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A DFT analysis of structure and energetics of Mg/Nb multilayers

ANIL KUMAR, IRENE BEYERLEIN, JIAN WANG, Los Alamos National Laboratory — Magnesium and its alloys, the lightest structural materials, have attracted the attention of the automotive industry for reducing the vehicle's weight to increase its fuel efficiency. The magnesium phase characterized within Mg/Nb multilayers can adopt either body-centered cubic (bcc-Mg) or hexagonal close packed (hcp-Mg) structure depending on the Mg layer thickness. The bcc-Mg has a similar weight density as the hcp-Mg, but low Young's modulus, high shear modulus and conventional slip systems of bcc structure. In this work, using first-principles density functional theory, we studied both structural and mechanical properties of bcc-Mg and hcp-Mg in Mg/Nb multilayers as a function of Mg layer thickness and developed a simple theoretical model to predict the structural stability of the bcc-Mg/Nb and hcp-Mg/Nb multilayers. We show that the bcc-Mg/Nb multilayer is energetically favorable when the bcc-Mg layer is less than 4.2 nm. We also studied the mechanism such as inter-mixing of Mg and Nb atoms, creation of vacancies and doping of solute atoms at Mg/Nb interface to minimize the Mg/Nb interface energy. We found that solute atoms such as Zr, Cd and Zn, whose metallic radius are smaller than Mg, can easily segregate at Mg/Nb interface and lower the interface energy.

Anil Kumar
Los Alamos National Laboratory

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