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Dimension reduction of defect properties for application in 2D dislocation dynamics

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ABSTRACT

In this study, a dimension reduction procedure of defect properties is proposed together with a two dimensional dislocation dynamics framework in order to simulate tensile response of the materials at different levels of external conditions such as radiation. This procedure delivers ordered pairs of strength and line density according to the changes in the geometrical properties of the defects. Plain strain deformation of irradiated oxygen-free high conductivity copper is investigated by using experimental information about the evolution of stacking-fault tetrahedra at the irradiation doses of 0–0.2 dpa.

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1. Introduction

Exposure to intense radiation fields, high temperatures, and high pressures for long periods of time are characteristics of many materials in nuclear reactors. Since their satisfactory performance is vital, modeling and simulations of nuclear materials constitute a major part in development and design.

Face-centered cubic (FCC) materials are also in the service of nuclear industry for their beneficial properties such as high thermal and electrical conductivity. The micromechanical properties of FCC materials have been investigated by many experiments [1–6]. Below the limit of $0.3T_m$, where T_m is the melting temperature, major irradiation-induced defects in FCC materials are stacking-fault tetrahedra (SFT), dislocation loops, and vacancies [3,5]. Beyond $0.3T_m$, aggregation of vacancies results in the formation of voids. Including the presence of the precipitates [7–9] in the alloys, these defects behave as an obstacle for dislocations and change the yield strength [4–8]. Plastic deformation due to irradiation-induced defects is the basic aspect to model failure of the nuclear materials.

In the present study, a dimension reduction procedure that will fit on 2D dislocation dynamics (DD) [10] is proposed in order to represent multi-type defects. In Section 2, a brief description of 2D DD framework is present. Section 3 describes the determination of average 2D profile by using Delesse Principle and its adaptation to the formulations of defect strength. Section 4 introduces the notion of line density and spacing based on Rosiwal Principle. Finally, in Section 5, tensile response of oxygen-free high conductivity (OFHC) copper under the condition of plain-strain deformation, is presented by using experimental defect data [6] for the irradiation levels of 0–0.2 dpa.

2. 2D DD model

A 2D DD [10] framework, which is illustrated in Fig. 1 is proposed to perform simulations for the constitutive behavior of irradiated materials. This model is based on plain strain deformation with small strain approximation where three slip systems with only edge dislocations (⊥) exist. Dislocations are generated in the form of dipole via Frank–Read (FR) sources (◯), and edge dislocations are allowed to move, annihilate, pin and release at obstacles (•) on slip lines which are the side view of slip planes. Each slip line is impenetrable in order to give the effect of grain boundaries. Although 2D DD is a simplified model in terms of dislocation motion, reduction of slip planes to slip lines complicates the representation of heterogeneous materials. Together with the absence of classification based on defects, this problem concludes the arbitrary selection of fundamental terms such as density and strength of the defects [10–14]. In order to realize a more accurate description, 3D geometrical properties of defects may be translated to the basis of 1D information, since edge dislocations move on slip lines. A dimension reduction procedure for representation of defects in 2D DD requires two main phases. In the first phase, adaptation of defect strength formulations to 2D DD computational cell is accomplished by the illustration of an average 2D profile assuming that 2D average spacing is preserved inside the

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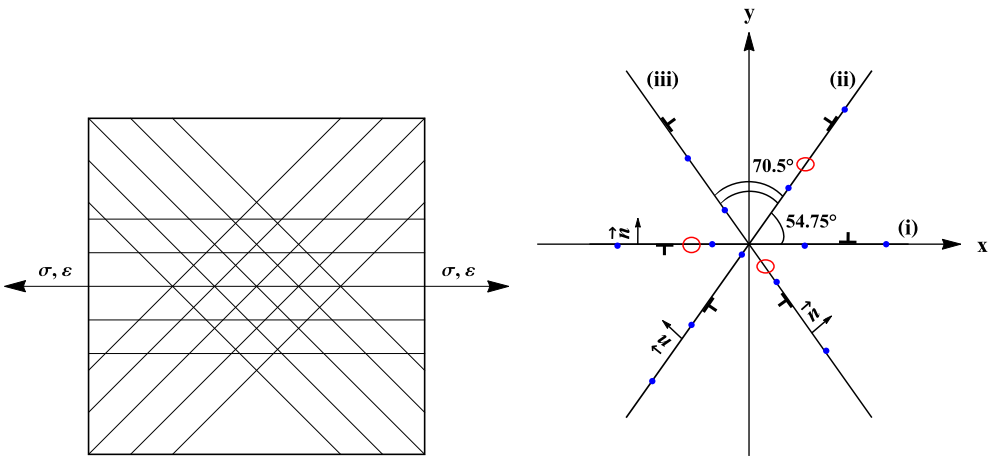

Fig. 1. DD unit cell model (left) for the tensile response. A grain has three slip systems (right) on which dislocations (⊥) can be generated from sources (◯), can glide and be halted by obstacles (•).

geometrical cell. In the latter phase, determination of intersections between slip lines and defects finalizes the procedure with the acquisition of necessary information to represent defects on the path of dislocations.

3. Strength of defects

Defects may block moving dislocations if their resistance is greater than the absolute value of resolved shear stress of interacting dislocation. Theories developed for defect strength in mesoscale simulations are based on the estimates of line tension in a generic dislocation as it propagates through a dispersion of 2D objects over its glide plane. As a consequence, strength of obstacles is a function of 2D spacing between defects. In this section, current formulations of barrier strength are modified according to 2D profile which is obtained by a slicing process.

First type of defects, on which slicing is applied, are the precipitates which are elementary defects in any alloy. Although precipitates exist in various shapes, they can be considered as spherical objects in a first approximation. The basic information that may be provided by using experimental or computational techniques is the density of these precipitates which is defined as:

$$\rho^{3D}_{Objects} = \frac{\text{Number of objects}}{\text{Volume}} \tag{1}$$

Since Eq. (1) doesn't give sufficient detail about the geometrical properties such as total volume, an additional expression is required to achieve further steps. Herein, fraction is the ideal expression that supplies the missing information in Eq. (1). N such precipitates of an average radius R inside a representative cubic volume of edge size W correspond to a volume fraction given by:

$$P_{3D} = \frac{4}{3} N \pi \left(\frac{R}{W}\right)^3 \tag{2}$$

After the determination of necessary terms in 3D, next step is to precise the effects made by slicing on 2D. It is trivial that discs will be generated by slicing a sphere as illustrated in Fig. 2 (left). If m discs are present on a square area of edge size W, then introduction of a fraction between the total area of m discs and square cross-section yields:

$$P_{2D} = m\pi \left(\frac{R^{2D}}{W}\right)^2 \tag{3}$$

The average radius of the discs is different from the radius of the spheres due the slicing process. The relation between R and R^{2D} is determined by averaging over the sphere:

$$R^{2D} \approx \frac{1}{\pi}\int_0^{\pi} R\sin\theta d\theta = \frac{2}{\pi}R \tag{4}$$

When one performs infinitely many slices, both areal fraction on the cross-section and volumetric fraction are expected to be equal. This conservation is called Delesse Principle [15–19] and states that:

$$P_{2D} = P_{3D} \tag{5}$$

Equivalence of fractions is a constraint which gives a chance to determine the number of objects in 2D. Practically, it is possible to express m in terms of 3D quantities using Eqs. (2), (3), and (5):

$$m = \frac{1}{3} N \pi^2 \frac{R}{W} \tag{6}$$

Since the average number of discs that should be present on 2D cross-section is identified, 2D density gets the following form with 3D geometrical inputs:

$$\rho^{2D}_{Discs} = \frac{\pi^2}{3}\rho^{3D}_{Spheres} R \tag{7}$$

Eq. (7) may be considered as the final step of transition from 3D to 2D because, not only density is calculated but also the average distance between the discs is characterized. Thus, the average spacing between discs is approximated via:

$$L_{Discs} \approx \frac{1}{\sqrt{\frac{\pi^2}{3}\rho^{3D}_{Spheres} R}} \tag{8}$$

Eventually, the completion of calculations enables to describe an average 2D profile in Fig. 3 (left). One should also note that 2D spacing calculated via Eq. (8) is conserved inside the picture.

Determination of 2D geometrical quantities permits to calculate the strength of precipitates. Many formulations developed for precipitate hardening overestimate the strength values in comparison to DD simulations. Hence, it has been shown [20] that the Orowan strengthening due to the presence of precipitate is consistently modeled by the Bacon, Kocks, and Scattergood (BKS) approximation [21]:

$$\tau_{precipitates} = \frac{A\mu b}{L_{Discs}}\left[\ln\left(\frac{\overline{D}}{r_0}\right) + B\right] \tag{9}$$

where relative diameter due to Orowan loop, $\overline{D}$, is given by:

$$\overline{D} = \left(D^{-1} + L^{-1}_{Discs}\right)^{-1} \tag{10}$$

If parameters of BKS formula are investigated, A is a coefficient depending on the character of the dislocation, $A = 1/2\pi(1-\nu)$ for

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