ICSMA19 Metz, France, June 26 - July 1, 2022
International Conference on Strength of Materials

Solute effects on prismatic slip in Mg alloys

Masoud Rahbar Niazi[a] , W. A. Curtin[a]

[a]*Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, CH-1015, Lausanne, Switzerland*

[a]*william.curtin@epfl.ch*

The poor ductility of the Mg alloys is attributed to the low activity of non-basal slip systems and limits their use in many applications. Activation of prismatic slip can increase the ductility by providing three additional $< a >$ slip systems. Experimental studies have shown that the addition of small amounts of alloying elements such as Zn and Al soften the prismatic slip at low temperatures. Focusing on Mg-Zn system, the work presented here aims at uncovering the mechanisms behind the effects of solute atoms on prism edge and screw dislocations by atomic scale simulation methods. Solute strengthening of edge dislocations, assessed using theory and first-principles DFT, provides some strengthening but remains well below experiments. Dynamic strain aging by cross-core diffusion contributes additional strengthening, and the total may approach experiments, suggesting that edge dislocations increasingly contribute to prism strengthening at elevated temperatures. The addition of Zn can also stabilize the screw $< a >$ dislocation on the prismatic plane, and may soften and enhance prismatic slip. Study of these mechanisms at larger scales by direct simulations is facilitated by the development and use of an Mg-Zn neural-network interatomic potential.

Keywords : Mg-Zn; prismatic slip; solute strengthening; cross-core diffusion; DFT

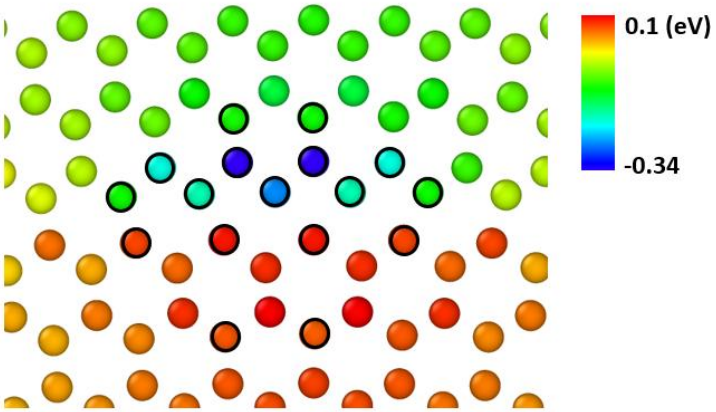

Fig.1 Solute/dislocation interaction energy map for prism edge dislocation in Mg-Zn alloy.