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ACCEPTED MANUSCRIPT Influence of local stresses on motion of edge dislocation in aluminum

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On the basis of theoretical consideration and analysis of molecular dynamic (MD) simulation data, we show that the dislocation motion is determined by the stress field in its local environment. These stresses differ from the values averaged over even such tiny microscopic regions, which are usually used in MD study of dislocation motion. As a result, the slip velocity of dislocations can remain virtually constant with a gradual decrease in the average stresses in the calculation area. When a dislocation enters the trace of the previous dislocation, that is, into a region plastically relaxed by the slip of the previous dislocation, its velocity, on the contrary, decreases sharply, even if the average stresses in the region vary slightly. The revealed complex behavior leads to variable final average stress after the completion of the movement of dislocations; the average stress sometimes even changes its sign in the course of plastic relaxation. All these features can influence the response of the dislocation system to mechanical loading. Therefore, the action of the local stresses should be taken into account when analyzing the MD results, in the development of continuum models of plasticity, as well as in discrete dislocation dynamics. A dislocation motion equation is proposed with accounting of local stresses, and the constants for the edge dislocation in Al are determined by comparison with the results of MD simulations. An asymptotic solution of this equation is proposed, which can be used in the numerical solution of the equations of continuum dislocation plasticity. Alternative dependencies of the drag force on the dislocation velocity are analyzed; it is shown that they describe the results of MD simulations worse than the equation proposed by us.

Keywords: A dislocations; A stress relaxation; mobility law; molecular dynamics

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