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Interaction between Dislocation and Coherent Twin Boundary by quasicontinuum model

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ABSTRACT

The mechanical strength of polycrystalline materials is greatly affected by the structures of dislocations, grain boundaries and the dislocation–grain boundary interactions.

The interaction between lattice dislocations and coherent twin boundary Σ3 {111} of copper has been studied using the quasicontinuum method. It appears that the coherent twin boundary provides high barrier to slip transmission. We show three interaction mechanisms between the dislocations and this grain boundary (pile-up, dissociation and transmission through twin grain boundary).

The dislocation pile-up modifies the stress field at its intersection with the grain boundary. A different reaction process compared with the case of single dislocations is noticed. One observes the nucleation of a Lomer-type dislocation with Burgers vector of ½ <110 > and glides on the (100) cube plane in the adjacent grain. This phenomenon has been observed with Transmission Electron Microscopy at room temperature [1,2] and in other Molecular dynamics simulations [3].

We show also a novel interaction mechanism between Lomer-type dislocation and Twin Boundary. This penetration process leaves a glissile dislocation with Burgers vectors coincident with the Displacement Shift Complete lattice of twin boundary.

A quantitative estimation of critical stress for various transmission phenomena is performed by using the virial stress. Such information can be used as input for Dislocation Dynamics models.

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