

Temperature dependence of dislocation core configuration in pure Ti

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The glide of a dislocation on a selected crystallographic plane is dependent on the dislocation core configuration. In pure Ti, the dislocation motion has been described as jerky, gliding during an extended period at high velocity on the {10-10} prismatic plane and cross-slipping slowly during a limited period on the {10-11} pyramidal plane[1]. The rate of cross-slip is an important parameter that influences the ductility and strength of the material. The study of the temperature dependence of dislocation core configurations will allow us to know which glide plane is favored at a given temperature. We've computed the temperature dependence of the dislocation core Gibbs free energy for different core configurations to study the thermodynamic stability of these configurations. These computations have been done using molecular dynamics simulations using a nonequilibrium free energy calculation method[2] and a MEAM potential describing the properties of Ti. Different ground state core configurations are reached by applying a non-Schmid stress on the simulation cell, and the changes in the core structures are characterized using an elastic stability parameter[3]. An energy barrier between the prismatic and the pyramidal orientation of the core is measured. It is shown that the pyramidal core orientation becomes more easily accessible to the core as temperature increases.

Keywords: Dislocation core, Titanium, Non-equilibrium free energy calculation, Molecular dynamics, Temperature dependence.

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