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Ab initio guided design of bcc Mg-Li alloys for ultra light-weight applications MARTIN FRIÁK, WILLIAM ART COUNTS, DIERK RAABE, JÖRG NEUGEBAUER, Max-Planck-Institut fuer Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Duesseldorf, Germany — 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. In this paper, fundamental physical properties (like formation energies and elastic constants) of 11 bcc Mg-Li compounds are calculated using density-functional theory (DFT) and compared with available experimental data. These DFT-determined properties are in turn used to calculate engineering parameters like (i) specific Young's modulus (Y/ρ) or (ii) bulk over shear modulus ratio (B/G) differentiating between brittle and ductile behavior. The engineering parameters are then used to identify alloys that have optimal mechanical properties needed for a light weight structural material. It was found that the stiffest bcc magnesium-lithium alloys contain about 70 at.% Mg while the most ductile alloys have 0-20 at.% Mg. The specific modulus for alloys with 70 at.% Mg is equal to that of Al-Mg alloys. An Ashby map containing Y/ρ vs. B/G shows that it is not possible to increase both Y/ρ and B/G by changing only the composition or local order of a binary alloy (W. A. Counts, M. Friák, D. Raabe and J. Neugebauer, Acta Mater 57 (2009) 69-76).

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