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First Principles Stability and Coherency Strain in Mg3RE (RE=rare earth) D019 Metastable Precipitates in Mg A. ISSA, J. SAAL, C. WOLVERTON, Northwestern University — As the need for strong yet lightweight materials intensifies, magnesium alloys have become increasingly important. Although lightweight, these alloys exhibit low strength, particularly in comparison to aluminum alloys. The potential to greatly strengthen magnesium alloys has driven current research, with a recent focus on strengthening precipitates, particularly involving rare earth (RE) dopants. The morphology of these precipitates dictates their effect on the strength of the alloy, and quantifying the coherency strain between the precipitates and the Mg matrix is key to determining the morphology of the precipitate. The large size of the potential composition space makes a systematic experimental study costly and time consuming. Therefore, we apply density functional theory (DFT) to systematically predict the formation energies and coherency strains of D019 precipitates in Mg-RE systems along several crystallographic directions. In particular, we look for D019 precipitates that favorably form plate-shaped morphologies along non-basal planes, as this morphology should be effective obstacles to plastic deformation. These Mg-RE systems also provide an interesting testing ground for the accuracy of DFT methods for intermetallic compounds containing f-electrons.

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