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The effects of Li concentration on the structure and mechanics in the Li-Mg binary system OLIVIA PAVLIC, West Virginia University, IRAIS VALENCIA-JAIME, CINVESTAV-Queretaro, ALDO ROMERO, West Virginia University-Department of Physics and Astronomy — Magnesium (Mg) is a low density and naturally abundant material that has received much attention due to structural, mechanical, electrical, and thermal properties. Unfortunately, due to its hexagonal close packed (hcp) structure Mg materials exhibit low ductility and are difficult to work with at room temperature. One way to make Mg suitable for industrial applications is to change its structure by alloying. Lithium (Li) is a good candidate to alloy with Mg because of its more workable body centered cubic (bcc) structure and low density, making LiMg compounds regarded as ultralight materials. We study the Li-Mg binary compounds over varying percents of Li from $0 - 100\%$ using the minima hopping method for structural search. On our convex hull we find four structures, Li1Mg2 space group I4/mmm, Li1Mg1 space group Pm-3m, Li7Mg2 space group Ibam, and Li9Mg1 space group C12/m1. We note that the Li1Mg2, Li2Mg7, and Li9Mg1 structures are previously unreported. A mechanical and structural characterization is performed over these and six other structures. We present elastic constants, mechanical properties, and structures which outline the effect of the added Li.

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