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Irradiation defect dispersions and effective dislocation mobility in strained ferritic grains: A statistical analysis based on 3D dislocation dynamics simulations

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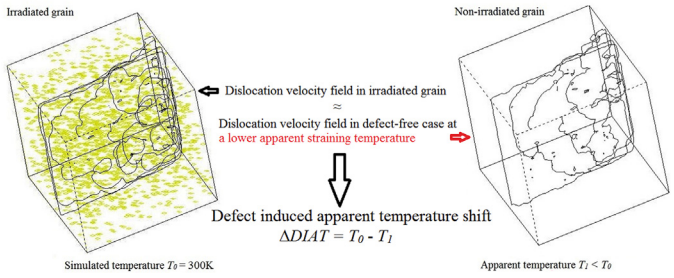
HIGHLIGHTS

- Effective dislocation mobility in presence of defects is lower than in un-irradiated grains.
- The defect-induced evolutions of the Effective dislocation mobility are interpreted using ΔDIAT concept.
- The predicted ΔDIAT levels closely replicate the ductile to brittle transition temperature shifts in various Fe-Cr materials.
- The ΔDIAT evolutions can be described using a simple dose-dependent analytical expression.
- The proposed approach in principle applies to any dispersion of hard or soft defects (e.g. precipitates, cavities, etc.).

GRAPHICAL ABSTRACT



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ABSTRACT

The influence of irradiation defect dispersions on plastic strain spreading is investigated by means of three-dimensional dislocation dynamics (DD) simulations, accounting for thermally activated slip and cross-slip mechanisms in Fe-2.5%Cr grains. The defect-induced evolutions of the *effective* screw dislocation mobility are evaluated by means of statistical comparisons, for various defect number density and defect size cases. Each comparison is systematically associated with a quantitative Defect-Induced Apparent Straining Temperature shift (or «ΔDIAT»), calculated without any adjustable parameters. In the investigated cases, the ΔDIAT level associated with a given defect dispersion closely replicates the measured ductile to brittle transition temperature shift (ΔDBTT) due to the same, actual defect dispersion. The results are further analyzed in terms of dislocation-based plasticity mechanisms and their possible relations with the dose-dependent changes of the ductile to brittle transition temperature.

1. Introduction

Ferritic steels are widely used as structural nuclear materials, thereby submitted to dose-dependent evolutions including: embrittlement, hardening, ductility loss, swelling, etc. [1–4]. These

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materials have a well-defined ductile-to-brittle transition (DBT), which strongly depends on irradiation temperature and dose [5–7]. In absence of radiation-induced defects, the temperature-dependent fracture response is ascribed to a given screw dislocation mobility level [8–10]. At fixed testing temperature T_0 however, the fracture toughness level K_0 is generally higher than its post-irradiated counterpart, K_1 [2,11]. Interestingly, the usual experimental trend curves indicate that this $K_0 \rightarrow K_1$ evolution can be replicated in a non-irradiated specimens, by depressing the test temperature $T_0 \rightarrow T_1$ (where $T_1 < T_0$). This perception implies that the fracture toughness gap $K_0 \rightarrow K_1$ (at T_0) is possibly caused by a defect-induced shift of the *effective* dislocation mobility (see Section 3.3).

It is well-known that radiation defect clusters strongly interact with mobile dislocations, according to transmission electron microscopy (TEM) observations [12,13]; molecular dynamics (MD) [14,15] and dislocation dynamics (DD) simulations [16–18]. Several grain-scale plasticity mechanisms in post-irradiated bcc metals have been conducted in the past few years [19–22]. A statistical description of dislocation mobility in presence of dispersed defects and how it possibly relates to the ductile to brittle transition temperature are missing, however. Our goal of this work is to explore the analog effect of straining-temperature and dispersed defect populations on dislocation mobility, using three-dimensional DD simulations.

This paper contains two core sections. Section 2 presents the adopted investigation methodology, including: the thermally-activated dislocation mobility rules (Section 2.1), the different simulation setups (Section 2.2), the defect-induced apparent straining temperature shift (ΔDIAT) concept (Section 2.3). Section 3 presents the DD simulation results obtained using different defect dispersions, including: the stress-strain response and dislocation density spreading (Section 3.1), the effective resolved shear stress and dislocation velocity evolutions (Section 3.2), the associated ΔDIAT trends (Section 3.3). The present results provide quantitative insight on post-irradiation plasticity mechanisms that cannot be deemed through any other existing method (see Section 3.4). This information can then be used to parametrize continuum mechanics calculations (like crystal plasticity or local approach of fracture models), for achieving a more global picture of the irradiation hardening and fracture response issues (see Ref. [23], for example).

This study however focuses on the Fe-2.25%Cr system, for which all the required data is available in the open literature. Namely: strain rate jump and temperature jump data to estimate the thermal activation input parameters and post-irradiation fracture response evolutions, to compare/validate the DD modelling (output) results.

2. Model and method descriptions

2.1. Dislocation mobility rules

The present 3D dislocation dynamics simulations were performed using TRIDIS code, where the dislocation lines are described through series of discrete linked sections, in the form of orthogonal edge and screw segments [24].

These segments glide in discrete body center cubic lattice, where the lattice spacing parameter corresponds to 10 times the Burgers vector magnitude b. The dislocation segment lengths correspond to discrete multiples of the lattice spacing, capturing the complexity of the dislocation network caused by all the implemented obstacles. The displacement of a mobile segment during a given time step is calculated according to its stress-dependent velocity. It is usually assumed that screw dislocation velocity in bcc metals is controlled by thermally activated, kink pair nucleation. The corresponding stress-velocity rule used in our DD simulations has been described in Refs. [25,26], where the screw segment velocity is given by:

$$v_{screw} = hJX' \tag{1}$$

where h is the Peierls valley width, J is the kink pair nucleation rate per unit dislocation length and X' the kink pair propagation distance before annihilation with an opposite propagating kink pair, along a screw dislocation of finite length. In practice, this length is taken as:

$$X' = \frac{X_\infty L}{X_\infty + L} \tag{2}$$

X_∞ is the average (and finite) distance swept by a kink pair before annihilation with another kink pair along an infinitely long screw dislocation; and L is the finite length of the dislocation segment considered. Distance X_∞ can be expressed as:

$$X_\infty = 2\left(\frac{v_k}{J}\right)^{1/2} \tag{3}$$

where v_k is taken as equal to the (stress-dependent) edge dislocation velocity; while J is calculated as explained in Refs. [22,25], namely:

$$J(\tau^*, T) = \frac{8\pi(\tau^*)^2}{\mu B h}\exp\left(-\frac{\Delta G(\tau^*)}{k_B T}\right) \tag{4}$$

The pre-factor appearing in Eq. (4) can be interpreted as the kink-pair area generated per unit of time; B is the viscous drag coefficient, μ is the shear modulus, k_B the Boltzmann's constant, T is the test temperature, τ^* is the effective resolved shear stress acting on the dislocation segment considered and $\Delta\Delta G$ the kink-pair formation enthalpy [22]. The latter quantity is calculated using the following («Kock's») expression:

$$\Delta G(\tau^*) = \Delta H_0\left[1 - \left(\frac{\tau^*}{\tau_0}\right)^p\right]^q \tag{5}$$

where ΔH_0 and τ_0 are the kink-pair formation energy and Peierls shear stress at 0 K. Quantities p and q characterize the shape of the thermal activation barrier, being either sharp or more gradual, with respect to τ^* variations [26].

Using fixed strain rate loading conditions means $\dot{\varepsilon} = \rho_{mobile} v b = constant$ and implies that $\Delta G(\tau^*) \approx C k_B T$ (see Eq. (4)), where quantity C is a dimensionless, material-dependent scaling factor. This condition applies at least at low straining temperature, where $L \ll X_\infty$ [26]. Inserting $\Delta G = C k_B T$ in the left-hand part of Eq. (5) and solving for τ^* yields:

$$\tau^*(T) = \tau_0\left[1 - \left(\frac{C k_B T}{\Delta H_0}\right)^{1/q}\right]^{1/p} \tag{6}$$

Quantity $\tau^*(T)$ here scales with the material yield stress evolution with temperature. The bracketed term vanishes at $T = T_{athermal}$ and then:

$$T_{athermal} = \Delta H_0 / C k_B \tag{7}$$

Inserting Eq. (7) in Eq. (5) taking $p = 0.5$ and $q = 1$ (based on atomistic calculations [27]) and differentiating with respect to T finally gives: