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Crystal plasticity modeling of irradiation effects on flow stress in pure-iron and iron-copper alloys

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ABSTRACT

The mechanistic modeling of irradiation induced embrittlement of reactor pressure vessel steels strongly depends on the precise evaluation of flow stress behavior. This requires accurate characterization of change in both the yield strength as well as the strain-hardening capacity. A dislocation-density based crystal plasticity model is thus developed in this work to quantify these variations with irradiation. The model considers the interaction between dislocations and irradiation induced defects such as self-interstitial atomic loops, vacancy clusters and precipitates to obtain flow stress variations in irradiated ferritic alloys. The model is calibrated and validated for polycrystalline pure-iron and iron-copper alloys, neutron-irradiated to different dose levels under typical pressure vessel operating conditions. A comparison with experimental results show that the model is able to quantify the changes in flow stress behavior accurately. At 0.2 dpa a loss of strain-hardening capacity beyond 2% strain is also obtained from the model. The yield strength increase with irradiation obtained from the model is also compared with analytical strengthening models based on Orowan's equation.

1. Introduction

The long-term exposure of Reactor Pressure Vessels (RPVs) to neutron irradiation increase their failure probability due to the precipitation and segregation of secondary phases, as well as formation and growth of vacancy clusters and self interstitial atomic loops (English and Hyde, 2012). For instance, an increase in the yield strength and a decrease in the post-yield hardening exponent can be observed with increasing irradiation dose levels, and is due to the interaction of the dislocations with the defects. Also, the ductile-to-brittle transition temperature (DBTT) has been observed to increase with irradiation dose levels. Since, the RPV is one of the critical components whose integrity determines the safe extension of the operational lifetime of the exisiting nuclear reactors beyond the 60 year period, hence, accurate assessment of RPV steel embrittlement is essential.

The present approach to quantify embrittlement in RPVs rely on semi-empirical models that are calibrated using the surveillance samples in the reactors (Eason et al., 2013). Though these models have successfully quantified DBTT shifts and yield stress increase for the 40–60 year life extension, their accuracy for extrapolation can be hindered due to the lack of experimental data and appearance of late-blooming phases. Multi-scale models of irradiation induced aging can assist in improving the predictive ability of the semi-emperical models by providing surrogate data, and, exploring the mechanisms that can emerge due to longer exposures beyond the designed period (Massoud et. al., 2010). These models span across widely differing length and time-scales from atomistics to engineering scale, and attempts to provide physical understanding of defect formation, their interaction and effect on mechanical behavior.

At the scale of the fracture specimens, the models developed to characterize DBTT shifts primarily incorporate the mechanisms causing stable ductile damage and probabilistic cleavage initiation. For ductile damage, pressure sensitive plasticity models characterizing void nucleation, growth and coalescence are utilized (Gurson, 1997; Rousselier, 1987). The model parameters are calibrated from tensile tests and/or fracture tests at the upper shelf. The cleavage initiation models are based on the weakest link theory, which incorporates the mechanism of plasticity induced micro-crack initiation from grain-boundary carbides and their growth into a macro-crack causing unstable failure. The Beremin model (Beremin, 1983), using the weakest link theory based Weibull distribution (Weibull, 1953) for probabilistic cleavage initiation, is typically employed to capture the scattered fracture energy and toughness observed in the transition regime. The Beremin model parameters are typically calibrated near the lower shelf.

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A combination of the ductile damage and Beremin model has been used in Finite Element Method (FEM) simulations of fracture specimens to obtain DBTT by several authors (Tanguy et al., 2005; 2006; Samal et al., 2008; Chakraborty and Biner, 2014). In Samal et al. (2008), the calibrated ductile damage and Beremin model parameters are kept constant and only the temperature sensitive flow stress is varied to obtain the DBTT of unirradiated RPV steels. In Tanguy et al. (2005), temperature dependent Beremin model parameters are considered additionally to obtain improved comparison with experiments. Under irradiated condition it has been observed that both the ductile damage and cleavage model parameters vary with dose levels (Tanguy et al., 2006). Also, the DBTT shifts are sensitive to the post-yield hardening behavior. In Chakraborty and Biner (2014), temperature dependent cohesive zone model and flow stress parameters were utilized to obtain DBTT in RPV steels. In a parametric study using tensile test data for ferritic-martensitic steels (Chakraborty and Biner, 2015), it has been shown that the variation of ductile damage parameters saturate with increasing irradiation dose levels, whereas the flow stress parameters still evolve. From these numerical studies it can be concluded that precise evaluation of flow stress variation with temperature and irradiation dose levels is essential to characterize DBTT shifts accurately. Also, quantifying the yield stress variations alone is not sufficient to obtain the DBTT shifts and evaluation of flow stress variations upto a critical plastic strain is necessary (Odette et al., 2007).

Modeling the evolution of flow stress with irradiation involves the development of methods to track defect evolution and their interaction with dislocations. Atomistic scale method such as Molecular Dynamics (MD) can provide insight into the fundamental mechanisms and the associated energetics. Coarse grained methods such as Atomistic Kinetic Monte Carlo (AKMC) and Dislocation Dynamics (DD), can subsequently utilize the information from MD to model larger spatial and temporal scales. Meso-scale methods such as phase-field, cluster dynamics and crystal plasticity can further extend the length and time scales of defect evolution and interaction to polycrystalline systems. The predictions from the crystal-plasticity models can then be utilized to obtain the flow stress variations at the specimen-scale simulations. Hence in the present work, a crystal plasticity based modeling approach is being developed to quantify the interaction between irradiation induced defects and dislocations with the objective to obtain correlations between irradiation dose levels and flow stress variations in RPV steels.

In the present work, pure-iron and iron-copper model alloy systems for RPV steels are considered to quantify the effect of neutron irradiation on flow stress variation. The experimental results presented in Lambrecht et al. (2008); 2010); Meslin et al. (2010) are utilized for this purpose. In Lambrecht et al. (2008); 2010), specimens made from a RPV steel and the model alloys were irradiated around 290 °C and 15 MPa to a maximum dose-level of 0.1 dpa followed by defect and flow stress characterization. To quantify the defect type, number density and size, different techniques such as Transmission Electron Microscopy (TEM), Positron Annihilation Spectroscopy (PAS), Atom Probe Tomography (APT) and Small Angle Neutron Scattering (SANS) were used. Flow stress variations were obtained from quasi-static tensile testing performed at room temperature. Furthermore, the analytical model based on Orowan strengthening was utilized to investigate the effect of different defect types on the yield stress (Lambrecht et al., 2010). From their analysis it was concluded that the self-interstitial atomic (SIA) loops, and, vacancy and copper clusters are the strongest obstacle to dislocation motion in pure-iron and iron-copper alloys. The contribution of very small vacancy clusters to overall hardening was insignificant. These observations were included in the crystal plasticity model where the strengthening effect of SIA loops, and vacancy and copper clusters was only considered. Subsequently, the parameters are calibrated from and validated with unirradiated and irradiated microstructures and flow stress data, to establish the workability of the model.

The organization of the paper is as follows. In Section 2, the dislocation density based crystal plasticity model considering the self-interactions of dislocations and with irradiation induced defects, is presented. A comparison of the model predictions with dislocation dynamics simulation (Arsenlis et al., 2012) is presented in sub-Section 3.1. Subsequently, the model parameters are calibrated and validated for unirradiated and irradiated pure-iron and iron-copper alloys, and presented in sub-Section 3.2. Finally in sub-Section 3.3, the prediction of increase in yield strength from the crystal plasticity model is compared with an analytical model. The paper is concluded in Section 4.

2. Dislocation-density based crystal plasticity model

In the crystal plasticity model (Roters et al., 2010), the deformation gradient tensor, $\underline{\underline{F}}$, is multiplicatively split as

$$\underline{\underline{F}} = \underline{\underline{F}}^e \underline{\underline{F}}^p \tag{1}$$

where $\underline{\underline{F}}^e$ and $\underline{\underline{F}}^p$ are the elastic and plastic deformation gradients, respectively. The multiplicative split assumes an intermediate configuration where the inelastic deformation occurs through dislocation motion along specific slip systems. This configuration is subsequently stretched and rotated elastically to the current configuration by $\underline{\underline{F}}^e$. The rate of evolution of $\underline{\underline{F}}^p$ occurs through glide of dislocations along different slip systems as

$$\dot{\underline{\underline{F}}}^p = \sum_\alpha \dot{\gamma}^\alpha \underline{m}_0^\alpha \otimes \underline{n}_0^\alpha \tag{2}$$

where $\dot{\gamma}^\alpha$ is the glide rate on a slip system, α, and, $\underline{m}_0^\alpha$ and $\underline{n}_0^\alpha$ is the glide direction and plane normal, respectively, in the intermediate configuration. The glide rate on a slip system in Eq. 2 evolves following the Orowan's equation

$$\dot{\gamma}^\alpha = \rho_M^\alpha b^\alpha v^\alpha \tag{3}$$

where ρ_M^α is the density of mobile dislocation, b^α is the Burger's vector and v^α is velocity of mobile dislocations on the slip system. In this model, the density of dislocations that has the potential to be thermally activated is identified as mobile. The converse holds true for the immobile dislocation density, as discussed in Lagneborg and Forsen (1973). This is consistent with the observation that when the grains are initially deforming elastically, though none of the dislocations are moving, a finite density of dislocations have the potential to be mobile once they can overcome the barriers. These barriers could be intrinsic, such as the Peierls barrier, as well as extrinsic in the form of precipitates, parallel and forest dislocations (Ma and Roters, 2004). The v^α is defined using the activation enthalpy driven flow rule (Patra and McDowell, 2013) as

$$v^\alpha = \begin{cases} l^\alpha \nu \exp\left(-\frac{\Delta F}{K_B T}\left(1 - \left[\frac{|\tau^\alpha| - s_a^\alpha}{s_t^\alpha}\right]^p\right)^q\right) sgn(\tau^\alpha), & \text{for } |\tau^\alpha| > s_a^\alpha \\ 0, & \text{otherwise} \end{cases} \tag{4}$$

where l^α is the average dislocation glide distance between barriers, ν is the jump frequency, ΔF is the activation energy under zero stress, K_B is the Boltzmann's constant, T is the temperature in Kelvin, τ^α is the resolved shear stress, and, s_a^α and s_t^α are the athermal and thermal resistances to slip, respectively. The τ^α is related to the 2^{nd} Piola-Kirchhoff stress in the intermediate configuration ($\underline{\underline{T}}^*$) following

$$\tau^\alpha = \underline{\underline{T}}^* : \underline{m}_0^\alpha \otimes \underline{n}_0^\alpha \tag{5}$$