Available online at ScienceDirect

Nuclear Engineering and Technology

journal homepage: www.elsevier.com/locate/net

Original Article

Multiscale Simulation of Yield Strength in Reduced-Activation Ferritic/Martensitic Steel

Chenchong Wang [a], *Chi Zhang* [a,*], *Zhigang Yang* [a], *and Jijun Zhao* [b]

[a] *Key Laboratory of Advanced Materials of Ministry of Education, School of Materials Science and Engineering, Tsinghua University, No.1 Qinghua Yuan, North Zhongguancun Street, Beijing, China*

[b] *State Key Laboratory of Materials Modification by Laser, Electron, and Ion Beams, School of Physics and Optoelectronic Technology and College of Advanced Science and Technology, Dalian University of Technology, No.2, Linggong Street, Dalian, China*

ARTICLE INFO

Article history:
Received 24 July 2016
Received in revised form
25 September 2016
Accepted 2 October 2016
Available online xxx

Keywords:
High Temperature
Irradiation
Multiscale Simulation
Yield Strength

ABSTRACT

One of the important requirements for the application of reduced-activation ferritic/martensitic (RAFM) steel is to retain proper mechanical properties under irradiation and high-temperature conditions. To simulate the yield strength and stress-strain curve of steels during high-temperature and irradiation conditions, a multiscale simulation method consisting of both microstructure and strengthening simulations was established. The simulation results of microstructure parameters were added to a superposition strengthening model, which consisted of constitutive models of different strengthening methods. Based on the simulation results, the strength contribution for different strengthening methods at both room temperature and high-temperature conditions was analyzed. The simulation results of the yield strength in irradiation and high-temperature conditions were mainly consistent with the experimental results. The optimal application field of this multiscale model was 9Cr series (7–9 wt.%Cr) RAFM steels in a condition characterized by 0.1–5 dpa (or 0 dpa) and a temperature range of 25–500°C.

1. Introduction

One of the most important requirements of reduced-activation ferritic/martensitic (RAFM) steels is to retain proper mechanical properties in irradiation and high-temperature conditions [1–6]. However, testing the mechanical properties of materials under irradiation and high-temperature conditions is complicated and costly. To verify the accuracy of experimental results and to analyze the mechanisms associated with irradiation and high temperatures, much attention has been paid to simulations of the mechanical properties of RAFM steels under these conditions.

As a long-standing problem, yield strength simulations have been studied by many researchers, and many classical models have been established, including the Peierls–Nabarro (P–N) model [7,8], the Hall–Petch model [9,10], the Orowan dislocation looping model [11], Friedel's shear cutting model [12], and the Kocks–Mecking model [13–15]. Most of these models express one main strengthening method, with no

---

* *Corresponding author.*

E-mail address: chizhang@tsinghua.edu.cn (C. Zhang).

http://dx.doi.org/10.1016/j.net.2016.10.006

relationships among them. To widen the application range of yield strength simulations, a superposition model [16], which combined different classical models, was built and used to calculate the yield strength of gear steels. However, this superposition model was only feasible for use under normal conditions (no irradiation at room temperature). In 2015, a self-consistent thermomechanical model was devised by Terentyev and co-workers [17] to simulate the strain-hardening behavior of polycrystalline tungsten at high temperatures. However, this model mainly expressed the effect of the temperature on dislocation strengthening without considering irradiation effects or other factors. Moreover, the Friedel–Kroupa–Hirsch model [12,18] and a dispersed barrier hardening model [19] have been widely used to calculate the irradiation effect on the yield strength of steels. However, these models only express factors related to He bubbles and dislocation loops [20].

In this work, a multiscale model, which consists of models at different scales and theories of different strength methods, is established to simulate the yield strength and stress-strain curve of RAFM steels in both irradiation and high-temperature conditions.

2. Simulation method

The applied model mainly consists of four strengthening models. Fig. 1 shows the overall simulation procedure of the proposed multiscale simulation model. To evaluate the accuracy and rationality of this model, it was used to analyze the effects of irradiation and high temperatures on the yield strength of F28H steel (Japanese RAFM steel tempered at 750°C for 1 h).

2.1. *Microstructure simulation*

2.1.1. *Precipitation and solid solution*

Thermodynamic theory is commonly used to simulate the volume fraction of precipitation, commonly using the Thermo-Calc software package (Thermo-Calc Software AB Company, Stockholm, Sweden) [21]. Previous work reported that the main precipitations that form in RAFM steels were MX, $M_{23}C_6$, and the Laves phase [22,23]. As $M_{23}C_6$ and the Laves phase typically form at the grain boundary and at much higher coarsening rates than the MX phase [23,24], the MX phase is regarded as the main reinforcement for dispersion strengthening. Fig. 2 shows the simulation results of the volume fraction of the MX phase and the concentration of the solid-solution element in the matrix of F28H steel.

2.1.2. *Shear modulus*

For steels, small changes in the atomic configuration triggered by temperature changes can change the magnetic interactions responsible for the nonrandom atomic spin orientation. In such a case, different magnetic states lead to different macroscopic properties, such as the shear modulus and elastic modulus [25,26]. Recently, many simulation results pertaining to ideal strength levels were obtained by first-principles methods. Based on these simulation results [25,27] and on experimental findings, a linear hypothesis was used to express the effect of the temperature on the shear modulus from 25°C to 500°C in RAFM steels, as shown in the following equation:

$$\mu = \mu_0 - k_{\text{shear}}\Delta T \tag{1}$$

where μ_0 is the shear modulus at 25°C and ΔT denotes the temperature increment.

2.1.3. *He bubbles and dislocation loops*

The formation of He bubbles and dislocation loops under an irradiation condition is a complicated problem that has been studied by many different simulation methods, including phase field theory, rate theory, and molecular dynamics [28–31]. A linear function passing through zero has been used to express the relationship between the irradiation and density/size of the dislocation loops. Based on both simulation and experimental results, a linear hypothesis has been used to express the effects of accumulated displacement damage on

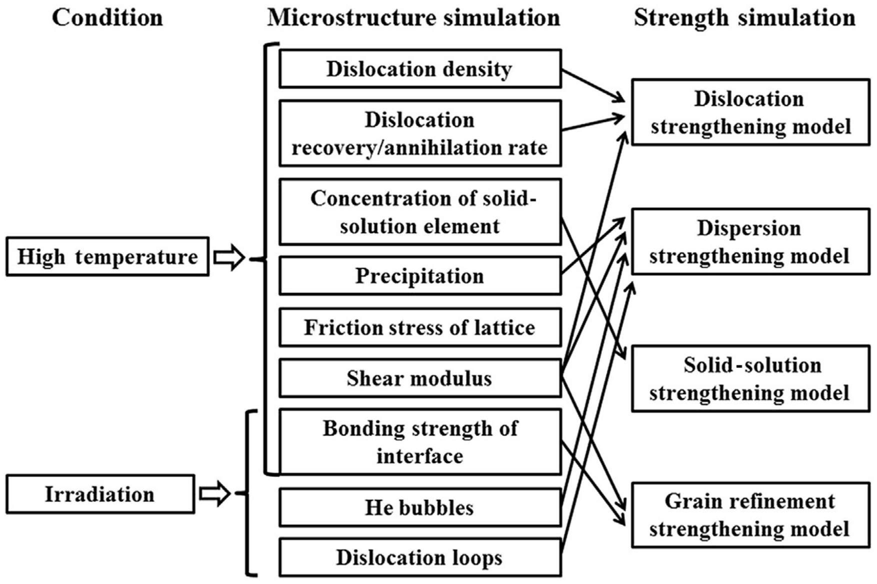

Fig. 1 – Simulation procedure of the multiscale simulation model.

Please cite this article in press as: C. Wang et al., Multiscale Simulation of Yield Strength in Reduced-Activation Ferritic/Martensitic Steel, Nuclear Engineering and Technology (2016), http://dx.doi.org/10.1016/j.net.2016.10.006