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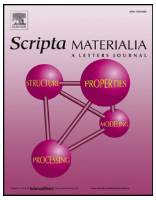

Suppression of Localized Plastic Flow in Irradiated Materials

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ABSTRACT

Suppressing deformation localization caused by dislocation channels is crucial in the reliable service of irradiated materials. Through 3D Discrete Dislocation Dynamics simulations, the evolution of deformation localization extent is quantitatively studied, and the effect of internal dislocation structure and slip mode are revealed. Results show that to inhibit dislocation channel formation, the material is required to be pretreated so as to enhance short-range dislocation interactions. This can be attained by introducing a homogeneously dense dislocation structure before irradiation, and by loading along orientations that activate multiple slip systems. Implications for the design of radiation-resistant materials are discussed.

Reliable operation of structural materials in nuclear energy requires resistance to irradiation-induced failure. One of the vexing problems is the localization of plastic flow in very narrow regions called dislocation channels (DC) [1-5]. Such deformation localization is believed to be an important origin of catastrophic fracture and irradiation-assisted stress corrosion cracking [6]. Therefore, a deeper understanding of the DC formation mechanisms and conditions is critical for lifetime extension of nuclear reactors.

One universally observed feature is that DC is easy to form at high irradiation dose [7-10]. However, the irradiation dose depends on the service environment, which cannot be easily changed. On the other hand, the state of irradiated materials, such as the initial dislocation structure or the loading orientation, can possibly to be controlled. A clearer understanding of the influence of the material microstructure and loading mode on DC may shed light on designing radiation-resistant materials. However, and until recently, microstructure parameters that affect DC formation remain largely unknown.

Numerous Molecular Dynamics (MD) simulations have recently revealed atomistic details of individual irradiation defect-dislocation interaction mechanisms [11-14]. Such studies help in gaining a fundamental understanding of the mechanisms responsible for the partial damage or complete destruction of irradiation defects by gliding dislocations. However, due to computational restrictions on the simulation time and spatial scales, collective interactions between irradiation defects and dislocations are not currently possible with MD studies alone. Under such circumstances, recourse to large-scale, continuous crystal plasticity models have been used [15-19]. These continuum studies have helped in understanding of irradiation hardening and channel formation in bulk irradiated materials, but various ad-hoc assumptions are included. To avoid this restriction, mechanism based Discrete Dislocation Dynamics (DDD) simulations have become a natural choice. Nevertheless, dealing with the huge amount of irradiation defects that have characteristic size that is much smaller than a typical dislocation segment length in DDD is not trivial [14]. Therefore, only limited computational DDD research on DC formation has been reported till now [4, 9, 20, 21]. To make further advances in the computational capabilities of DDD, we recently developed a model which couples DDD with a continuum irradiation defect field model [10] by coarse-graining dislocation-irradiation defect interactions. The model is an efficient and effective method to investigate the DC formation problem, without losing microscopic details [10,22]. This raises the possibility of revisiting the influence of the microstructural state and loading mode on DC formation.

The investigative tool employed here is the MoDELib (Mechanics of Defect Evolution Library) computer code [23] built on the theoretical foundations of the parametric variational method, described in detail in our previous papers [24,25]. In the present study, a series of DDD simulations of the tension test are performed on irradiated Fe single crystal pillars. Since previous work showed that a sample with

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edge length 1.3 μm is capable of capturing bulk-like DC formation behavior [9], the simulated sample here is of 1.5 μm diameter and 3.0 μm height. An atomistically-informed dislocation mobility law for bcc crystals is used [26]. The material parameters are given in [27], and model details are described in detail in [10]. Similar to the experiments reported in reference [28], the 7.5×10^{-3} dpa and 3.75×10^{-1} dpa irradiation doses are considered at a temperature of 320 K. These conditions correspond to initial irradiation defect densities of N_0 1×10^{21} m^{-3} and 3×10^{22} m^{-3} in irradiated Fe, respectively. For simplicity, hereafter we will call these two doses as low-dose (Low N_0) and high-dose (high N_0), respectively [28]. To reveal loading mode effect, simulations of tensile loading tests along the [001] and $[\bar{2}35]$ directions are performed to achieve multi-slip and single-slip conditions. To disclose the role of the initial dislocation structure, a range of initial dislocation densities ρ_0 $(0.3 \sim 10) \times 10^{12}$ m^{-2} are considered. We will call ρ_0 $(0.3 \sim 2) \times 10^{12}$ m^{-2} as low ρ_0, and other density as high ρ_0 to facilitate discussions.

To quantitatively characterize the extent of deformation localization, a "deformation localization index" (DLI) is used. This is defined as the percent of the volume with plastic strain that is lower than the volume average $(\overline{\gamma}^p)$ [22]. A value of DLI=0 corresponds to perfectly homogeneous deformation, while DLI is close to 1 means that deformation is highly localized. Therefore, the observation of a clear DC generally corresponds to a higher DLI [22]. As one example, Fig. 1 (a) shows two sets of DLI evolution during plastic deformation in low-dose and high-dose irradiated Fe pillar with low ρ_0 and [001]-orientation. It demonstrates that under low-dose conditions, DLI first decreases and then stabilizes without the appearance of a clear DC (see Fig. 2 (e)). The plastic strain for reaching relatively stable DLI is dependent of the initial dislocation microstructure. In contrast, for the high-dose case, the DLI first decreases and then increases as DCs are more clearly formed (see curve #2 and microstructure C and D). After DCs are well-developed, the DLI exhibits a very slow decrease due to a gradual widening of DCs and some dislocation activities outside them (see stage AB in curve #1 and microstructure A and B in Fig. 1 (a)). Several observations are consistent with experiments [5, 28-30]. First, DCs only appear under high dose irradiation. Second, the critical strain of observing clear DCs is low (see point A and D in

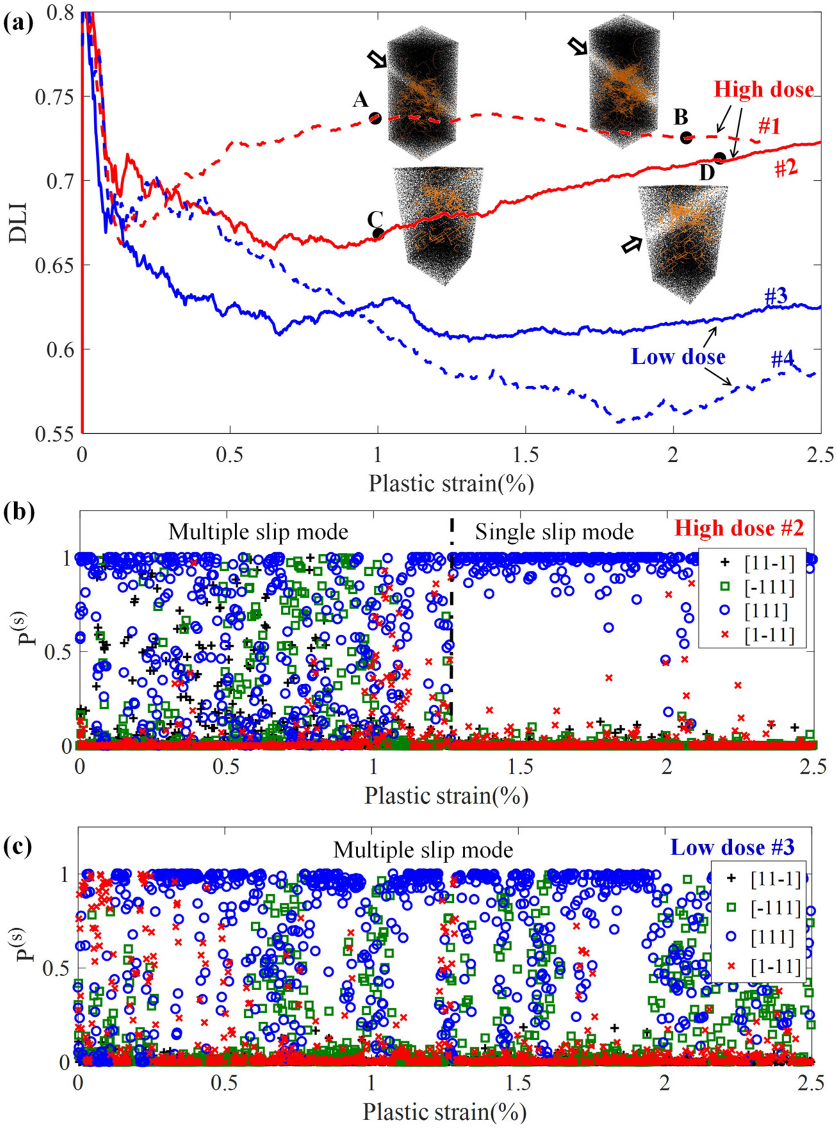

Fig. 1. Typical simulation results for irradiated Fe pillars with d=1.5 μm when loading is along the [001]-direction. (a) Evolution of the deformation localization index (DLI). The insets in (a) are snapshots of irradiation defect (dark grey dots) and dislocation configuration s (orange lines) corresponding to the marked points. Hollow arrows indicate a dislocation channel. (b-c) Evolution of plastic strain rate fraction $P^{(s)}$ induced by dislocations with different Burgers vectors under high-dose and low-dose conditions, respectively.