Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Engineering materials-design parameters of the Mg-Li Alloy System from ab initio calculations WILLIAM COUNTS, MARTIN FRIAK, DIERK RAABE, JORG NEUGEBAUER, Max-Planck Institute for Iron Research — Ab initio calculations are becoming increasingly useful to engineers interested in designing new alloys because these calculations are able to accurately predict basic material properties only knowing the atomic composition of the material. Fundamental physical properties (like formation energy and elastic constants) of 11 bcc magnesium-lithium alloys were calculated using density-functional theory (DFT) and compared with available experimental data. These DFT determined properties were in turn used to calculate engineering parameters like the bulk modulus/shear modulus (B/G) and Young's modulus/density (E/ρ). From these engineering parameters, alloys with optimal mechanical properties need for a light weight structural material were identified. It was found that the stiffest bcc magnesium-lithium alloys contain about 70 at.% magnesium while the most ductile alloys have 0-20 at.% magnesium. In addition, the specific modulus for alloys with 70 at.% magnesium was found to be equal to that of aluminum-magnesium alloys and slightly lower than that of aluminum-lithium alloys.

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Date submitted: 23 Nov 2007 Electronic form version 1.4