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High-throughput study of crystal structures and stability of strengthening precipitates in Mg alloys DONGSHU WANG, MAXMILIAN AMSLER, VINAY HEGDE, JAMES SAAL, AHMED ISSA, Northwestern University, XIAOQIN ZENG, Shanghai Jiao Tong University, CHRISTOPHER WOLVERTON, Northwestern University — Age hardening, in which precipitates form and impede the movement of dislocations, can be applied to magnesium alloys in order to increase their limited strengthening behavior. To help clarify the energetics of precipitation hardening of Mg alloys, we employed first principles density functional theory calculations to elucidate both crystal structures and energetics of a very large set of precipitates in Mg alloys. We find the enthalpy changes of (stable and metastable) observed precipitates during the age hardening process are consistent with the experimental sequence of formation for many Mg binary alloys (Mg- {Nd, Gd, Y, Sn, Al, Zn}). For cases where the metastable precipitate crystal structure is unavailable, we search over several prototypes and predict structures/stoichiometries for several ternary precipitates. In addition, high-throughput calculations are performed to construct hcp-based based convex hulls, which assist the identification of coherent GP zones and new metastable phases in age-hardened hcp systems.

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