1 T_1 + S_5 R_1 R_1) + T_1 T_1 (S_6 L_1 L_1 + S_2 T_1 T_1 + S_4 R_1 R_1) \\
+ R_1 R_1 (S_5 L_1 L_1 + S_4 T_1 T_1 + S_3 R_1 R_1) + \frac{S_7}{2} (T_1 T_1 R_1 R_1 + T_1 T_1 R_1 R_1) \\
+ \frac{S_8}{2} (L_1 L_1 R_1 R_1 + L_1 L_1 R_1 R_1) + \frac{S_9}{2} (L_1 L_1 T_1 T_1 + L_4 L_1 T_1 T_1)
\]

\[
S_{1122} = S_6 = L_2 L_2 (S_1 L_1 L_1 + S_6 T_1 T_1 + S_5 R_1 R_1) + T_2 T_2 (S_6 L_1 L_1 + S_2 T_1 T_1 + S_4 R_1 R_1) \\
+ R_2 R_2 (S_5 L_1 L_1 + S_4 T_1 T_1 + S_3 R_1 R_1) + \frac{S_7}{2} (T_1 T_2 R_1 R_2 + T_1 T_2 R_1 R_2) \\
+ \frac{S_8}{2} (L_1 L_2 R_1 R_2 + L_1 L_2 R_1 R_2) + \frac{S_9}{2} (L_1 L_2 T_1 T_2 + L_1 L_2 T_1 T_2)
\]

\[
S_{1133} = S_5 = L_3 L_3 (S_1 L_1 L_1 + S_6 T_1 T_1 + S_5 R_1 R_1) + T_3 T_3 (S_6 L_1 L_1 + S_2 T_1 T_1 + S_4 R_1 R_1) \\
+ R_3 R_3 (S_5 L_1 L_1 + S_4 T_1 T_1 + S_3 R_1 R_1) + \frac{S_7}{2} (T_1 T_3 R_1 R_3 + T_1 T_3 R_1 R_3) \\
+ \frac{S_8}{2} (L_1 L_3 R_1 R_3 + L_1 L_3 R_1 R_3) + \frac{S_9}{2} (L_1 L_3 T_1 T_3 + L_1 L_3 T_1 T_3)
\]

\[
S_{2233} = S_4 = L_3 L_3 (S_1 L_2 L_2 + S_6 T_2 T_2 + S_5 R_2 R_2) + T_3 T_3 (S_6 L_2 L_2 + S_2 T_2 T_2 + S_4 R_2 R_2) \\
+ R_3 R_3 (S_5 L_2 L_2 + S_4 T_2 T_2 + S_3 R_2 R_2) + \frac{S_7}{2} (T_2 T_3 R_2 R_3 + T_2 T_3 R_2 R_3) \\
+ \frac{S_8}{2} (L_2 L_3 R_2 R_3 + L_2 L_3 R_2 R_3) + \frac{S_9}{2} (L_2 L_3 T_2 T_3 + L_2 L_3 T_2 T_3)
\]

\[
S_{2222} = S_2 = L_2 L_2 (S_1 L_2 L_2 + S_6 T_2 T_2 + S_5 R_2 R_2) + T_2 T_2 (S_6 L_2 L_2 + S_2 T_2 T_2 + S_4 R_2 R_2) \\
+ R_2 R_2 (S_5 L_2 L_2 + S_4 T_2 T_2 + S_3 R_2 R_2) + \frac{S_7}{2} (T_2 T_2 R_2 R_2 + T_2 T_2 R_2 R_2) \\
+ \frac{S_8}{2} (L_2 L_2 R_2 R_2 + L_2 L_2 R_2 R_2) + \frac{S_9}{2} (L_2 L_2 T_2 T_2 + L_2 L_2 T_2 T_2)
\]

\[
S_{3333} = S_3 = L_3 L_3 (S_1 L_3 L_3 + S_6 T_3 T_3 + S_5 R_3 R_3) + T_3 T_3 (S_6 L_3 L_3 + S_2 T_3 T_3 + S_4 R_3 R_3) \\
+ R_3 R_3 (S_5 L_3 L_3 + S_4 T_3 T_3 + S_3 R_3 R_3) + \frac{S_7}{2} (T_3 T_3 R_3 R_3 + T_3 T_3 R_3 R_3) \\
+ \frac{S_8}{2} (L_3 L_3 R_3 R_3 + L_3 L_3 R_3 R_3) + \frac{S_9}{2} (L_3 L_3 T_3 T_3 + L_3 L_3 T_3 T_3)
\]

H-7
$$S_{2323} = S_7 = L_2L_3(S_1L_2L_3 + S_6T_2T_3 + S_5R_2R_3) + T_2T_3(S_6L_2L_3 + S_2T_2T_3 + S_4R_2R_3) + R_2R_3(S_5L_2L_3 + S_4T_2T_3 + S_3R_2R_3) + \frac{S_7}{2}(T_2T_2R_3R_3 + T_3T_2R_2R_3) + \frac{S_8}{2}(L_2L_2R_3R_3 + L_3L_2R_2R_3) + \frac{S_9}{2}(L_2L_2T_3T_3 + L_3L_2T_2T_3)$$

$$S_{1313} = S_8 = L_1L_3(S_1L_1L_3 + S_6T_1T_3 + S_5R_1R_3) + T_1T_3(S_6L_1L_3 + S_2T_1T_3 + S_4R_1R_3) + R_1R_3(S_5L_1L_3 + S_4T_1T_3 + S_3R_1R_3) + \frac{S_7}{2}(T_1T_1R_3R_3 + T_3T_1R_2R_3) + \frac{S_8}{2}(L_1L_1R_3R_3 + L_3L_1R_1R_3) + \frac{S_9}{2}(L_1L_1T_3T_3 + L_3L_1T_2T_3)$$

$$S_{1212} = S_9 = L_1L_2(S_1L_1L_2 + S_6T_1T_2 + S_5R_1R_2) + T_1T_2(S_6L_1L_2 + S_2T_1T_2 + S_4R_1R_2) + R_1R_2(S_5L_1L_2 + S_4T_1T_2 + S_3R_1R_2) + \frac{S_7}{2}(T_1T_1R_2R_2 + T_2T_1R_1R_2) + \frac{S_8}{2}(L_1L_1R_2R_2 + L_2L_1R_1R_2) + \frac{S_9}{2}(L_1L_1T_2T_2 + L_2L_1T_1T_2)$$
Table H-3  Direction cosines for in-plane rotation

<table>
<thead>
<tr>
<th></th>
<th>( L )</th>
<th>( T )</th>
<th>( R )</th>
</tr>
</thead>
<tbody>
<tr>
<td>i</td>
<td>( L_1 = \cos(\theta) )</td>
<td>( T_1 = \cos\left(\frac{\pi}{2} - \theta\right) )</td>
<td>( R_1 = 0 )</td>
</tr>
<tr>
<td>j</td>
<td>( L_2 = \cos\left(\frac{\pi}{2} + \theta\right) )</td>
<td>( T_2 = \cos(\theta) )</td>
<td>( R_2 = 0 )</td>
</tr>
<tr>
<td>k</td>
<td>( L_3 = 0 )</td>
<td>( T_3 = 0 )</td>
<td>( R_3 = 1 )</td>
</tr>
</tbody>
</table>

\[
S_1 = L_1 L_1 (S_1 L_1 L_1 + S_6 T_1 T_1) + T_1 T_1 (S_6 L_1 L_1 + S_2 T_1 T_1) + \frac{S_9}{2} (L_1 L_1 T_1 T_1 + L_1 L_1 T_1 T_1)
\]

\[
S_2 = L_2 L_2 (S_1 L_2 L_2 + S_6 T_2 T_2) + T_2 T_2 (S_6 L_2 L_2 + S_2 T_2 T_2) + \frac{S_9}{2} (L_2 L_2 T_2 T_2 + L_2 L_2 T_2 T_2)
\]

\[
S_3 = R_3 R_3 (S_3 R_3 R_3)
\]

\[
S_4 = R_3 R_3 (S_5 L_2 L_2 + S_4 T_2 T_2)
\]

\[
S_5 = R_3 R_3 (S_5 L_1 L_1 + S_4 T_1 T_1)
\]

\[
S_6 = L_1 L_2 (S_1 L_1 L_1 + S_6 T_1 T_1) + T_2 T_2 (S_6 L_1 L_1 + S_2 T_1 T_1) + \frac{S_9}{2} (L_1 L_2 T_1 T_2 + L_1 L_2 T_1 T_2)
\]

\[
S_7 = \frac{S_7}{2} (T_2 T_2 R_3 R_3) + \frac{S_8}{2} (L_2 L_2 R_3 R_3)
\]

\[
S_8 = \frac{S_7}{2} (T_1 T_1 R_3 R_3) + \frac{S_8}{2} (L_1 L_1 R_3 R_3)
\]

\[
S_9 = L_1 L_2 (S_1 L_1 L_1 + S_6 T_1 T_2) + T_1 T_2 (S_6 L_1 L_1 + S_2 T_1 T_2) + \frac{S_9}{2} (L_1 L_1 T_2 T_2 + L_1 L_1 T_2 T_2)
\]

\[
S = \begin{bmatrix}
S_1[S_1, S_2, S_6, S_9] & S_6[S_1, S_2, S_6, S_9] & S_5[S_4, S_5] & 0 & 0 & 0 \\
S_6[S_1, S_2, S_6, S_9] & S_2[S_1, S_2, S_6, S_9] & S_4[S_4, S_5] & 0 & 0 & 0 \\
S_5[S_4, S_5] & S_4[S_4, S_5] & S_3[S_3] & 0 & 0 & 0 \\
0 & 0 & 0 & S_7[S_7, S_8] & 0 & 0 \\
0 & 0 & 0 & 0 & S_8[S_7, S_8] & 0 \\
0 & 0 & 0 & 0 & 0 & S_9[S_1, S_2, S_6, S_9]
\end{bmatrix}
\]

\[ H-9 \]
Table H-4  Constants invoked by choice of experiment for orthotropic material – load not applied in principal directions rotated relative to material preferred direction with an in-plane rotation

<table>
<thead>
<tr>
<th>Load $\sigma_1 \neq 0$ or $\sigma_2 \neq 0$</th>
<th>Measure</th>
<th>$S_1$</th>
<th>$S_2$</th>
<th>$S_3$</th>
<th>$S_4$</th>
<th>$S_5$</th>
<th>$S_6$</th>
<th>$S_7$</th>
<th>$S_8$</th>
<th>$S_9$</th>
</tr>
</thead>
<tbody>
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<td>$\varepsilon_1$</td>
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<td>X</td>
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<td></td>
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</tr>
<tr>
<td></td>
<td>$\varepsilon_2$</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\varepsilon_3$</td>
<td></td>
<td></td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>$\sigma_4 \neq 0$</td>
<td>$\varepsilon_4$</td>
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<tr>
<td>$\sigma_5 \neq 0$</td>
<td>$\varepsilon_5$</td>
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<td></td>
<td></td>
<td></td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>$\sigma_6 \neq 0$</td>
<td>$\varepsilon_6$</td>
<td>X</td>
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</tr>
</tbody>
</table>

Table H-5  Constants invoked by choice of experiment for orthotropic material – invoking single crystal dependency

See H.1.3

<table>
<thead>
<tr>
<th>Load</th>
<th>Measure</th>
<th>$s_{11}^{sc}$</th>
<th>$s_{33}^{sc}$</th>
<th>$s_{12}^{sc}$</th>
<th>$s_{13}^{sc}$</th>
<th>$s_{44}^{sc}$</th>
<th>$S_1$</th>
<th>$S_2$</th>
<th>$S_3$</th>
<th>$S_4$</th>
<th>$S_5$</th>
<th>$S_6$</th>
<th>$S_7$</th>
<th>$S_8$</th>
<th>$S_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Any unidirectional</td>
<td>In direction of load</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>

65 This table is made through inspection of Equation (H-1) and the dependencies shown between $S$ and $S$ summarized at the bottom of Table H-3.
H.5. Figures Appendix H

(Note - Rotation around the R axis is shown for illustrative purposes and is used in the subsequent discussions.)

<table>
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<tr>
<th></th>
<th>L</th>
<th>T</th>
<th>R</th>
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<td>T₁</td>
<td>R₁</td>
</tr>
<tr>
<td>j</td>
<td>L₂</td>
<td>T₂</td>
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</tr>
<tr>
<td>k</td>
<td>L₃</td>
<td>T₃</td>
<td>R₃</td>
</tr>
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Figure H-1  Direction cosines between unit vectors in LTR and 123 coordinate systems