Simulation of crystal plasticity of P92 heat resistant steel considering martensitic lath structure

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Abstract: Based on the theory of crystal plasticity, coupled with dislocation and lath hardening models, this paper establishes a crystal plasticity finite element model describing the high temperature creep of P92 steel. Open source software was used to generate lath models with an average size of 350nm, 650nm and 950nm to explore the effect of lath coarsening on the high-temperature creep behavior of P92 steel. The results show that the roughening of the slats increases the rate of creep deformation, resulting in a decrease in the service life of the material. Observing the slat model, it can be seen that the roughening of the slats enlarges the numerical gradient of stress and strain, and aggravates the overall plastic strain of the model. The coarsening of the slats accelerates the movement of dislocations, causing the density of movable dislocations to increase, and at the same time the shear strain amplitude of the slip system increases, thereby reducing the hardening behavior of the material.

1. Introduction
Improving efficiency and reducing environmental pollution are the long-term development goals of thermal power industry. P92 heat resistant steel is the representative of thermal power steel. It is widely used in ultra (ultra) critical thermal power units. However, during high temperature service, the microstructure evolution of P92 heat resistant steel will affect the mechanical properties and reduce the service life. Therefore, in order to improve the service life of P92 steel, it is necessary to evaluate the relationship between microstructure and creep rupture behavior.

P92 steel shows tempered martensite structure after heat treatment. There are a lot of dislocations in the martensitic lath, and the lath structure hinders the dislocation. The excellent creep properties of P92 steel mainly benefit from this. During service, the coarsening of martensitic laths will lead to the decrease of the overall dislocation density of the material. Xiao Jin [1] found that the high temperature strength of P92 steel is mainly affected by lath and dislocation hardening in the early stage of service. With the increase of time, the strengthening mechanism changes to lath strengthening and precipitation strengthening. Therefore, the strip structure plays an important role in the mechanical properties of P92 steel.

Based on experiments, it is difficult to accurately describe the effect of single microstructure on micromechanical properties. It is necessary to establish a multi-scale creep mechanical model considering microstructure. The mechanism of metal plastic deformation is fully considered by crystal
plastic finite element technology (CPFEM). It can accurately simulate and predict the local plastic deformation of metal grain size (Roters et al. [2]).

Based on CPFEM, a creep constitutive model of P92 steel considering dislocation and size effect is established in this paper. The representative volume elements (RVE) model containing martensitic laths is generated. The effect of lath coarsening on high temperature creep properties of P92 heat resistant steel was investigated.

2. Crystal plasticity finite element model

2.1 Constitutive model

This study is based on the rate-dependent crystal plasticity constitutive model proposed by Asaro and Needleman[3]. The Orowan dislocation dynamic equation is used to describe the relationship between the dislocation slip rate and the movable dislocation density and the average velocity of movable dislocations[2].

\[
\begin{align*}
\dot{\gamma}^{(\alpha)} &= \rho^{\alpha} b v^{\alpha} \quad (|\tau^{\alpha}| \geq |\tau_c|) \\
\dot{\gamma}^{(\alpha)} &= 0 \quad (|\tau^{\alpha}| \leq |\tau_c|)
\end{align*}
\]

\( \rho^{\alpha} \) represents the dislocation density of the \( \alpha \)-th slip system; \( b \) represents the burgers vector, \( b=0.248 \text{nm} \), where the average moving velocity of movable dislocations \( v^{\alpha} \) is expressed as:

\[
v^{\alpha} = \xi \cdot \exp\left(-\frac{F}{RT}\right) \frac{\tau^{\alpha} d}{\tau_c} \text{sign}\left(\frac{\tau^{\alpha}}{\tau_c}\right)
\]

Where \( \xi \) is the fitting coefficient of dislocation motion; \( T \) is the absolute temperature (Kelvin temperature); \( F \) is the thermal activation energy; \( R \) is the Boltzmann constant; \( d \) is the rate sensitivity index; \( \tau^{\alpha} \) is the resolved shear stress of the slip system \( \alpha \), \( \tau_c \) represents the flow stress of the sliding system. \( \tau_c \) consists of two parts:

\[
\tau_c = \tau_l + \tau_p
\]

\( \tau_p \) and \( \tau_l \) represent the slip resistance caused by dislocation hardening and slab hardening. Based on Taylor's hardening criterion[4], the dislocation resistance is proportional to the square root of the dislocation density. The dependence of flow stress on the size of the slab can be expressed by the Hall-Petch relationship [5].

\[
\tau_l = 10 G b / \lambda_l
\]

\[
\tau_p = \tau_0 + G b \sqrt{\sum_{\beta=1}^{N} A^{\alpha\beta} \rho^\beta}
\]

\( \lambda_l \) is the average size of the strip; \( G \) is the shear modulus; \( \tau_0 \) indicates the strength of the initial slip system. Refer to reference [25] to determine \( A^{\alpha\alpha}=1.0 \); \( A^{\alpha\beta}=0.2 \); The dislocation motion of the slip system \( \alpha \) is divided into two parts: dislocation increment and dislocation extinction, as shown in formula (13):

\[
\dot{\rho} = \frac{1}{b} \left( \sqrt{\frac{\sum_{\alpha=1}^{N} A^{\alpha\beta} \rho^\beta}{\psi}} - 2 \chi_c \rho^{\alpha} \right) |\dot{\gamma}^{\alpha}|
\]

\( \psi \) represents the fitting coefficient of dislocation increment. \( \chi_c \) represents the length of critical dislocation extinction, which is related to dynamic recovery. Through the secondary development of the UMAT subroutine in the ABAQUS finite element software, the above-mentioned dislocation-based crystal plasticity theory formula is written into the subroutine in the form of Fortran language.

2.2 RVE model

In practical research, it is found that P92 steel as a whole shows body centered cubic crystal structure (BCC) [6]. According to the microcolumn compression experiment conducted by Du [7], the slip in bcc structure mainly occurs on the \{110\} [111] slip system (Table 1). Therefore, only \{110\} [111] slip system is considered in this study.
Table 1 {110} [111] 12 slip surfaces and slip directions of slip system

| Number | Slip surface | Slip direction | Number | Slip surface | Slip direction |
|--------|--------------|----------------|--------|--------------|----------------|
| S1     | (011)        | <1-11>         | S7     | (01-1)       | <111>          |
| S2     | (011)        | <11-1>         | S8     | (01-1)       | <-111>         |
| S3     | (101)        | <-111>         | S9     | (10-1)       | <111>          |
| S4     | (101)        | <11-1>         | S10    | (10-1)       | <1-11>         |
| S5     | (110)        | <1-11>         | S11    | (-110)       | <11-1>         |
| S6     | (110)        | <1-11>         | S12    | (-110)       | <111>          |

Transmission electron microscopy was used to quantify the strip size of P92 steel at different service times (Xiao Jin et al. [1], 2020). After 75000 hours of service, the average size of the strip increased from the initial 350 nm to 800 nm. With the extension of service time, the strip size always shows an upward trend. To this end, RVE models of P92 steel with average strip widths of 350 nm, 650 nm and 950 nm were established using neper software (Quey et al [8], 2011). Different regions represent different laths, and the initial crystal orientation of laths is randomly distributed. The model applies periodic boundary conditions and is loaded in the X direction.

Fig.1 Lath models of different sizes (a)350nm, (b)650nm, (c)950nm; (d)Boundary conditions;

The material parameters used in crystal plasticity calculation are generally obtained by fitting the experimental curve. Refer to the simulation parameters [9-11] of relevant BCC materials, and constantly select some trial values for parameter sensitivity analysis and correction. The material parameters of relevant crystal calculations are obtained. Fig.2 shows the creep fitting curve of P92 heat resistant steel under 140 MPa stress at 650°C. The fitted material parameters (Table2) reflect the creep deformation behavior of P92 heat resistant steel at 650°C.

Fig.2 Creep fitting curve of experiment and simulation under stress of 140MPa
Fig. 3 Macro creep curves of different slab size models
Table 2. P92 heat-resistant steel crystal plasticity calculation parameters

| Parameter | Numerical value | Unit | Parameter | Numerical value | Unit |
|-----------|-----------------|------|-----------|-----------------|------|
| $C_{11}$  | 130             | GPa  | $\tau_0$  | 450             | MPa  |
| $C_{12}$  | 90              | GPa  | $d$       | 5               |      |
| $C_{44}$  | 85              | GPa  | $\psi$    | 32              |      |
| $b$       | 0.248           | nm   | $\lambda$ | 0.016           |      |
| $T$       | 873             | K    | $\gamma_c$| 2.1             | nm   |
| $Q$       | $4.48E-21$      | J    | $A^\alpha/A^\alpha$ | 0.2 / 1 |       |
| $\rho_0$  | $8E+7$          | mm$^{-2}$ | $R$ | $1.38E-23$ | J/K |

3. Results and discussion

3.1 Effect of lath coarsening on macro creep mechanical properties

The creep mechanical curves of different lath sizes at 650 °C and 140MPa tensile stress are given in the figure 3. It is observed that the strain in the third stage of creep increases significantly with the increase of lath size. When the tensile time is 70 h, the creep strain of the model strip size of 350 nm is 1%, but the creep strain of 950 nm increases to 3.3%. It shows that strip coarsening has a significant effect on the mechanical properties in the third stage of creep. Strip coarsening accelerates the creep fracture rate and reduces the service life of P92 steel.

3.2 Micromechanical response of lath coarsening

The figure 4 shows the stress-strain nephogram of different lath sizes at 650 °C and 140MPa tensile stress. After creep, the stress-strain distribution of the strip is obviously uneven. It has obvious strip structure characteristics. There is stress-strain concentration at the grain boundary and inside some laths. Due to the different size and crystal orientation of the strip, the strip will have a "hard" or "soft" orientation response. At the same time, it is necessary to ensure deformation coordination between laths. Affected by the size of adjacent grain boundaries and laths, it eventually leads to the non-uniformity of stress and strain.

![Fig.4 Stress-strain nephogram of model under 350nm lath sizes](image)

Draw the stress-strain numerical diagram of the same path (A-B) element to observe the specific effect of lath size on stress-strain. In figure 5(a), the stress under different sizes of laths fluctuates up and down, and the stress at the same position is different. The stress under the three dimensions is maintained between 120-180mpa. It shows that strip coarsening has little effect on stress. In Figure 5(b), the model strain value with the lath size of 350nm is the smallest, and the strain value mainly fluctuates between 0-2%. However, as the lath size increases to 650 nm and 950 nm, the overall strain value increases to 3-8%. It shows that the lath coarsening reduces the hardening strength and accelerates the creep deformation. It aggravates the non-uniformity of plastic deformation.
Figure 6 shows the maximum stress-strain values and average stress-strain values of the three strip models. With the strip coarsening, the overall maximum stress of the model increases from 253MPa to 276MPa. However, the average stress value changes little and is basically stable at 150MPa. It shows that the lath coarsening has little effect on the overall stress of the model. The overall strain of the model changes greatly, the maximum strain increases from 2.8% to 10%, and the average strain increases linearly from 1% to 3%. It shows that the lath coarsening intensifies the stress-strain concentration of the model, which is easy to lead to crack initiation and damage cracking.

3.3 The effect of slat coarsening on dislocation slip

The average dislocation density of the three different slab size models was calculated, and the evolution of the model's average dislocation density under different stretching times was drawn. It can be seen from Figure 7 that the movable dislocation density remains unchanged at the initial stage of deformation. With the increase of creep deformation, the dislocation density of the three models increased sequentially after 35h. At the same time, the larger the slab size, the higher the dislocation density of the model.

Select the same position element in three lath models with different sizes, count the shear strain of each slip system of the element, and observe the start-up of the slip system. The results are shown in the figure. It is observed that there are obvious differences in the actuation of the slip system, which is closely related to the orientation and size of the lath. Figure 8 (a-350nm) the maximum shear strain of the slip system is 1.1%. With the increase of slab size, the maximum shear strain of slip system in Figure 8 (c-950nm) increases to 5.3%. It shows that slab coarsening promotes the start of slip system. The shear strain of slip system increases and accelerates the creep deformation at high temperature.
Figure 8. Shear strain of slip system at the same position

4. Conclusion
(1) Based on the theory of crystal plasticity, coupled with Taylor's dislocation hardening model and Hallpage formula, this paper establishes a microscopic creep mechanics model that considers the effect of slab hardening. The calculation parameters of crystal plasticity at 140 MPa and 650°C are determined.
(2) Comparing the creep behavior of the average lath size at 350 nm, 650 nm and 950 nm, lath coarsening aggravates the unevenness of plastic deformation, reduces the ability to hinder the movement of dislocations, causes the creep rate to rise, and accelerates the damage Cracked.

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