Atomistic Calculations of Dislocation Locks: Effects of Hydrogen*

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A basic mechanism determining the mechanical behavior of materials is the response of a dislocation lock to an applied stress field. Both the work hardening and the fracture behavior of materials have been related to this mechanism. In this presentation we present the results of atomistic calculations of a dislocation lock in nickel modeled using the Embedded Atom Method (EAM). The stability of the lock as a function of applied strain at various temperatures has been determined. The effects of an important environmental impurity, hydrogen, on this stability is quantified. It is found that depending on the character of the applied strain field, hydrogen can either reduce the strain necessary to break the dislocation lock or enhance the propensity of void formation at the lock.

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