Mobility and cross-slip of the 1/2< 110> scriw dislocation in UO2

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Abstract

The plastic deformation of UO2 single crystal is characterized by dislocations gliding mainly in the primary slip systems $\frac{1}{2}$ {001} of the fluorite structure. However, recent numerical studies conducted at the meso-scale have highlighted the possible role of dislocation cross-slip in secondary slip systems, $\frac{1}{2}$ {110} and $\frac{1}{2}$ {111}, as a possible explanation for the Schmid law breakdown and the anisotropic mechanical response observed in UO2 single crystal experiments performed at high-temperature (1,2,3). Despite these insights, hypothesis relying on elementary deformation processes in UO2 remain qualitative for now, primarily due to the limited understanding of the screw dislocation structure and mobility at elevated temperature.
In this study, we employ a combination atomistic and discrete dislocation dynamics simulation to investigate the mobility of the $\frac{1}{2}$ screw dislocation in UO2. The fundamental deformation mechanisms of dislocation motion at the atomic scale are explored from room temperature to 2200 K, with a particular emphasis on the progressive activation of cross-slip in the {111} planes. Models for the screw dislocation mobility and cross-slip are developed based on the tendency of the screw dislocation core to spread across the various crystallographic planes of the fluorite structure, and are tested within a discrete dislocation dynamics framework. In addition to a through comparison with atomistic simulations, meso-scale simulations are employed to validate the the cross-slip models through test-cases relevant to irradiation and strain hardening in UO2.

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