# Predicting steady-state thermal creep rate of Zr-2.5wt%Nb pressure tube using two physical models: VPSC model and Crystal plasticity FEM

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## 1. Introduction

Zr-2.5wt%Nb alloy is used for pressure tube in a CANDU pressurized heavy water reactor. The pressure tube is an important structural component, which supports burning fuels and pressurized heavy water. During the operation, the creep deformation in the pressure tube occurs and affects the safety and the efficiency of the reactor. Due to the anisotropic physical properties of the hexagonal crystal structure of zirconium and strong texture introduced by manufacturing process, the pressure tube shows the highly anisotropic deformation trend depending on the state of stress.

Actually thermal creep is less dominant than the irradiation creep during the operation because the stress state by the pressure of the heavy water is relatively low. However, when the defects such as a notch or volumetric flaw increase the stresses in the vicinity of them, the thermal creep deformation becomes important. Since dislocation glide is the main mechanism of the thermal creep of the tube [1], the physical model based on crystal plasticity is needed to properly predict the anisotropic deformation behavior. In this study, two physical models were used to describe the thermal creep behavior of the tube and they were compared.

## 2. Modeling

Visco-plastic self-consistent (VPSC) model and crystal plasticity finite element model (CPFEM) are governed by the following constitutive law for a single crystal:

$$\dot{\varepsilon}_{ij} = \dot{\gamma}_0 \sum_\alpha m_{ij}^\alpha \left(\frac{m_{kl}\sigma_{kl}}{\tau_0^\alpha}\right)^n \quad (1)$$

where $\dot{\varepsilon}_{ij}$ and $\sigma_{kl}$ are a strain rate tensor in a single crystal and the applied stress on the given crystal, respectively. $\dot{\gamma}_0$ and $n$ are the reference strain rate constant for a normalization and the strain rate sensitivity exponent, respectively. $m_{ij}^\alpha$ is the Schmid tensor for α slip system which is expressed by $\frac{1}{2}\left(n_i^\alpha b_j^\alpha + n_j^\alpha b_i^\alpha\right)$ where $n^\alpha$ and $b^\alpha$ are the slip normal and direction vector of α slip system. $\tau_0^\alpha$ is the critical resolved shear stress (CRSS) for α slip system.

### *2.1. VPSC model*

In the self-consistent model, it is assumed that a grain can be described with the uniform stress and strain states, and their constitutive relation can be linearized as the following equation,

$$\dot{\varepsilon}_{ij} = M_{ijkl}^c \sigma_{kl} + \varepsilon_{ij}^0 \quad (2)$$

where $M_{ijkl}^c$ and $\varepsilon_{ij}^0$ are the compliance and the back-extrapolated strain rate for a crystal. These values can be defined differently depending on what linearization method is used.

The bulk polycrystal is approximated to the aggregate as a homogeneous equivalent medium (HEM) consisting of crystals and, their constitutive relation between overall strain rate and the applied overall stress can be written in the similar linear form with a single crystal law,

$$\dot{E}_{ij} = M_{ijkl}\Sigma_{kl} + \dot{E}_{ij}^0 \quad (3)$$

where $\dot{E}_{ij}$ and $\Sigma_{kl}$ are the strain rate and the stress for polycrystal, respectively. $M_{ijkl}$ and $\dot{E}_{ij}^0$ are the bulk compliance and the bulk back-extrapolation term.

In order to relate each crystal and the HEM, a grain is regarded as an inclusion embedded in the HEM and the interaction between them is solved using the Eshelby theory, which gives the following interaction form,

$$\left(\dot{\varepsilon}_{ij} - \dot{E}_{ij}\right) = -\widetilde{M}_{ijkl}(\sigma_{kl} - \Sigma_{kl}) \quad (4)$$

where $\widetilde{M}_{ijkl}$ is the interaction tensor defined as,

$$\widetilde{\boldsymbol{M}} = (\boldsymbol{I} - \boldsymbol{S})^{-1}\boldsymbol{S}\boldsymbol{M} \quad (5)$$

where $\boldsymbol{S}$ is the Eshelby tensor, which is a function of the shape of the grain and the bulk modulus. Using the above equations and the condition that the weighted averages of stresses and strain rates over the crystals has to coincide with the corresponding macroscopic magnitude provides the expression from which the bulk compliance can be calculated in a self-consistent iterative way. Complete equations and their detailed solutions can be found in [2].

### *2.2. CPFEM*

CPFEM has more straightforward application than VPSC model. In contrast to VPSC model, defining linearization method, homogenization scheme, and interaction tensor is not necessary in CPFEM. FEM framework provides convenience for them. Of course, additional considerations are required such as the development of time integration procedure and the

calculation of Jacobian matrix, which are requirements of FE analysis.

For the time integration procedure, the basic framework about kinematic relation should be taken account of. In the kinematic relation, the deformation gradient can be expressed by a multiplicative decomposition into elastic and plastic components as:

$$\boldsymbol{F} = \boldsymbol{F^e F^p} \text{ where } \det \boldsymbol{F^e} > 0 \; and \; \det \boldsymbol{F^p} = \boldsymbol{1} \quad (6)$$

where $\boldsymbol{F^e}$ *and* $\boldsymbol{F^p}$ are deformation gradient tensor about the elastic deformation accounting the elastic stretching and the rigid-body rotation of crystal lattice and the incompressible plastic deformation due to dislocation slip, etc., respectively.

Since stress is a function of not the plastic deformation but the elastic one, the second Piola-Kirchoff stress ($\boldsymbol{S}$) can be expressed by the following simple linear form

$$\boldsymbol{S} = \mathbb{C}^e : \boldsymbol{E^e} \quad (7)$$

where $\mathbb{C}^e$ and $\boldsymbol{E^e}$ are the fourth-order anisotropic elastic tensor and the elastic Green-Lagrange strain tensor defined as $\boldsymbol{E^e} = \frac{1}{2}(\boldsymbol{F^{eT}F^e} - \boldsymbol{I})$, respectively.

For FE analysis, the stress should be computed through decomposing the elastic deformation tensor and the plastic one. The change of the plastic deformation tensor with a finite time increment can be derived by the following equation concerning the evolution of plastic deformation

$$\boldsymbol{L^p} = \dot{\boldsymbol{F}}^{\boldsymbol{p}} \boldsymbol{F^{p-1}} = \sum_{\alpha} \dot{\gamma}^{\alpha} \boldsymbol{m}^{\alpha}$$

The right term is identical with the basic constitutive equation (1). With the parameters dealt in the equation (1), the time integration procedure can be developed, then, the stress can be calculated.

Although the Jacobian matrix does not affect the accuracy of the final solution, for the convergence rate during FE analysis, the Jacobian matrix should be properly defined. The derivation of the matrix demands complex numerical consideration. More explanation about the Jacobian and more details about the CPFEM theory can be found in [3].

## 3. Thermal creep behavior

For the application of the two model, we borrowed the data about thermal creep tests on Zr-2.5wt%Nb pressure tube from [1]. They performed uniaxial and bi-axial thermal creep tests at many different stress levels and temperatures. The steady-state creep rates were taken and they were compared with the creep rates calculated using the models.

Figure 1 shows the axial steady-state creep rates as a function of the applied stress. Even though the same conditions of the applied stress and temperature were used, the scatter that cannot be ignored was found. The reason for the scatter is the variations in the microstructure and texture of the specimen.

In the process of finding the model parameters, such variation is not specially considered. Instead of selecting some data that seem to have a consistent tendency, we do use all data including those having the same condition but different creep rates.

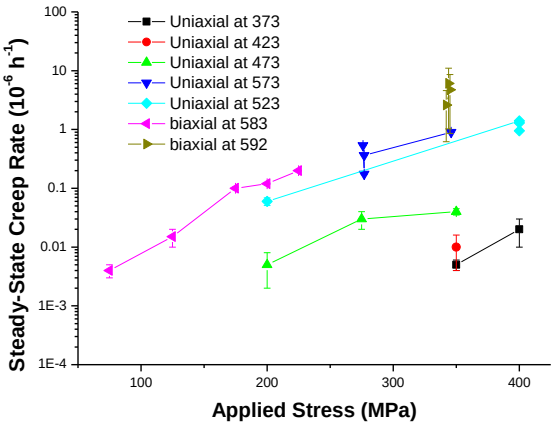


Figure 1. The axial steady-state thermal creep rates of the Zr-2.5wt%Nb pressure tube as a function of the applied stress from [1]

## 4. Finding model parameters

To optimize the parameters of the models, the loop codes written in Python language 3.6 were developed. The goal of the codes is to find the parameters that introduce the minimum difference between the calculated creep rate and the experimentally obtained creep rate. For an efficient search process, the evolutionary strategy, which generate the next generation of the parameter based on the previous generation, was used. Figure 2 and 3 show the schematic flows of the codes for VPSC model and CPFEM, respectively.

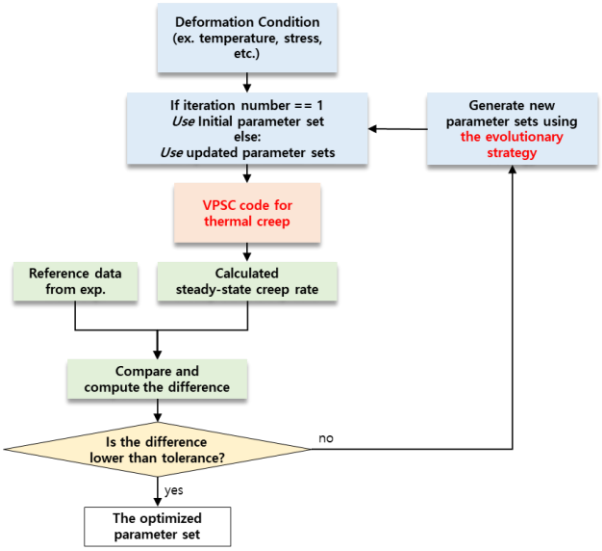


Figure 2. The schematic code flow used for optimizing parameters in VPSC model.

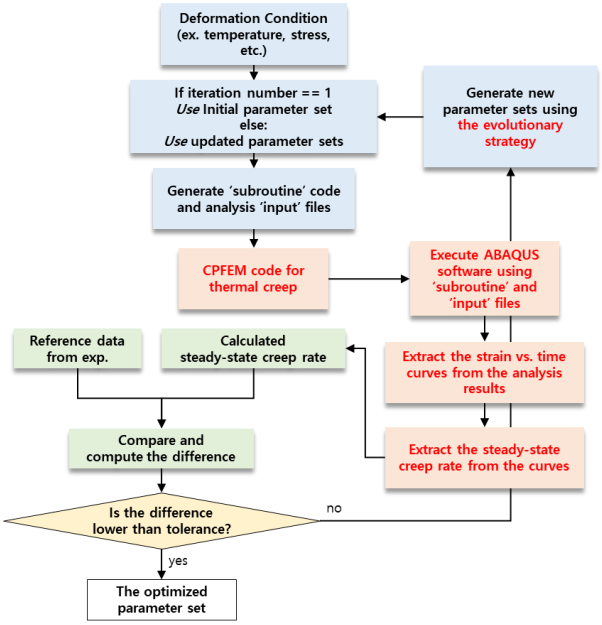


Figure 3. The schematic code flow used for optimizing parameters in CPFEM.

## 5. Results

After over 100 iterations, the optimized parameter sets for VPSC model and CPFEM were acquired with reasonable differences. In the both models, calculating a steady-state creep strain rate requires four model parameters: three critical resolved shear stresses (CRSSs) for basal, prismatic and pyramidal slip system and a reference shear strain rate. Other model parameters except them were fixed. We assumed that CRSSs do not change with changing temperature, instead, the reference shear strain rate does. Therefore, through the iterations, total 10 parameters (three CRSSs and the reference shear strain rates at 7 different temperatures) were found.

Figure 4 (a) and (b) shows the obtained reference shear strain rates as a function of temperature for VPSC model and CPFEM, respectively. Although the absolute values from VPSC model are slightly higher than those from CPFEM, the tendencies found in the dependency on temperature are almost identical. The similarity is the predictable result when considering the same basic constitutive model of the dislocation slip mechanism. The other parameters, CRSSs, from both models also show quite similar values due to the same reason as the reference shear strain rate.

The predicted steady-state creep strain rates by VPSC model and CPFEM using the optimized parameters are within an order of magnitude with measurements, which are quite satisfied predictions because the variation in the experimental data has the same order of deviation. There are minor differences between the results from both models, which can be attributed to the method how to expand the constitutive law from a single crystal to polycrystal.

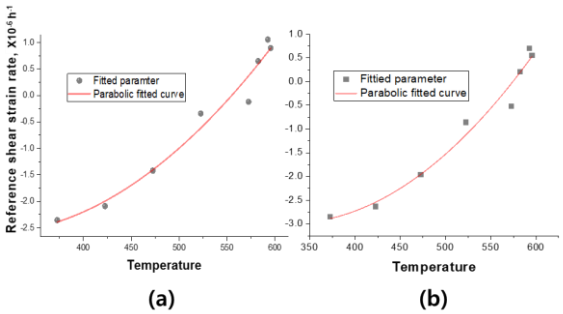


Figure 4. The obtained reference shear strain rate through the optimization code (dots) and the parabolic fitted line (red line) for (a) VPSC and (b) CPFEM.

## 6. Conclusions

In the study, the steady-state thermal creep strain rates of the Zr-2.5wt%Nb pressure tube were described using two crystal plasticity model: VPSC model and CPFEM. Through iterating calculations with the in-house optimization codes, the fitted parameters have been obtained. With the parameters, the both models well predicted the creep strain rates under very different stress states and temperatures. Although different bulk homogenization schemes are adopted to VPSC model and CPFEM, only minor difference were found between the obtained parameters and the predicted results from the models. The non-dramatic variation indicates the basic crystal constitutive law is more dominant factor than the homogenization scheme for predicting the thermal creep strain rates of the pressure tube.

## REFERENCES

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