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Atomic-scale modeling of clear band formation in FCC metals

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Abstract

Molecular Dynamics simulations are employed to simulate at the atomic scale the interactions between dislocations and several irradiation defects in FCC crystals: glissile interstitial loops, stacking fault tetrahedra and interstitial Frank loops. The simulations reveal different interaction mechanisms (absorption, unfaulting and shear), depending on the nature and shape of the defects and show that athermal cross-slip events are systematically involved when screw dislocations are considered. In the case of Frank loops, the classical unfaulting mechanism is observed but is not the general rule, defect shearing being more frequent than usually assumed. Consequences of these observations on clear band formation are discussed.

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1. Introduction

It is well established that metals irradiated at low temperature (typically below half their melting temperature) generally deform inhomogeneously [1,2]: the deformation is localized in shear bands which are called clear bands (or defect-free zones) because, after deformation, they are clear of all irradiation defects visible in transmission electron microscopy (TEM).

Clear bands are a common feature of deformed irradiated metals, since they are observed in all crystallographic structures and irradiation microstructures. For example, in the case of FCC metals of specific interest here, clear bands develop in copper where the microstructure is dominated by vacancy-type stacking fault tetrahedra [3] and in austenitic steels where the microstructure is mainly composed of interstitial Frank loops [4]. Note also that clear bands develop both in single and polycrystals, and are observed without irradiation, for example, in the case of alloys hardened by coherent shearable particles [2]. Clear bands have a width independent of the strain rate and the deformation, which therefore proceeds by a

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multiplication of the clear bands and a corresponding decrease in the spacing between them. As a reference, in metals deformed to a neutron dose of $10^{18}\,\mathrm{cm}^{-2}$ and extended by 4% at 293 K, channels have a width of 0.15 μm and a spacing of 2.5 μm. The shear in the bands is high, 0.5 μm, corresponding to the passage of several thousand dislocations, or said in other words, to the passage of two to three dislocations per slip plane, assuming homogeneous deformation in the clear bands [1].

Disappearance of the irradiation defects from the shear bands means that the mobile dislocations remove the defects in the course of their glide, which can occur by three mechanisms. The first possibility is a *Drag* of the defects, either via long-range elastic interactions or after absorption of the defects in dislocation cores. Drag is possible only with edge dislocations, which locally climb with the formation of jogs or superjogs, and not with screw dislocations, since in the latter case, a helical turn would form on the dislocation line that would pin the screw dislocation because it can glide only in the Burgers vector direction and not in the glide direction. The second mechanism involves a *Transformation* of the defects: they may react with dislocations and transform into less-pinning defects. An example is the well known unfaulting of Frank loops, which are transformed into glissile prismatic loops [5]. The third possibility is the *Shear* of the defects, as in the case of precipitate-hardened alloys. The defects have then to be sheared by the moving dislocations until they are too small to be visible in TEM, or until they become unstable and/or are absorbed in the dislocation cores.

Clear band formation is usually attributed to the *drag* of glissile defects and the *transformation* of sessile defects into glissile ones, generally involving unfaulting of the latter. It is in particular the case for Frank loops [1,6] and SFTs [7].

In order to understand the interplay between these mechanisms, atomistic information and atomic-scale Molecular Dynamics (MD) simulations are required. The reason is that all three mechanisms (except for long-range drag) involve contact and short-range core interactions between the dislocations and the irradiation defects, which can be modeled with precision only by means of atomic-scale simulations. Also, all TEM studies of clear band formation report traces of cross-slip which is another atomic-scale core process [1,8]. Finally, irradiation defects are at the atomic scale, since their size and relative separation are in the range of a few nanometers. For example, SFTs in irradiated copper have an average size of $2.5\,\mathrm{nm} \pm 0.5\,\mathrm{nm}$ and an average separation of 20 nm [3]. These defects can therefore be simulated at the atomic scale, by MD, with realistic dimensions, taking advantage of the actual computational speed and computer storage capacity.

Several irradiation defects have been studied using similar MD techniques, mostly in FCC crystals. The defects considered are small glissile interstitial loops [9,10], SFTs [11,12] and more recently, interstitial Frank loops [13,14]. The aim of the present article is to review the main results of these studies. They show that all three interaction mechanisms mentioned above are encountered, depending on the nature of the defects, will pay a particular attention to interstitial Frank loops, where the classical unfaulting mechanism is observed at the atomic scale, assisted by athermal cross-slip events. However, we show that this mechanism is not the general rule. Instead, depending in particular on the shape of the loop, shearing is observed and appears, from the simulations, to be more frequent than generally postulated.

In Section 2, we present the main characteristics of the MD simulations and particularly the boundary conditions. In Section 3, we review the simulations on glissile interstitial loops and SFTs. In Section 4, we focus on interactions between screw dislocations and Frank loops, and in Section 5, we consider the case not studied up to now, of screw dislocations in interaction with SFTs. Finally, in Section 6, we discuss the implications of the present simulations on our understanding of clear band formation.

2. Computational model

Classical MD techniques are used, with only two items specific to the present simulations: the