

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

**First-principles thermodynamics of point defects and off-stoichiometry in  $\beta$ -Mg<sub>17</sub>Al<sub>12</sub>** DONGWON SHIN, CHRISTOPHER WOLVERTON, Northwestern University — The mechanical strength of Mg-Al alloys may be enhanced by a fine spatial dispersion of  $\beta$ -Mg<sub>17</sub>Al<sub>12</sub> precipitates. Native point defects, i.e. vacancies and anti-sites, in Mg<sub>17</sub>Al<sub>12</sub> 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<sub>17</sub>Al<sub>12</sub>. 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<sub>17</sub>Al<sub>12</sub> 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<sub>17</sub>Al<sub>12</sub>, consistent with the strong asymmetry in the observed Mg-Al phase diagram.

Dongwon Shin  
Northwestern University

Date submitted: 30 Nov 2008

Electronic form version 1.4