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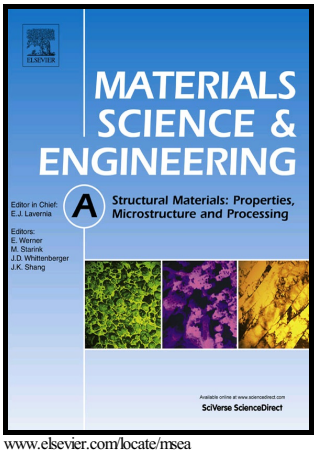

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Stacking fault tetrahedron induced plasticity in copper single crystal

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Abstract

Stacking fault tetrahedron (SFT) is the most common type of vacancy clustered defects in fcc metals and alloys, and can play an important role in the mechanical properties of metallic materials. In this study, molecular dynamics (MD) simulations were carried out to investigate the incipience of plasticity and the underlying atomic mechanisms in copper single crystals with SFT. Different deformation mechanisms of SFT were reported due to the crystal orientations and loading directions (compression and tension). The results showed that the incipient plasticity in crystals with SFT resulted from the heterogeneous dislocation nucleation from SFT, so the stress required for plastic deformation was less than that needed for perfect single crystals. Three crystal orientations ([1 0 0], [1 1 0] and [1 1 1]) were specified in this study because they can represent most of the typical deformation mechanisms of SFT. MD simulations revealed that the structural transformation of SFT was frequent under the applied loading; a metastable SFT structure and the collapse of SFT were usually observed. The structural transformation resulted in a different reduction of yield stress in compression and tension, and also caused a decreased or reversed compression/tension asymmetry. Compressive stress can result in the unfaulting of Frank loop in some crystal orientations. According to the elastic theory of dislocation, the process of unfaulting was closely related to the size of the dislocation loop and the