

Abstract Submitted
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Link between structural and mechanical stability of fcc- and bcc-based ordered Mg-Li alloys. MAJE PHASHA, Materials Science and Manufacturing, CSIR, Pretoria, SA, PHUTI NGOEPE, Materials Modeling Centre, University of Limpopo, SOVENGA, SA, HASANI CHAUKE, Materials Modeling Centre, University of Limpopo, SOVENGA, SA, DUC NGUYEN-MANH, UKAEA, Culham Science Centre, Oxfordshire, UK, DAVID PETTIFOR, Materials Modeling Laboratory, Department of Materials, University of Oxford, Oxford, UK — The first principles pseudopotential calculations based on the Perdew-Burke-Ernzerhof (PBE) form of generalized gradient approximation (GGA) within density functional theory (DFT) have been used to successfully investigate the electronic and elastic properties of cubic-based Mg-Li alloys. The heats of formation, Jones-type analysis and mechanical elasticity were utilized in predicting structural stability profile, and their results consistent with each other. An interesting correlation between shear modulus (C') and the predicted energy differences of corresponding bcc and fcc ordered compounds relative to hcp Mg and Li lattices is observed.

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