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Thermodynamics of plastic flow of BCC metals from atomistic studies of isolated screw dislocations ROMAN GRÖGER, Institute of Physics of Materials and CEITEC IPM, Academy of Sciences of the Czech Republic, VACLAV VITEK, Department of Materials Science and Engineering, University of Pennsylvania — The thermodynamic description of dislocation glide in BCC metals depends crucially on the shape of the Peierls barrier that $1/2\langle 111\rangle$ screw dislocations have to overcome when moving in the lattice. While the height of this barrier can be obtained unequivocally using saddle-point search algorithms such as the Nudged Elastic Band (NEB) method, its exact shape depends on the chosen approximation of the transition pathway of the system. We formulate a procedure that allows to identify the position of the dislocation directly from the displacements of atoms in its core. We investigate the performance of this model by calculating curved paths of a $1/2\langle 111\rangle$ screw dislocation in tungsten from a series of images obtained recently using the NEB method at zero applied stress and for positive/negative shear stresses perpendicular to the slip direction. The Peierls barriers plotted along these curved paths are shown to be quite different from those obtained previously by assuming a straight dislocation path. We demonstrate how these results can be utilized to develop a new thermodynamic model of plasticity of BCC metals that is systematically linked to the atomic-level properties of isolated $1/2\langle 111\rangle$ screw dislocations.

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