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Towards further understanding of stacking fault tetrahedron absorption and defect-free channels – A molecular dynamics study

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HIGHLIGHTS

- Stacking fault tetrahedron (SFT) is fully absorbed by screw dislocation.
- Absorbed SFT becomes moveable with the aid of Lomer dislocations.
- Finally SFT is removed from the specimen or from defect-free channels.
- Two scenarios responsible for the formation of defect-free channels were proposed.

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ABSTRACT

The mechanisms leading to stacking fault tetrahedron (SFT) absorption via interactions with dislocations, and subsequent formation of plastic flow localization in defect-free channels, which were frequently observed in irradiated materials in transmission electron microscopy experiments, are still unclear. To address this, screw dislocation interactions with SFTs in copper were investigated using molecular dynamics (MD) simulations. The interaction details reveal that a screw dislocation can fully absorb an SFT through the thermally activated transformation of Lomer–Cottrell lock into Lomer dislocations. After absorption, almost all the vacancies in the SFT are transferred into Lomer dislocations, which are able to move transversely under complex loading conditions. As a result, SFTs can be removed from the material (for SFTs near surface) or from defect-free channels (for SFTs in the bulk) with the aid of Lomer dislocations. In addition, it was shown that this absorption process is favorable only at high temperature, low applied shear stress and/or high SFT density. These results are in good agreement with *in situ* TEM observations. The current simulations and analyses provide useful insights into the formation mechanisms of defect-free channels in irradiated materials.

1. Introduction

The structural integrity of materials operating in an irradiation environment is of utmost importance for maintaining the outstanding performance of components as well as to guarantee safety requirements. For instance materials used in nuclear power plants need to demonstrate superior properties including irradiation-resistance, corrosion-resistance, and high strength. Irradiation can significantly change the micro structure of metallic materials by the formation of voids, stacking fault tetrahedrons (SFTs), and Frank loops. These defects degrade and reduce the material lifetime, due to irradiation-induced hardening, ductility loss and irradiation-induced creep [1–3]. Thus, the demand for accurate models, that can predict the mechanical behavior of materials exposed to irradiation, is of utmost importance.

Frank loops and SFTs are two important defects in irradiated metals, depending on the material character [3–8]. Generally speaking, in the stainless steels (304 and 316), Frank loops are usually observed after irradiation. Irradiation of metals with low stacking fault energy, e.g. copper and gold, results mainly in the formation of very dense SFTs (10^{22}–10^{24} m^{-3}) [5,9,10]. It has been experimentally observed that, during the plastic deformation process of almost all the irradiated metals, SFTs are removed via interactions with dislocations, and lead to the creation of defect-free channels [11–15]. Subsequent dislocations are able to glide freely

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in these channels, leading to plastic flow localization and ductility loss [16]. So far, the interactions between Frank loops and dislocations, as well as Frank loop-free channels have been studied widely [4,17–21]. On the other hand, fewer efforts have been devoted to the SFT-related research, and some basic questions on dislocation–SFT interactions are still open or even under dispute.

In situ straining experiments revealed that dislocation interactions with SFTs result in many different phenomena, including SFT complete absorption [6,22,23]; SFT partial absorption resulting in a smaller SFT [6,24,25]; SFT destruction leaving a super jogged dislocation [22,23]; and SFT collapse into a triangular Frank loop via the inverse Silcox–Hirsch mechanism [22]. These experimental observations provide useful insights into the formation of defect-free channels in irradiated materials. However, the irradiation-induced and quenching-induced SFTs are so small that it is difficult to identify the interaction details clearly [6,22]. On the other hand, molecular dynamics (MD) simulations are capable of reproducing *in situ* interaction processes, and consequently have been widely used to explore the interaction mechanisms between dislocations and SFTs [26–32]. These simulations showed that the results of the dislocation–SFT interactions depend on the dislocation character as well as the position at which the dislocation intersects the SFT. Osetsky et al. [28,33] showed that an edge dislocation cutting an SFT leaves ledges on the SFT faces. They also showed that a sequence of edge dislocations separates an SFT into a smaller SFT and a vacancy cluster. In addition, screw dislocation can cross slip on the SFT face and transform the SFT into a smaller one with a truncated base [34,35]. On the other hand, a sequence of four screw dislocations was shown to shear the SFT into two separate defects, namely a smaller perfect SFT and a partially dissociated Frank loop. Furthermore, Lee and Wirth [30] studied the interaction between a 60° mixed dislocation and an SFT and concluded that the inverse Silcox–Hirsch process occurs when the 60° dislocation approaches the SFT from its base plane, which agrees well with TEM observations [22]. Finally, a number of discrete dislocation dynamics (DDD) simulations have also been performed to gain insights into the dislocation–SFT interaction mechanisms [36–40,41].

Although full SFT absorption through interaction with a gliding dislocation has been frequently observed in experiments [6,22,23], the details of this process are still unclear. The Kimura–Maddin model [42] remains the most common to explain this absorption process [22]. However, some dislocation reactions described by this model are not favorable [34,39,43,44], and so far no MD or DDD simulations have been able to confirm this model. A recent special case study by Fan and Wang [27] showed that a screw dislocation intersecting an SFT at its base plane can completely annihilate the SFT under a shock shear stress. However, the dislocation was observed to be pinned at the end of the annihilation process and questions still remain on how subsequent increases in the applied stresses will affect the outcome of this interaction. Further, this interaction with the SFT base plane is a very specific configuration with small probability of occurrence, and the details of the general interaction process still are missing. It is also worth noting that in most previous MD simulations, the interactions between dislocations and other defect clusters (SFTs, Frank loops, voids and so on) were usually performed under simple planar shear conditions. Nevertheless, complex loading conditions are rarely studied, which are very common in *in situ* TEM experiments.

In order to address the formation mechanisms of defect-free channels, here we perform detailed MD simulations that shed light on the complete SFT absorption process by a screw dislocation intersecting an SFT face under more realistic loading conditions. In addition, the influences of temperature, boundary condition, loading condition, and SFT density on the interaction are also discussed. The paper is organized as follows. The computational method is discussed in Section 2, and the simulation results are presented and discussed in Section 3. Finally, concluding remarks are made in Section 4.

2. Computational method

The simulations performed here employ the three-dimensional MD code LAMMPS [45]. The embedded-atom method (EAM) potential chosen for these simulations is the one developed for copper by Mishin et al. [46]. This potential accurately predicts the properties of copper crystals, especially the stacking fault energy. All atomic configurations are visualized using Atomeye [47], and atoms are colored based on their atomic centro-symmetry parameter [48]. The simulation cells are parallelepiped cells shown schematically in Fig. 1. The *x*-, *y*-, and *z*-axes are oriented along the $[\bar{1}\,\bar{1}\,\bar{1}]$, $[\bar{1}\,1\,0]$, and $[1\,1\,\bar{2}]$ directions, respectively. Unless otherwise stated, the cell dimensions are l_x = 29.8 nm, l_y = 23.8 nm, and l_z = 40.0 nm along the three coordinate directions, and the initial distance between the dislocation and SFT is 31.3 nm. The resulting SFT density in the simulation volume is $3.52 \times 1022\ \mathrm{m}^{-3}$, which is equivalent to those reported experimentally for irradiated copper [5]. The dislocation slip plane is 1.9 nm above SFT base plane in all simulations, and subsequently the dislocation comes into contact with the SFT face "ABD".

An SFT is introduced into the simulation cell by first employing periodic boundary conditions along the *y*-direction only, followed by removing 276 atoms within a triangular platelet on the $(\bar{1}\,\bar{1}\,\bar{1})$ plane, and then relaxing the system. This leads to the generation of an SFT with an edge length of 6.0 nm. A screw dislocation having Burgers vector $b = a/2[\bar{1}\,1\,0]$ is then introduced into the simulation cell by fixing atoms in regions-II, -III, and -IV (see Fig. 1), and applying a positive velocity in the *y*-direction on atoms in region-I until the total displacement is equal to the magnitude of the Burgers vector, *b* [49,50]. Periodic boundary conditions are then imposed along the *y*- and *z*-directions, while the two surfaces along the *x*-direction are free. Finally, all atoms in the simulation cell are relaxed again before subsequent heating and loading. In order to study the influence of boundary conditions on the interaction, free surface boundary conditions along the *y*-axis are also employed in some simulations (see Section 3.2).

In order to simulate the interaction at high temperatures, the system is heated up to 400 K and 600 K, respectively, and the temperature is maintained using the NVT ensemble throughout the simulation. A shear stress τ_{xy} is applied to drive the screw dislocation towards the SFT, by constraining all the atoms within 0.9 nm from the upper and lower surfaces in the *x*- and *z*-directions, while

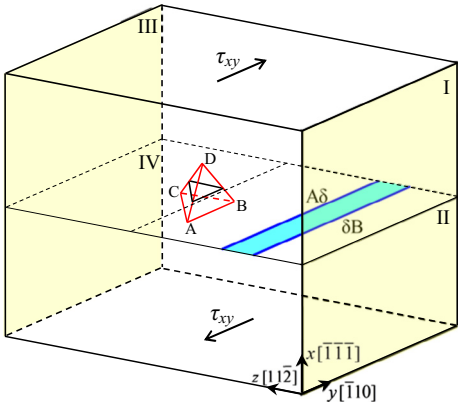

Fig. 1. Simulation volume schematic showing a dissociated screw dislocation with partials "Aδ" and "δB", and an SFT "ABCD". Under the applied load τ_{xy}, the screw dislocation will glide towards the SFT face ABD.