Proceedings of the Conference on Computational Engineering and Science JSCES
Vol. 30, Jun. 2025

A multiscale modeling strategy for diffusional creep mechanisms: application to Coble creep deformation

Yi Liu[1)], Kota Sagara[2)] and Kazuki Shibanuma[3)]

1) Ph.D, Student of the University of Tokyo (Postal Address, E-mail: yi-liu1127@g.ecc.u-tokyo.ac.jp)
2) Ph.D, Student of the University of Tokyo (Postal Address, E-mail: sagarakota@g.ecc.u-tokyo.ac.jp)
3) Dr. Eng. Associate Professor (Postal Address, E-mail: shibanuma@struct.t.u-tokyo.ac.jp)

The importance of micro-macro coupling methods lies in their ability to bridge microscopic mechanisms and the performance of macroscopic structures, and providing powerful tools for material design. Designing of novel materials with high temperature creep resistance is important since it related with thermal efficiency and environmental problems. In this study, the framework for the creation of surrogate modelling of micro-macro coupling problem for diffusion creep is established, and the application into two-scale boundary value problems (BVPs) for Coble creep deformation is developed.

Key Words: *Surrogate model; Multiscale analysis; Coble creep deformation; Finite element method*

1. Introduction

With the development of computational science, several coupling schemes for two-scale (micro-macro scale) boundary value problems (BVPs) were developed, which made it possible to apply the microscopic physical quantities into macroscopic model [1].

Coble creep is one of the most important mechanisms in metal creep behavior, and the corresponding microscopic Coble creep deformation representative volume element (RVE) model was well developed [2], which is an important basis of this study.

The purpose of this study is to realize the two-scale coupling analysis between microscopic model and macroscopic model in diffusional creep mechanism.

In this study, the framework for the creation of surrogate modelling of micro-macro coupling problem is established, and the application into two-scale BVPs for Coble creep deformation is developed. There are three steps in this study, and the brief outline of this study is shown in Fig.1:

(1) Use the prepared microscopic model to create the databases: the numerical material tests (NMTs) are performed on variety microscopic RVE models for Coble creep deformation, and each RVE model is subjected to various patterns of systematically defined stress fields in order to create the database that contains sufficient deformed configurations. Each database contains the constitutive relationship between strain vectors and coefficient matrix for Norton's equation;

(2) Determine the parameters of surrogate model: the polynomial fitting model is applied to build the continuous constitutive relationship between strain vectors and coefficient matrices, and both accuracy and efficiency of polynomial fitting model are compared with other surrogate models (local radial basis function (LRBF) model and inverse distance weighting (IDW) model);

(3) Simulation using macroscopic finite element analysis (FEA) model: two macroscopic specimen models are simulated based on the macroscopic FEA model that including the constitutive law from step (2) and the tensor form of yield criterion.

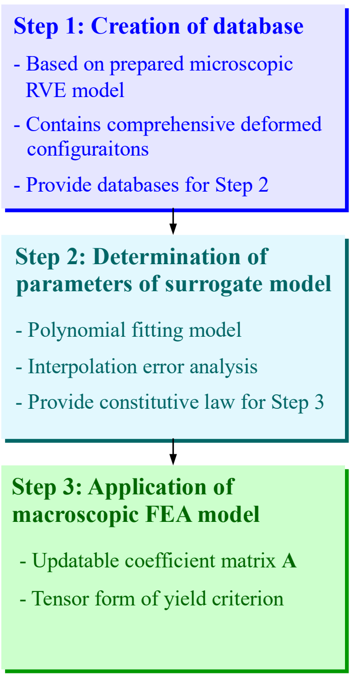


Fig. 1 Brief outline of this study

The results show that our framework of surrogate modelling is applicable in micro-macro coupling analysis for Coble creep deformation.

2. Creation of the database

The microscopic RVE model for Coble creep deformation applied in this study is already well developed [2]. In this model, for a given stress, the creep strain rate could be obtained based on grain boundary diffusion theory.

According to the constitutive relationship between creep strain rate and stress in Norton's equation for Coble creep, the target coefficient matrix $\mathbf{A}$ could be calculated by applying six kinds of unit stresses on a certain deformed configuration of RVE model, as shown in Eq.(1).

$$\dot{\boldsymbol{\varepsilon}}_{unit}^{(I)} = \mathbf{A}^{(I)} \cdot \boldsymbol{\sigma}_{unit}^{(I)}, I = 1,2,\ldots,6 \qquad (1)$$

Where $\dot{\boldsymbol{\varepsilon}}_{unit}^{(I)}$ is the creep strain rate under the I-th unit stress field; $\mathbf{A}^{(I)}$ is the I-th component of the target coefficient matrix $\mathbf{A}$; $\boldsymbol{\sigma}_{unit}^{(I)}$ is the I-th unit stress vector. In other words, we can obtain a 6 by 6 coefficient matrix $\mathbf{A}$ by applying 6 kinds of unit stress fields.

One of the important factors of the robustness of surrogate model is the density of data points of database that used to determine its parameters. Therefore, comprehensive deformed configurations of microscopic RVE model are needed in this study, and we can achieve this by applying several systematically defined stress fields, as shown in Fig.2.

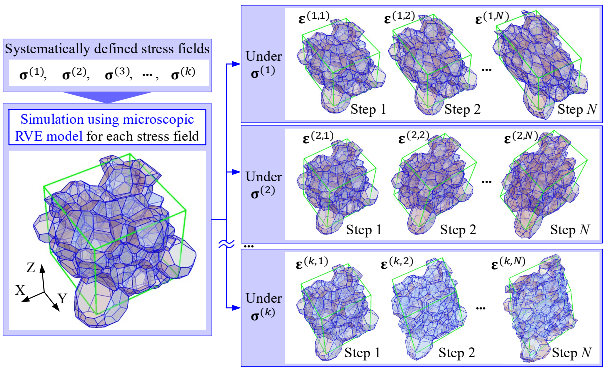


Fig. 2 Creation of comprehensive deformed configurations

For each deformed configuration, we apply six kinds of unit stress fields respectively based on Eq.(1), and obtain the coefficient matrix $\mathbf{A}$.

The systemically defined stress fields are generated from the normal stress choice set: $\{0, 1, 2, \ldots, p\}$, shear stress choice set: $\{0, -1, 1, -2, 2, \ldots, -q, q\}$ and magnitude of multipliers for normal stress and shear stress σ and τ. The total number of the combination from two stress choice sets (without all zero components case) could be calculated as: $(p+1)^3 \times (2q+1)^3 - 1$. After all the combinations are created, the systemically defined stress fields could be created by multiplying the pre-defined stress multipliers σ and τ.

To be more specific, the calculation flow chart to create the database is shown in Fig.3.

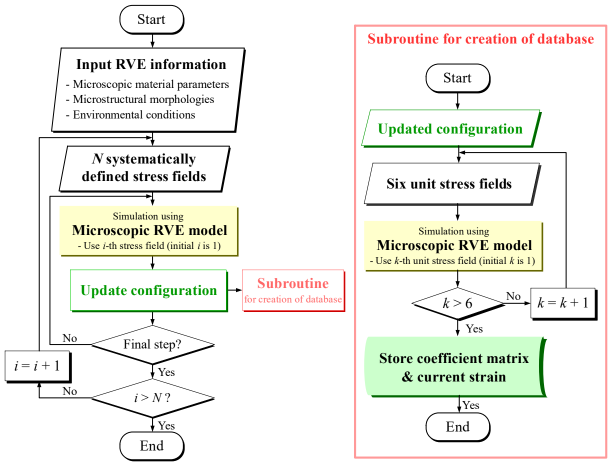


Fig. 3 Calculation flow chart for the creation of the database.

3. Determination of parameters of surrogate model

There are various well-developed surrogate models to connect the macroscopic performances and microscopic mechanisms. In this study, polynomial fitting model is selected as the surrogate model for multiscale coupling analysis, as shown in Eq.(2) to Eq.(4).

$$A_{IJ} = f(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}_{IJ}) \qquad I,J = 1,2,\ldots,6 \qquad (2)$$

$$\boldsymbol{\alpha}_{IJ}(L) = \left[\alpha_{IJ}^{(0)}, \alpha_{IJ}^{(1)}, \ldots, \alpha_{IJ}^{M(L)}\right] \qquad (3)$$

$$M(L) = \frac{(5+L)!}{5!\,L!} \qquad (4)$$

Where A_{IJ} is one component of coefficient matrix $\mathbf{A}$; $\boldsymbol{\alpha}_{IJ}(L)$ is the set of polynomial fitting coefficients for A_{IJ}; L is the maximum polynomial order; $M(L)$ is the maximum number of polynomial fitting coefficients.

3.1 Determine maximum polynomial order L

The maximum polynomial order L could be determined based on the interpolation error analysis between parent database and child database. To be more specific, we can obtain the polynomial equation under order i' based on linear regression process (LRP) from child database, then use this equation and each strain vector of parent database to calculate the predicted matrix $\mathbf{A}'$, and compare with the corresponding real matrix $\mathbf{A}$ from parent database. We can apply higher i' until the error is smaller than certain threshold, as shown in Fig.4.

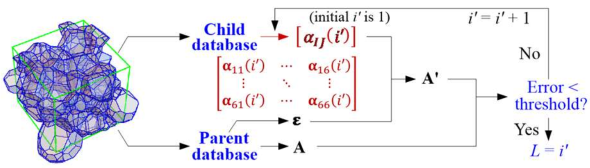


Fig. 4 Determination of maximum polynomial order

3.2 Determine polynomial fitting coefficients

In this study, the robustness of surrogate model also related with the variation of morphologies of microscopic RVE model. Therefore, sufficient number of databases generated from different RVE models are needed.

Based on LRP, we can obtain $\boldsymbol{\alpha}_{IJ}(L)$ for each database. Then, the accumulated ratio for each component of $\boldsymbol{\alpha}_{IJ}(L)$ could be obtained. Finally, the average value for each component of $\boldsymbol{\alpha}_{IJ}(L)$ could be used as the parameters of surrogate model by verify the coefficient of variation (CV) for each accumulated ratio curve, as shown in Fig.5.

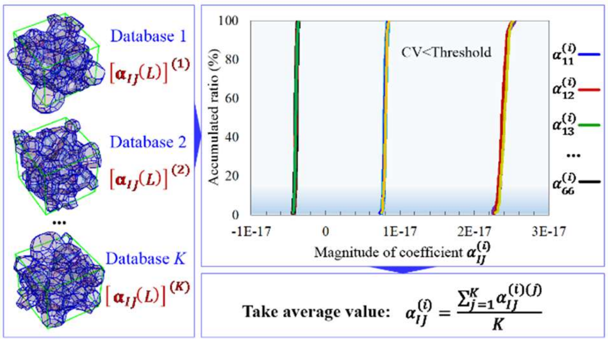


Fig. 5 Determination of polynomial fitting coefficients

4. Application to macroscopic FEA model

After we obtain the constitutive law, the corresponding FEA model is needed for further simulation (the verification of FEA model is shown in Appendix 1). To be more specific, the calculation flow chart of macroscopic FEA model in this study is shown in Fig.6.

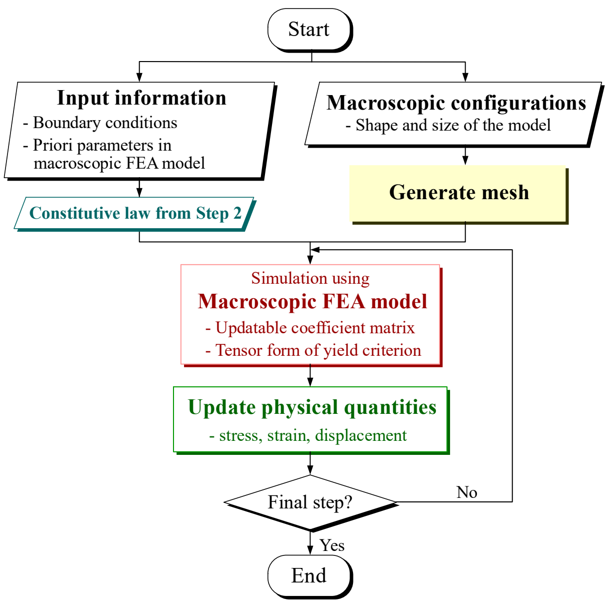


Fig. 6 Calculation flow chart of macroscopic FEA model

In practice, creep phenomenon in metals is regarded as visco-plastic behavior. In order to accommodate the coefficient matrix derived from the microscopic RVE model, the corresponding tensor form of yield criterion is need.

In this study, the Newton-Raphson (NR) iteration is used for visco-plasticity. By considering the complementary condition, the tensor function $\tilde{\boldsymbol{\Phi}}$ of creep strain increment $\Delta\boldsymbol{\varepsilon}^c$ could be expressed as:

$$\tilde{\boldsymbol{\Phi}}(\Delta\boldsymbol{\varepsilon}^c) \equiv \mathbf{s}_{n+1}^{trial} - 2G\mathbf{I}_d : \Delta\boldsymbol{\varepsilon}^c - \mathbf{s}_{n+1} = 0 \quad (5)$$

Where n is the number of time step; $\mathbf{s}_{n+1}^{trial}$ is the trial deviatoric stress vector in step $n+1$.; G is shear modulus; $\mathbf{I}_d$ is the deviatoric matrix; $\mathbf{s}_{n+1}$ is the deviatoric stress vector in step $n+1$.

After we obtained $\Delta\boldsymbol{\varepsilon}^c$, the following physical quantities could be updated:

$$\mathbf{s}_{n+1} = \mathbf{s}_{n+1}^{trial} - 2G \cdot \Delta\boldsymbol{\varepsilon}^c \quad (6)$$

$$\boldsymbol{\sigma}_{n+1} = \mathbf{s}_{n+1} + p_{n+1}^{trial} \cdot \mathbf{I} \quad (7)$$

$$\boldsymbol{\varepsilon}_{n+1}^c = \boldsymbol{\varepsilon}_n^c + \Delta\boldsymbol{\varepsilon}^c \quad (8)$$

$$\mathbf{D}^{ep} = \frac{\partial \boldsymbol{\sigma}_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}^{e,trial}} = \mathbf{D}^e - \frac{4G^2 \cdot \mathbf{I}_d}{2G\mathbf{I}_d + \mathbf{H}} \quad (9)$$

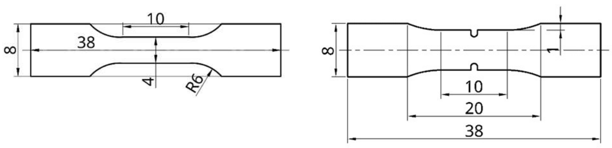
Where $\boldsymbol{\sigma}_{n+1}$ is the stress vector in step $n+1$; p_{n+1}^{trial} is the trial value of hydrostatic pressure in step $n+1$; $\mathbf{I}$ is identical matrix; $\mathbf{D}^{ep}$ is elastoplastic matrix; $\boldsymbol{\varepsilon}_{n+1}^{e,trial}$ is the trial elastic strain vector in step $n+1$, and $\mathbf{H}$ is the hardening coefficient matrix, which could be expressed as:

$$\mathbf{H} \equiv \frac{\partial \mathbf{s}_{n+1}}{\partial \Delta\boldsymbol{\varepsilon}^c} \quad (10)$$

5. Simulation results

Based on the interpolation error analysis and comparison of accuracy and efficiency between LRBF model and IDW model (as shown in Appendix 2), polynomial order 3 is applied in this study. Therefore, based on Eq.(4), 56 averaged values of polynomial fitting coefficients are used as the parameters of surrogate model.

The geometrical information of two kinds of specimen models are shown in Fig. 7.



(a) (b)

Fig. 7 Geometrical information of (a) smooth specimen; (b) notched specimen (unit: mm)

The necessary macroscopic material properties are shown in Table 1.

Table 1. necessary macroscopic material properties

Young's modulus	205 GPa
Poisson's ratio	0.30

The stress condition on cross-section for both smooth specimen model and notched specimen model are shown in Fig.8.

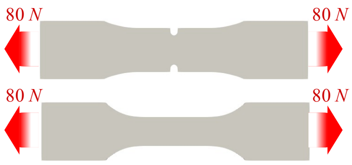


Fig. 8 Loading conditions for smooth specimen model and notched specimen model

The simulation results of strain contours for smooth specimen are shown in Fig.9, and the simulation results of strain contours for smooth specimen are shown in Fig.10.

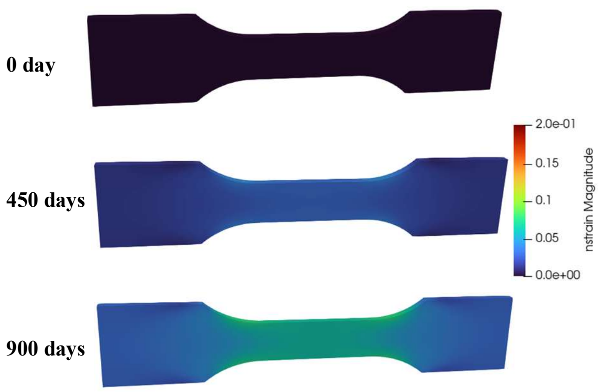


Fig. 9 Strain contours for smooth specimen model

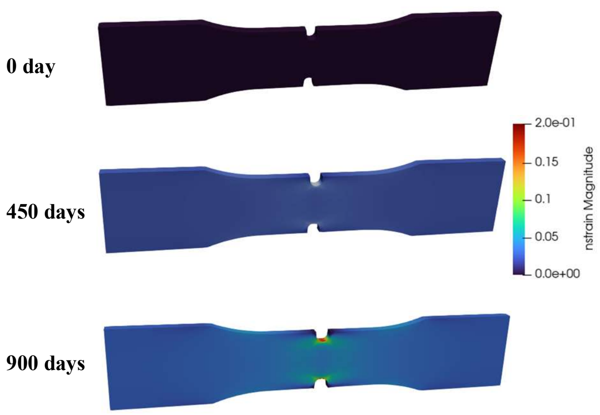


Fig. 10 Strain contours for notched specimen model

And the comparison of maximum displacement between two models are shown in Fig. 11.

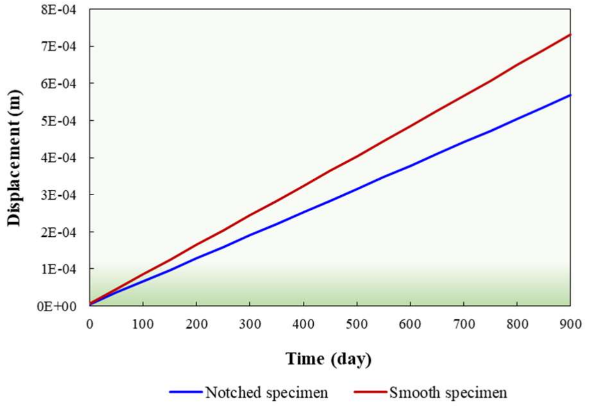


Fig. 11 Comparison of maximum value of displacement

6. CONCLUSIONS

In this study, the framework for the multiscale analysis of Coble creep deformation is established. By comparing both accuracy and efficiency with LRBF model and IDW model, polynomial fitting model with order 3 is applied as the surrogate model. In macroscopic FEA model, the tensor form of yield criterion was developed, and the simulations for smooth specimen model and notched specimen model are performed.

7. OUTLOOKS

In the future, the surrogate model considering void nucleation and growth in Coble creep should be further developed; the microscopic RVE model for dislocation creep should also be developed.

REFERENCES

[1] Yamanaka, Y., Matsubara, S., Hirayama, N., Moriguchi, S., & Terada, K. (2023). Surrogate modeling for the homogenization of elastoplastic composites based on RBF interpolation. Computer Methods in Applied Mechanics and Engineering, 415, 116282.

[2] Shibanuma, K., Fukada, T., Yasumoto, H., Tokuda, K., Kim, B. N., & Nikbin, K. (2023). Representative volume element model for quantitatively predicting the influence of 3D polycrystalline morphology on Coble creep deformation. Materials & Design, 226, 111635.