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Dynamic observations and atomistic simulations of dislocation–defect interactions in rapidly quenched copper and gold

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Abstract

Dislocation interactions with quenched-in defects, which are either partial or complete stacking-fault tetrahedra, in copper and gold have been studied by combining static and dynamic transmission electron microscope studies with molecular dynamics computer simulations. The interaction of a dislocation with a stacking-fault tetrahedron can result in the tetrahedron being sheared into two defects, converted to another defect type, or annihilated. These observations provide insight into defect interaction and annihilation mechanisms that are responsible for creating the defect-free channels in deformed irradiated material.

Keywords: In situ TEM; Stacking-fault tetrahedron; Dislocation interactions; Molecular dynamics simulations; Defect-free channels

1. Introduction

In the early stages of deformation of irradiated materials, dislocations emitted from grain boundaries and other localized regions of high stress concentration interact with and destroy radiation-induced defects to create the commonly observed defect-free channels [1–4]. Although the presence of these channels in a wide range of materials is well documented, the atomistic processes responsible for defect annihilation due to the interaction with dislocations [5–11] have not been experimentally verified. In low stacking-fault energy face-centered cubic (fcc) materials, most of the proposed annihilation mechanisms involve the generation of a Shockley partial dislocation that sweeps across the defect, thereby annihilating the stacking fault and converting the defect into a perfect dislocation loop that can be either absorbed by the slip dislocation or left behind. The interactions depend on the geometry of the interaction, as well as the character of the defects involved. A few of the possible interactions are reviewed here to illustrate the possibilities.

Screw dislocations, due to their ability to cross-slip, are efficient at annihilating non-coplanar Frank loops as first proposed by Silcox and Hirsch [12] and illustrated in Fig. 1; for convenience, the dislocations and slip planes are described using Thompson's notation employing the definition of handedness as given in Hirth and Lothe [13]. In Fig. 1, a right-handed screw dislocation with Burgers vector AB is mobile on the (*d*)-plane. It encounters a Frank loop with Burgers vector $C\gamma$, cross-slips onto the (*c*)-plane and dissociates into the partial dislocations $A\gamma + \gamma B$ (Fig. 1(b)). These partial dislocations move across the loop eliminating the fault and these interact with $C\gamma$ to produce perfect segments of Burgers vector BC and AC, according to the reactions $B\gamma + \gamma C = BC$ and $A\gamma + \gamma C = AC$ (Fig. 1(c)). The segments of dislocation AB outside the loop cross-slip from the (*d*)- to the (*c*)-plane and move toward points A and D, respectively (Fig. 1(d)). The dislocation segments comprising the loop collapse towards point C as indicated by the successive dislocation positions in Fig. 1(e). The result is the helical dislocation shown in Fig. 1(f).

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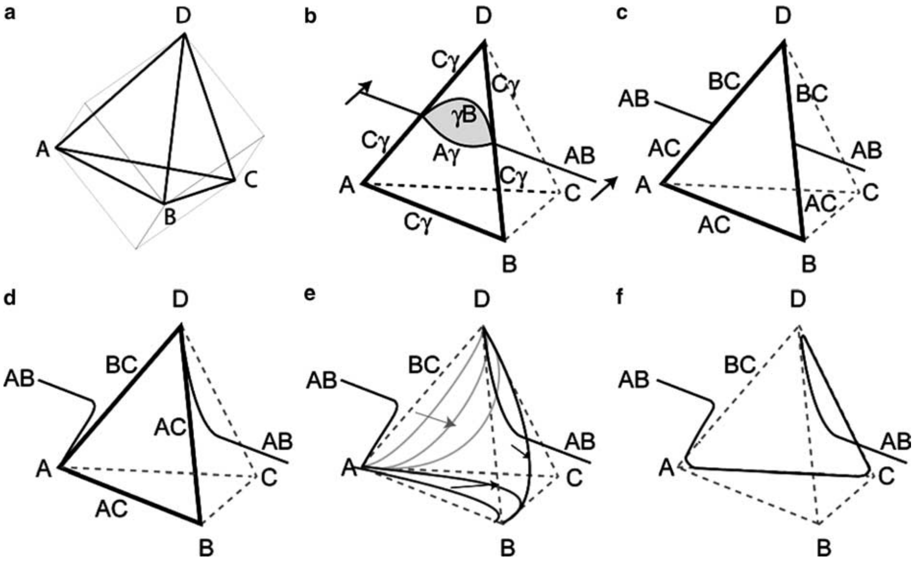

Fig. 1. Interaction of a right-handed screw dislocation with a Burgers vector AB with a Frank loop with a Burgers vector Cγ. The loop is annihilated by the interaction and the dislocation assumes a helical form. The relationship between the line direction and Burgers vector follows the convention detailed in Hirth and Lothe with observation from outside the tetrahedron.

Stacking-fault tetrahedra, found in low stacking-fault energy materials following neutron irradiation or thermal treatments of quenching from high temperature with lower temperature annealing, are formed from Frank loops through the Silcox–Hirsch mechanism [12]. Fig. 2 shows an example of the mechanism, proposed by Kimura and Maddin [9], for the unfaulting and annihilation of a stacking-fault tetrahedron through interaction with a screw dislocation. The pure screw dislocation has a Burgers vector AB and slips on the (*d*)-plane. It intersects the stacking-fault tetrahedron on the (*c*)-plane and dissociates into the partial dislocations Aγ and γB (Fig. 2(a)). It is important to note that if this plane was not faulted, the Burgers vectors Aγ and γB on the (*c*)-plane would be the same as the matrix and not reversed as shown. Assuming the partial γB moves toward D and eliminates the fault as it moves, it intersects the stair rod partial dislocations at FD and ED, and produces dislocations αB and βB according to the reactions $\alpha\gamma + \gamma B \rightarrow \alpha B$ and $\beta\gamma + \gamma B \rightarrow \beta B$, respectively. The partial αB is glissile on the (*a*)-plane and its motion eliminates the fault on that plane. It interacts with βα along DC to produce βB, with γα along FB to produce

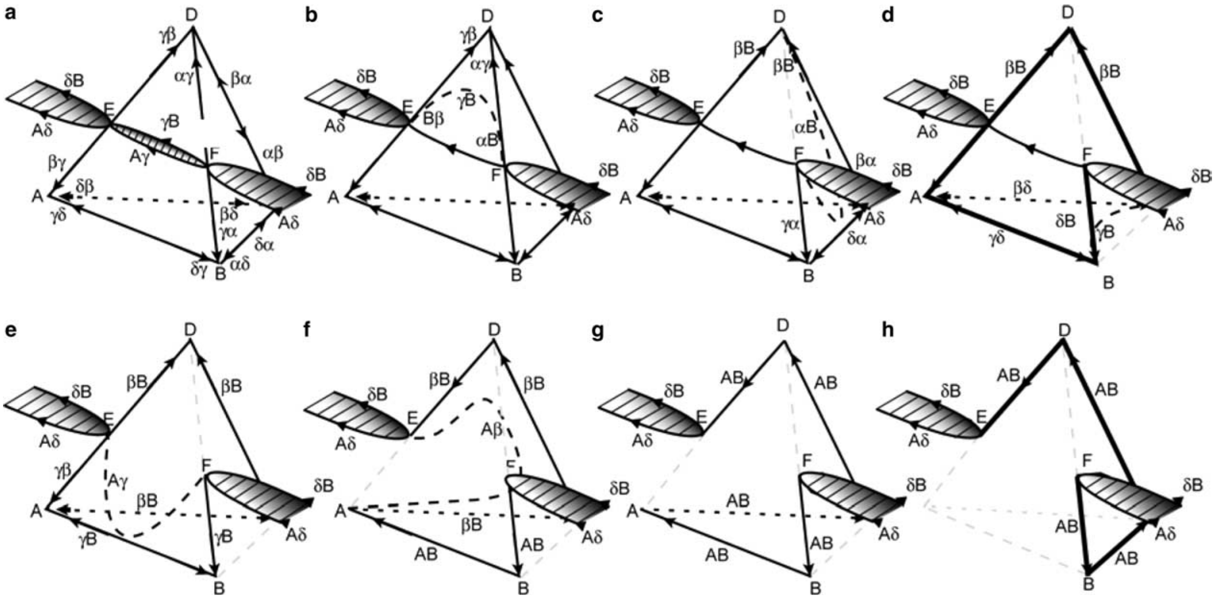

Fig. 2. Interaction of a left-handed screw dislocation with Burgers vector AB with a stacking-fault tetrahedron. The initial interaction occurs on the (*c*)-plane. The relationship between the line direction and Burgers vector follows the convention detailed in Hirth and Lothe with observation from outside the tetrahedron.