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Calculation of the Peierls barrier of screw dislocations in bcc metals and its dependence on stress ROMAN GROGER, Institute of Physics of Materials, Academy of Sciences of the Czech Republic, VACLAV VITEK, Department of Materials Science and Engineering, University of Pennsylvania — Plastic deformation of bcc metals at low temperatures is governed by thermally activated glide of $1/2\langle 111\rangle$ screw dislocations over Peierls barriers. Thermodynamic models of the dislocation glide depend on the shape of the Peierls barrier and its changes under stress. Atomistic simulations provide only the maximum slope of the Peierls barrier and, therefore, its overall shape as well as the path of the dislocation are generally unknown. We introduce a new approach by which the Peierls barrier and its changes under stress can be calculated if a suitable set of constraints is imposed to prevent the dislocation from falling into the nearest potential minima. The state of the system at any point along the path is described by the position of the intersection of the dislocation with the perpendicular $\{111\}$ plane. Hence, both the Peierls barrier and the transition path are obtained directly. This is a clear advantage over the currently used approach, where one calculates the path of the system of N atoms through the space of $3N$ degrees of freedom. We compare the results of these two approaches by employing the Finnis-Sinclair potential for tantalum.

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