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Damage of High-Chromium Steels under Deformation in a Wide Temperature Range

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Abstract. High-chromium steels have high strength properties, corrosion properties and resistance to neutron irradiation, thereby are considered as promising steels for nuclear reactors of generation IV. The deformation and damage of high chromium steels in a wide temperature range was studied by numerical simulation method. A model was proposed to predict the deformation and damage of high chromium steels under quasi–static loading within the temperature range from 295 to 1100 K. It is shown that the ductility of high-chromium steels increases proportionally to temperature in the range from 750 to 1100 K due to the growth of α′-phase precipitates.

INTRODUCTION

High chromium steels, including oxide dispersion strengthened (ODS) grades, are considered as structural materials for critical components of Gen-IV reactor. These steels form an important class of steels with a unique combination of properties such as high resistance to aqueous corrosion, high temperature oxidation resistance, high strength and ductility, resistance against thermal creep, weldability, and neutron irradiation hardening effect [1, 2]. The mechanical behavior of high chromium steels in a wide temperature range, including in combination with radiation and neutron radiation, is intensively studied using experimental methods and molecular dynamics method [1–5]. Terentyev showed the decomposition of high chromium steel into the Fe-rich α and Cr-rich α′ phases takes place under thermal aging [1]. The formation of the Cr-rich α′ phase occurs under irradiation at a temperature below the peak thermal aging temperature (753 K). This effect can be explained by the acceleration of the α′-phase formation due to the production of mobile point defects after the collision damage cascade [1–4].

Thus, damage at elevated temperatures is an important factor affecting the mechanical behavior of high chromium steels. The precipitates of α′- and σ-phases cause the hardening effect of Fe-Cr steel due to pinning dislocations. The yield strength decreases in the range from 473 to 1073 K due to reduction of the mole fraction of the α′- and σ-phase precipitates with increasing temperature [4].

The aim of this work is to predict the deformation and damage of Fe–Cr steels in a wide temperature range up to 1100 K.

COMPUTATIONAL MODEL

Tension tests of specimens (ASTM A242/A 242M-04) at constant strain rates and various initial temperatures were simulated by means of licensed software WB ANSYS 14.5 and AUTODYN. The standard specimen shape for sheet steel testing was considered. The calculations were carried out with solvers using a finite difference scheme of

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second-order accuracy. Mechanical behavior at the macroscopic level is described by a system of conservation equations (kinematic equations, equations of conservation of mass, momentum and energy), and a constitutive equation in which shear stress relaxation is calculated by a dislocation model of plastic flow [6, 7].

The constitutive equation is used in the form

$$\sigma_{ij} = \sigma_{ij}^{(m)}(1-D),\ \sigma_{ij}^{(m)} = -p^{(m)}\delta_{ij} + S_{ij}^{(m)}, \tag{1}$$

where D is the damage parameter, σ_{ij} is the stress tensor components, p is the pressure, and S_{ij} are the stress deviator components, respectively, δ_{ij} is the Kronecker delta, and the superscript m indicates an undamaged phase.

The Mie–Grüneisen equation of state is used for pressure calculation of the α-, γ- and ε-phases of Fe-Cr [7]. The deviator of stress tensor is calculated by the equation

$$\mathrm{d}S_{ij}^{(m)} \big/ \mathrm{d}t = 2\mu(\dot{e}_{ij} - \dot{e}_{ij}^{\mathrm{p}}), \tag{2}$$

where d/dt is the Jaumann derivative, μ is the shear modulus, and $\dot{e}_{ij}^{n}$ is the deviator of the inelastic strain rate tensor.

The components of the strain rate tensor $\dot{\varepsilon}_{ij}$ are determined by the relation

$$\dot{\varepsilon}_{ij} = \frac{1}{2}(\partial u_j \big/ \partial x_i + \partial u_i \big/ \partial x_j), \tag{3}$$

where $\bar{u}$ is the particle velocity with components u_i,

$$\dot{\varepsilon}_{ij} = (1/3)\dot{\theta}\delta_{ij} + \dot{e}_{ij}, \tag{4}$$

where $\dot{\theta} = \dot{\varepsilon}_{kk}$ is the bulk strain rate, and $\dot{e}_{ij}$ is the deviator of the strain rate tensor.

The shear modulus and the Poisson ratio at temperature T are calculated by the Hashin–Shtrikman bounds [8]. The shear modulus of the solid phase was calculated by the relation

$$\mu_K(T) = \mu_{0k}^{\mathrm{c}}(1-\alpha_d)[1 + A_{sk}p - B_{sk}(T/T_{\mathrm{m}} - 297\,\mathrm{K}/T_{\mathrm{m}})], \tag{5}$$

where μ_{0k}^{c} is the shear modulus of the k-solid phase, A_{sk} and B_{sk} are the constants for the k-solid phase, and T_{m} is the melting temperature of the Fe–Cr system.

Poisson's ratio can be described by the relation

$$\nu_k(T) = \nu_{0k} + k_{\nu T}T + k_{\nu p}p, \tag{6}$$

where ν_k is the Poisson's ratio of the k-phase, ν_{0k}, $k_{\nu T}$, and $k_{\nu\mathrm{p}}$ are the k-phase constants, p is given in GPa, and T is given in Kelvins. Calculations were done using $\nu_{0k} = 0.264$, $k_{\nu T} = 1.067$ (K^{-1}), $k_{\nu\mathrm{p}} = 0.0008$ (GPa^{-1}) for the α-phase of Fe-Cr steel.

The temperature dependence of the bulk modulus $B_{0k}(T)$ of the k-phase can be calculated as

$$B_{0k}(T) = \frac{2\mu_k(T)(1+\nu_k(T))}{3(1-2\nu_k(T))}. \tag{7}$$

The damage parameter is calculated by Eq. (8)

$$D = \int_0^{\varepsilon_{\mathrm{eq}}^{\mathrm{p}}} (1/\varepsilon_{\mathrm{f}})\mathrm{d}\varepsilon_{\mathrm{eq}}^{\mathrm{p}} = \frac{1}{C_1}\int_0^{\varepsilon_{\mathrm{eq}}^{\mathrm{p}}} \frac{\exp(-p/\sigma_{\mathrm{eq}}C_2)}{1 - C_3(T - T_{\mathrm{s}}^{\alpha'})\big/(T_{\mathrm{f}}^{\alpha'} - T_{\mathrm{s}}^{\alpha'})H(T_{\mathrm{f}}^{\alpha'} - T)H(T - T_{\mathrm{s}}^{\alpha'})}\mathrm{d}\varepsilon_{\mathrm{eq}}^{\mathrm{p}}, \tag{8}$$

where D is the damage parameter, $\varepsilon_{\mathrm{eq}}^{\mathrm{p}} = [(2/3)\varepsilon_{ij}^{\mathrm{p}}\varepsilon_{ij}^{\mathrm{p}}]^{1/2}$, ε_{f} is the strain to fracture, C_1, C_2, and C_3 are the material parameters, $\sigma_{\mathrm{eq}} = [1.5S_{ij}S_{ij}]^{1/2}$, p is the pressure, T is the temperature, $T_{\mathrm{s}}^{\alpha'} - T_{\mathrm{f}}^{\alpha'}$ is the temperature range in which the α'-phase exists ($T_s^{\alpha'} = 748$ K, $T_f^{\alpha'} = 1115$ K), H (.) is the Heaviside function, and p/σ_{eq} is the triaxiality stress factor [9].

The damage accumulation in a wide temperature range can be represented by a general law that accounts for both the growth of existing defects and nucleation of new damages (microcracks or voids). The local damage of material particles is described by the criterion

$$D = 1. \tag{9}$$

The yield criterion is used in the form

$$\sigma_{eq} \le \sigma_s, \tag{10}$$

where σ_s is the yield strength.

The deviator of the inelastic strain rate tensor is determined be the relation

$$\dot{e}_{ij}^{p} = (3/2)[S_{ij}\dot{e}_{eq}^{p}/\sigma_{eq}]. \tag{11}$$

The scalar function $\dot{e}_{eq}^{p(m)}$ is defined as the sum of the parts corresponding to dislocation movements and dislocation nucleation near precipitates [6, 7]

$$\dot{e}_{eq}^{p} = [\dot{e}_{eq}^{p}]_{disl} + [\dot{e}_{eq}^{p}]_{disl\ nucl},$$

$$[\dot{e}_{eq}^{p}]_{disl} = gbvN_m \exp(-\Delta G_1/kT),\ \Delta G_1 = \Delta G_0[1-(\sigma_{eq}/\sigma_{eq}^{*})^{n_1}]^{q},\ v = b(\sigma_{eq}-\sigma_{bs\,pr})/B_v, \tag{12}$$

$$[\dot{e}_{eq}^{p}]_{disl\ nucl} = gb\dot{N}_{nucl}l_0 \exp(-\Delta G_2/kT),\ \dot{N}_{nucl} = (p+(2/3)\sigma_{eq})^4 H[p+(2/3)\sigma_{eq}-\sigma^{*}],$$

where $g \sim 0.5$ is the orientation coefficient, b is the modulus of the Burgers vector, v is the mean dislocation velocity, N_m is the mobile dislocation density, k is the Boltzmann constant, ΔG_1 is the activation energy for slip systems, ΔG_2 is the activation energy of nucleation, $\sigma_{bs\ pr}$ is the back-stress increment caused by the presence of various precipitates, l_0 is the average size of dislocation loops, $B_v = 3kzT/(20C_s b^2)$, z is the number of atoms per unit cell of the phase, $C_s = [\mu_k(T)/\rho(T)]^{1/2}$, ρ is the mass density, σ^* is the threshold stress of the heterogeneous nucleation of dislocations in Fe–Cr, and H (.) is the Heaviside function. All calculations were done using b = 0.248 nm, $\Delta G_0 = 0.35\mu b^3$, $n_1 = 0.28$, and $q = 1.34$, $\sigma^* = 0.56$ GPa, $l_0 = 400$ nm, $\Delta G_2 = 562–329$ kJ mol^{-1}, while the Cr content varied in the range 9–27%. The constitutive equation was used to predict the yield strength of high chromium steels under deformation in a wide temperature range. The mechanisms of interaction between dislocations and irradiation-produced defects, such as voids and dislocation loops, are the same in Fe and Fe-Cr alloys.

The yield strength increment is described by the Orowan–Ashby equation

$$\sigma_{bs\,pr} = \frac{0.83\mu bM \ln(r_s/2b)}{(2\pi r_s\sqrt{1-\nu})(\sqrt{\pi/f_c}-2)}, \tag{13}$$

where μ is the shear modulus of the α-phase matrix (~78 GPa), $b = 0.248$ nm is the magnitude of the Burgers vector, $M \approx 3.06$ is the Taylor factor, r_s is the average radius of the cross section of Cr-rich clusters, ν is the Poisson's ratio (~0.33), and $f_c \approx 6.7 \times 10^{23}$ m^{-3} is the density of Cr-rich clusters.

We simulated the mechanical behavior of 9Cr–1MoV, Fe–14Cr–3W–0.4Ti–0.18O (14WT), Fe–14Cr–3W–0.4Ti–0.3Y–0.18O (14YWT) high chromium steels. The difference between the yield strengths of 14WT and 14YWT steels was caused by the concentration of nanoscale Y_2O_3 inclusions in 14YWT steel [10].

RESULTS AND DISCUSSION

Figure 1a shows the calculated strain to fracture versus temperature. Curves *1*, *2* correspond to 9Cr–1MoV. Curves *3*, *4* and *5*, *6* were calculated for 14WT and 14YWT, respectively.

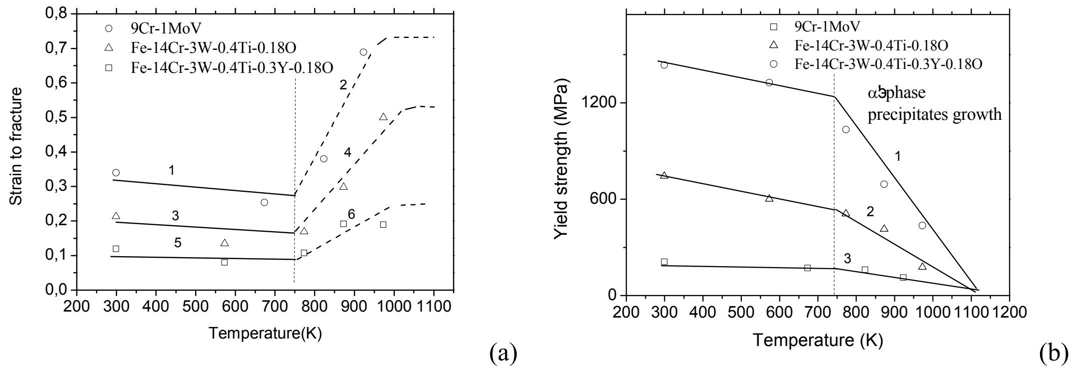

FIGURE 1. Calculated strain to fracture versus temperature (a), yield strength versus temperature (b), experimental data are designated by symbols [10]

The material parameter C_3 in Eq. (8) was taken equal to 0.8, 0.95, and 1.1 for 14YWT, 14WT, and 9Cr–1MoV steels, respectively. The strain to fracture of all the considered high chromium steels increased at temperature above 750 K. The curve slope changes when the temperature exceeds 750 K. The size of the α′-phase (Cr clusters) at the same duration of heating increases proportionally to temperature. The calculated values of strain to failure of high chromium steels increases proportionally to temperature growth in the range 750–1100 K. These results allow us to predict the delay of damage of high chromium steels under quasi-static tension at temperatures 750–1100 K. The calculated curve of the yield strength versus temperature is shown in Fig. 1b. The experimental data for Fe–Cr steel are denoted by symbols [10]. Curves *1–3* correspond to 14YWT, 14WT, and 9Cr–1MoV, respectively. It was assumed for Fe–Cr steel that the α′-phase concentration increased within the temperature range 750–1115 K. Recently, Yang has shown this effect for Fe–14% Cr steel [11]. Therefore, the volume fraction of the Cr-rich cluster f_c in Eq. (13) will depend only on temperature. It was assumed in the calculations that the steel was heated to the temperature T and kept at this temperature until the formation of the average equilibrium particle size r_s of the α′-phase. Curves *1* and *2* correspond to 14WT and 14YWT. The simulation results showed close values of softening of these steels in the range 295–750 K. The softening of 9Cr–1MoV steel is less than for 14WT and 14YWT, like the yield strength value. Thus, the simulation results indicate that the high chromium steels have similar mechanisms of plastic deformation and damage in the temperature range 297–750 K. This prediction agrees with experimental results obtained by Praud et al. [12]. The softening of all the considered high chromium steels is increased in the temperature range 750–1100 K.

SUMMARY

A multiscale approach was used to predict the mechanical behavior of precipitation-hardened 9Cr–1MoV, Fe–14Cr–3W–0.4Ti–0.18O (14WT), Fe–14Cr–3W–0.4Ti–0.3Y–0.18O (14YWT) high chromium steels in the temperature range up to 1100 K under quasi-static loading. A model was proposed to predict the deformation and damage of high chromium steels under quasi-static loading in the temperature range 295–1100 K.

The ductility of high chromium steels increases proportionally to temperature in the range from 750 to 1100 K.

The yield strength values of high chromium steels decrease faster with increasing temperature in the range 750–1115 K than in the range 295–750 K. This effect is associated with the growth of the α′-phase precipitates. The softening of high chromium steels is increased in the temperature range 750–1100 K.

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REFERENCES

1. D. Terentyev, S. M. H. Haghighat, and R. Schäublin, J. Appl. Phys. **107**, 061806 (2010).
2. G. Bonny, D. Terentyev, and L. Malerba, J. Phase Equilib. Diff. **31**, 439–444 (2010).
3. R. A. Barrett, P. E. O'Donoghue, and S. B. Leen, Comput. Mater. Sci. **92**, 286–297 (2014).
4. M. Samaras, W. Hoffelner, and M. Victoria, J. Nuclear Mater. **371**, 28–36 (2007).
5. R. A. Austin, and D. L. McDowell, Int. J. Plasticity **27**, 1–24 (2010).
6. V. A. Skripnyak, E. S. Emelyanova, M. V. Sergeev, N. V. Skripnyak, and O. S. Zinovieva, AIP Conf. Proc. **1783**, 020208 (2016).
7. V. A. Skripnyak, N. V. Skripnyak, V. V. Skripnyak, and E. G. Skripnyak, "Deformation and damage of Fe-Cr steels in a wide temperature range", in *Proc. of the 7th International Conference on Mechanics and Materials in Design, Albufeira/Portugal 11–15 June 2017*, edited by J. F. Silva Gomes and S. A. Meguid (Publ. INEGI/FEUP, 2017), vol. **1763**, p. 6602.
8. D. R. S. Talbot, J. R. Willis, and V. Nesi, J. Appl. Math. **54**, 97–107 (1995).
9. I. Kacker, S. S. Bhadauria, and V. Parashar, Int. J. Mech. Product. Eng. **3**, 2320–2092 (2015).
10. R. K. Nanstad, D. A. McClintock, D. T. Hoelzer, L. Tan, and T. R. Allen, J. Nucl. Mater. **392**, 331–340 (2009).
11. Y. Yang and J. T. Busby, J. Nucl. Mater. **448**, 282–293 (2014).
12. M. Praud, F. Mompiou, J. Malaplate, et al., J. Nucl. Mater. **428**, 90–97 (2012).