ATOMISTIC SIMULATIONS OF BAUSCHINGER EFFECTS OF METALS WITH HIGH ANGLE AND LOW ANGLE GRAIN BOUNDARIES

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In this paper, we examined Bauschinger effects in nickel single crystals and nickel containing arrays of high angle or low angle grain boundaries under shear deformation using molecular dynamics with Embedded Atom Method (EAM) potentials. In order to take into account dislocation nucleation under different boundary conditions and their effects on the stress-strain relationship, two limiting constraints were used to both high angle and low angle grain boundaries: fixed end on all sides and free ends on all sides. Stress-strain curves were then compared under these two boundary conditions for three cases: single crystal, high angle grain boundary arrays, and low angle grain boundary arrays. In each of the three cases, loading was reversed at different strain levels after yield and Bauschinger effects were examined on all the scenarios. The simulation results were also compared with macroscopic mechanics ideas for both high angle and low angle grain boundaries. The Bauschinger effect was found to be largest for the case of high angle boundaries and lowest for the single crystal.

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