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Magnesium Alloy Precipitate Formation Using Mixed Basis Cluster Expansions ROBERT LEONE, GUS HART[1], Northern Arizona University — Unlike steel and aluminum alloys, the basic science of magnesium alloys is poorly understood. The automotive industry is driving demand for lighter structural material, and readily available magnesium alloys have a higher strength-to-weight ratio than their aluminum counterparts. We seek to predict magnesium alloy properties from first principles, particularly the hardening effect of precipitate formation. Mixed basis cluster expansions (MBCE) have successfully modeled precipitate shapes and growth in aluminum alloys. Unfortunately, this methodology has not been extended to hcp-based materials such as magnesium alloys. In order to model binary magnesium alloys using the MBCE, particularly precipitate morphologies, we have constructed a coherency strain model for hcp structures to correctly represent the long range strain fields around precipitates. Coupling this generalized strain model to an Ising-like expansion methodology we have developed a mixed-basis cluster expansion for hexagonal symmetries. Results for several representative magnesium alloys will be presented.

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