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Molecular Dynamics simulation of dislocations in uranium dioxide

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Abstract

The plasticity of the fluorite structure in UO_2 is investigated with molecular dynamics simulation and empirical potential. The stacking fault energies and the dislocation core structures with Burgers vector $\frac{a}{2}\langle 110 \rangle$ are systematically calculated. All dislocation core structures show a significant increase of the oxygen sub-lattice disorder at temperatures higher than 1500 K. The threshold stress for dislocation glide is found to decrease with increasing temperature but its values is always very high, several GPa at 0 K and several hundred of MPa at 2000 K. A relation between the dislocation mobility dependence with temperature and the increase of the oxygen sub-lattice disorder in the dislocation cores is established.

Keywords: Molecular dynamics, uranium dioxide, dislocation, stacking fault

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