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First-principles thermodynamics of point defects and off-stoichiometry in β-$Mg_{17}Al_{12}$ DONGWON SHIN, CHRISTOPHER WOLVERTON, Northwestern University — The mechanical strength of Mg-Al alloys may be enhanced by a fine spatial dispersion of β-$Mg_{17}Al_{12}$ precipitates. Native point defects, i.e. vacancies and anti-sites, in $Mg_{17}Al_{12}$are important for understanding the phase stability and unusually asymmetric observed off-stoichiometry in this precipitate phase. In an effort to provide a quantitative picture of the phase stability of this system, we have performed a series of first-principles density functional theory calculations of bulk and defect properties of $Mg_{17}Al_{12}$. We consider not only the T=0K static energetics, but also key entropic terms such as the configurational and vibrational entropies. The vibrational entropies are calculated from DFT via the direct force-constant approach using the quasiharmonic approximation. We investigate the effect of atomic vibrations on native point defect free energies of $Mg_{17}Al_{12}$and combine the entropic contributions with the point defect formation energies to evaluate the thermodynamics of off-stoichiometry in this phase. We find there is a large vibrational entropy difference between Mg-rich and Mg-deficient defects in $Mg_{17}Al_{12}$, consistent with the strong asymmetry in the observed Mg-Al phase diagram.

Dongwon Shin
Northwestern University

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