Materials Science and Technology Division
Materials Theory Group

"Computer simulation of dislocations and dislocation loops in α-zirconium"

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Abstract

Zirconium is an important metal for nuclear industry, yet there have been few atomic-scale computer simulation studies of dislocations and their interaction with dislocation loops that are created by radiation damage. One reason is that it has proved difficult to produce interatomic potentials that reproduce the known preference for slip on the first-order prism planes, rather than the basal plane. This talk will present results obtained from simulations using a potential derived by Mendelev and Ackland (Philos. Mag. Lett. 87 (2007) 349). Its suitability has been assessed by modelling the core structure and Peierls stress of dislocations of the prism and basal systems, and these will be shown to be consistent with the slip behaviour of α-zirconium. As a result of this, the potential has been used to study the interaction of dislocations of the prismatic slip system with nano-scale interstitial loops. The reaction and absorption mechanisms of loops with both edge and screw dislocations will be described, and the pinning strength loops present to glide of these dislocations will be discussed.

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