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First-principles Calculations of Strengthening Compounds in Magnesium Alloy: A General Review

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First-principles computation methods play an important role in developing and designing new magnesium alloys. In this article, we present an overview of the first-principles modeling techniques used in recent years to simulate ideal models of the structure of strengthening compounds in Mg alloys. For typical Mg compounds, structural stability, mechanical properties, electronic structure and thermodynamic properties have been discussed. Specifically, the elastic anisotropies of these compounds are examined, which is highly correlated with the possibility of inducing micro-cracks. Furthermore, some heterogeneous nucleation interfaces investigated by first-principles method are reviewed. Some of the theoretical results are compared with available experimental observations, we hope to illustrate that the first-principles computation can help to accelerate the design of new Mg-based materials and the development of materials genome initiative. Remaining problems and future directions in this research field are considered.

Key words: Magnesium alloy; Strengthening compounds; First-principles calculation; Mechanical

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