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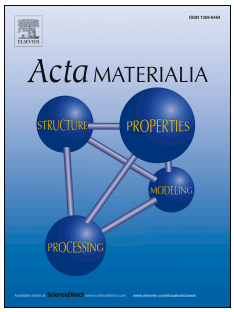

Atomistically-informed thermal glide model for edge dislocations in uranium dioxide

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Atomistically-informed thermal glide model for edge dislocations in uranium dioxide

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Abstract

We investigate the thermally activated glide mobility of dislocations in uranium dioxide (UO_2) from an atomistic point of view using a variable charge many-body empirical potential, the Second Moment Tight-Binding potential with charge equilibration (SMTB-Q). In order to determine the main glide system, we model the dislocation core structures for edge and screw orientations lying in different glide planes. Uncommon core structures with a double periodicity and a charge alternation are obtained. Straight dislocations motion is first considered to obtain the Peierls stress of each dislocation. We then address the thermally activated motion of the dislocations by the nucleation of kink pairs. Atomistic simulations give us the structure as well as the formation and migration energies of kink pairs. This information is finally combined with an elastic interaction model for kink pairs to obtain the dislocation velocities and the evolution of the critical resolved shear stress as a function of temperature. These quantities are compared to experimental data on urania single crystals.

Keywords: Uranium dioxide, Computer simulation, Dislocations, Kink pairs, Dislocation mobility