

# Ab Initio Guided Design of bcc Ternary Mg–Li–X (X = Ca, Al, Si, Zn, Cu) Alloys for Ultra-Lightweight Applications

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*Ab initio calculations are becoming increasingly important for designing new alloys as these calculations can accurately predict basic structural, mechanical, and functional properties using only the atomic composition as a basis. In this paper, fundamental physical properties (like formation energies and elastic constants) of a set of bcc Mg–Li and Mg–Li-based compounds are calculated using density functional theory (DFT). These DFT-determined properties are in turn used to calculate engineering parameters such as (i) specific Young's modulus ( $Y/\rho$ ) or (ii) shear over bulk modulus ratio ( $G/B$ ) differentiating between brittle and ductile behavior. These parameters are then used to identify those alloys that have optimal mechanical properties for lightweight structural applications. First, in case of the binary Mg–Li system, an Ashby map containing  $Y/\rho$  versus  $G/B$  shows that it is not possible to increase  $Y/\rho$  without simultaneously increasing  $G/B$  (i.e., brittleness) by changing only the composition of a binary alloy. In an attempt to bypass such a fundamental materials-design limitation, a set of Mg–Li–X ternaries (X = Ca, Al, Si, Cu, Zn) based on stoichiometric Mg–Li with CsCl structure was studied. It is shown that none of the studied ternary solutes is able to simultaneously improve both specific Young's modulus and ductility.*

The global challenges regarding energy savings and CO<sub>2</sub> reduction with the current worldwide trend toward an ever-increasing demand for global mobility are among the most essential tasks in materials science and engineering. Any successful attempt to achieve both goals requires the development of novel ultra-lightweight metallic materials with excellent mechanical and functional properties. This applies for both fossil-fuel and battery-driven units. In this context novel Mg alloys play a key role owing to their low mass density.<sup>[1–5]</sup> Pure Mg is a common, lightweight metal that can potentially be more widely applied as a structural material but the use of wrought Mg and Mg-alloys is limited in large-scale manufacturing operations: Mg and Mg-alloys are difficult to deform at room temperature, and once formed they often reveal undesirable mechanical properties. In this article we address two important aspects related to Mg alloys. First, how can the forming and anisotropy properties of Mg alloys

be improved? These properties are of particular relevance for instance in the field of advanced automotive manufacturing. Second, can we employ new alloy design strategies to achieve a more knowledge-driven rapid maturation of metallic materials that go beyond conventional empirical design approaches?

Regarding the first issue, we aim in this work at designing Mg alloys crystallizing in a phase that is more easily formable. The lack of room temperature ductility in Mg alloys is primarily due to the hexagonal closed packed (hcp) crystal structure of Mg. In hcp Mg, the critical resolved shear stress of the two basal slip systems is much lower than that of other slip systems. The two available slip systems are not enough to fulfill the von Mises criterion that requires five independent slip systems to accommodate an arbitrary deformation state via dislocation glide. The absence of room temperature ductility and the evolution of strong deformation textures are inherent limitations of the hcp crystal structure that to date have not been completely overcome.<sup>[6–10]</sup>

Changing the crystal structure fully or partially from hcp to either face centered cubic (fcc) or body centered cubic (bcc) is one way to realize Mg alloys that are less anisotropic and mechanically more compliant as this change increases the number of plastic degrees of freedom (higher number of available slip systems). The consequence would be better

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plastic formability at room temperature and a reduced tendency to form disadvantageous deformation textures. Cubic Mg would therefore be very attractive from a manufacturing point of view.

A number of Mg–X alloys are known to have a cubic structure. For example, the Mg–Li system has a stable bcc phase at room temperature and the bcc phase is stabilized with as little as 30 at% Li. Li does not only stabilize the bcc crystal structure; it also has the advantage of further decreasing the density of the Mg alloy since Li is the lightest known metal ( $\rho^{\text{Li}} = 0.58 \text{ g cm}^{-3}$ ,  $\rho^{\text{Mg}} = 1.74 \text{ g cm}^{-3}$ ). The resulting Mg–Li alloys are therefore among the lightest possible metallic alloys. Li additions on the other hand reduce the overall stiffness of Mg–Li alloys. Therefore, a systematic materials-design search (e.g., see Refs.<sup>[11–14]</sup>) is needed that accomplishes an optimization with respect to multiple, in part even contradicting, materials criteria.

This leads us to the second main point of how such a more systematic and knowledge-driven optimization can be pursued. In this context we choose a quantum-mechanics-based bottom-up approach to identify more rapidly not only suited compositions with regard to the thermodynamic stabilization of the desired phase but also scrutinize some of the basic structural and mechanical features of possible alloy candidates. In contrast to many top-down approaches that start from the macroscopic scale and continue downscale, here we are starting at the most fundamental level of materials science – the quantum-mechanical level – which describes the interaction of the fundamental constituents of any material without any experimental input. The only parameters entering the quantum-mechanical calculations are the nucleus number of the specific chemical element. These methods are called first principles methods or, using the corresponding Latin term, *ab initio* methods.

In order to carry out an *ab initio* guided materials-design strategy, a multi-disciplinary approach has been used in this paper. First, ground-state density functional theory (DFT) calculations were performed for a set of bcc and hcp ordered alloys in order to obtain information on thermodynamic phase-stabilities and linear-elasticity data at the atomic level. Second, polycrystalline elastic moduli and other engineering parameters measurable at macroscale were predicted employing linear-elasticity homogenization techniques that allow bridging the scale difference between atomistic and macroscopic levels. Using this methodological strategy, an alloy composition with desired properties may be suggested employing the following iterative steps. First, starting from an initial composition its properties are computed and compared to desired ones. Based on the residuum/deviation of the properties on the macroscale a new atomic composition is suggested and studied. These cycles are repeated until the desired properties are obtained. Of course, if the properties are not accessible by any chemical composition, a new set of properties has to be identified.

In this paper, we start with the Mg–Li bcc binary system. It was shown that (i) the resulting materials properties compare

very well with available experimental data, (ii) polycrystalline elastic constants (Young's modulus  $Y$  and shear modulus  $G$ ) possess nonlinear variations as a function of alloy composition, (iii) alloys with about 30 at% Li were the stiffest, and (iv) alloys with greater than 70 at% Li were the softest.<sup>[13,14]</sup> Using the DFT calculated data, an Ashby map containing (i) Young's specific modulus  $Y/\rho$  as a measure of the strength and (ii) the  $B/G$  as a suggested indicator of either brittle or ductile behavior was previously constructed.<sup>[15]</sup> Plotting the Reuss, Voigt, and self-consistent Hershey values of various local arrangements together in this map resulted in a universal master curve dependence that links increasing  $Y/\rho$  with decreasing  $B/G$ , i.e., increasing tendency toward an inherent brittleness. That such a universal master curve exists indicates that there is a fundamental materials-design limitation, i.e., it is not possible to increase both  $Y/\rho$  and  $B/G$  by changing only the composition or local order of a binary alloy. Here we show that the product of  $Y/\rho$  and  $G/B$  (i.e., an inverse of the originally proposed  $B/G$  ratio) is actually nearly constant for all studied bcc Mg–Li compounds. Next, in an attempt to bypass the identified materials-design limitation, the stoichiometric MgLi was chosen as a test system in which a ternary alloying was studied employing *ab initio* calculated thermodynamic and elasticity information. Specifically, properties of a set of MgLi–X ternaries ( $X = \text{Ca, Al, Si, Cu, Zn}$ ) were determined. It is shown that the studied solute additions have rather detrimental impact on the pair of studied materials properties and are not able to overcome the limitation.

#### Computational Methodology

DFT calculations<sup>[16,17]</sup> employing the generalized gradient approximation<sup>[18]</sup> were performed using a plane wave pseudopotential approach as implemented in the Vienna *Ab initio* Simulation Package (VASP) code.<sup>[19,20]</sup> Binary alloys were described by supercells consisting of  $2 \times 2 \times 2$  elementary cubic or hexagonal unit cells with a total of 16 atoms (see details in refs.[13,14]). Fifteen alloy compositions were studied by systematically replacing Mg and Li atoms. MgLi–X ternaries with solute additions were simulated using 16-atomic supercells formed from  $2 \times 2 \times 2$  MgLi CsCl (B2) cubic unit cells in which one (either Mg or Li) atom was replaced by one solute atom (Ca, Al, Si, Cu, or Zn). For each of the constructed supercells the equilibrium geometry has been calculated by minimizing the total energy with respect to atomic positions and supercell shape. The single-crystalline elastic constants of the calculated compounds were determined from the changes of the total energy as a function of the applied strain.<sup>[21]</sup> As all the computed compounds were of cubic symmetry, three elastic constants were determined from three independent cell-shape deformations, specifically (i) volumetric, (ii) tetragonal, and finally (iii) trigonal. For polycrystalline moduli, the self-consistent Hershey's<sup>[22]</sup> homogenization scheme for texture-free cubic aggregates (e.g., see also refs. [11,13,14,23–25]) based on the single-crystalline elastic constants  $C_{ij}$  was employed and compared

with the values within the Reuss and Voigt schemes<sup>[26,27]</sup> constituting the lower and upper bound, respectively, of the polycrystalline shear modulus. In this theoretical study, the properties of only one ordered atomic configuration per composition (with exception of 50 at%, B2 vs. B32) were calculated at  $T = 0$  K.

Results

The ground-state formation energies, lattice parameters, elastic constants, and moduli for various phases of pure Li and Mg, as well as both bcc- and hcp-based Mg–Li compounds are summarized in Refs.<sup>[13,14]</sup> The compositional dependence of the bulk modulus was shown to be nearly linear but the other characteristics, specifically the single-crystalline elastic  $C_{ij}$  constants or polycrystalline moduli, Young’s  $Y$  or shear  $G$ , are predicted to have strongly nonlinear character (see details in refs. [13,14]).

Regarding engineering processing-relevant materials characteristics, the  $B/G$  ratio<sup>[15]</sup> has been proposed as a metric to quantify whether a material will fail in a ductile or brittle fashion. Interestingly, it was shown<sup>[13,14]</sup> that the specific Young’s modulus  $Y/\rho$  is nearly inversely proportional to the  $B/G$  ratio. In order to obtain a deeper understating of the phenomena and to further investigate mutual connection between both engineering quantities,  $Y/\rho$  as a function of  $G/B$  is plotted below. Note, that this plot is plotted over  $G/B$  (rather than the inverse as in the original paper<sup>[15]</sup>) to emphasize the almost linear character. The corresponding Ashby map based on Voigt, Reuss, as well as Hershey’s self-consistent values for Mg–Li alloys with 6–80 at% Li is plotted in Figure 1. In terms of  $G/B$ , the value lower than 0.57 indicates ductile behavior, and  $G/B$  above 0.57 indicates brittle behavior. As can be seen, the Reuss, Voigt, and self-consistent values no longer form a lower bound, an upper bound, and an approximate average, but virtually coincide on a single (and for this alloy system) universal and nearly linear master curve. This result leads to the conclusion that it is not

possible to increase  $Y/\rho$  without increasing also  $G/B$  by changing only the composition or local atomic order in the distribution of atoms of this binary alloy. We expect that the existence of a universal master curve in this Ashby plot is not restricted to the Mg–Li alloys studied here, but will also be valid for other alloys.

In order to explore whether this fundamental materials-design limitation can be overcome, we go over from the binary Mg–Li alloys to ternary MgLi–X alloys with  $X = \text{Ca, Al, Si, Cu, Zn}$ . The selected set of solutes includes both elements that are industrially used in case of Mg–Li alloys, such as Al, Si, Cu, or Zn, and also Ca as the element that should solid-solution strength Mg–Li alloys due to its significant size mismatch. The 16-atomic supercell allows changing the composition by fractions of 1/16, i.e., approximately 6 at%, when either one Mg or Li atom is replaced by a solute atom. The homogenized polycrystalline elastic moduli obtained employing Hershey’s homogenization method, their ratios, as well as their densities are summarized in Table 1.

The results in Table 1 show that alloying does not guarantee improved elastic properties. A poor choice of the alloying element results in reduced elastic properties. In general, the elastic properties of  $\text{Mg}_8\text{Li}_7\text{X}$  are better than those of  $\text{Mg}_7\text{Li}_8\text{X}$ . Compared with  $\text{Mg}_8\text{Li}_8$ , the average increase in the bulk modulus for  $\text{Mg}_8\text{Li}_7\text{X}$  is 1.62 GPa compared with 0.56 GPa for the  $\text{Mg}_7\text{Li}_8\text{X}$  alloys. Similar trends are seen with Young’s modulus and shear modulus. The average increase in Young’s modulus is 7.9 GPa for  $\text{Mg}_8\text{Li}_7\text{X}$  compared with 4.1 GPa for  $\text{Mg}_7\text{Li}_8\text{X}$  alloys. The average increase in shear modulus for  $\text{Mg}_8\text{Li}_7\text{X}$  is 3.7 GPa compared to 2.0 GPa for  $\text{Mg}_7\text{Li}_8\text{X}$  alloys. These basic trends are not too surprising given the results shown in Figure 1 and the results in Refs.[13,14]: Adding Mg to a 50 at% MgLi binary alloy results in improved elastic properties. Thus  $\text{Mg}_8\text{Li}_7\text{X}$ -based alloys should also have improved elastic properties over  $\text{Mg}_7\text{Li}_8\text{X}$  alloys.

All of the individual elastic properties of MgLi can be improved via alloying. In fact, of the five alloying elements chosen for this study, only Ca reduces the individual elastic properties. The alloying element that provides the greatest

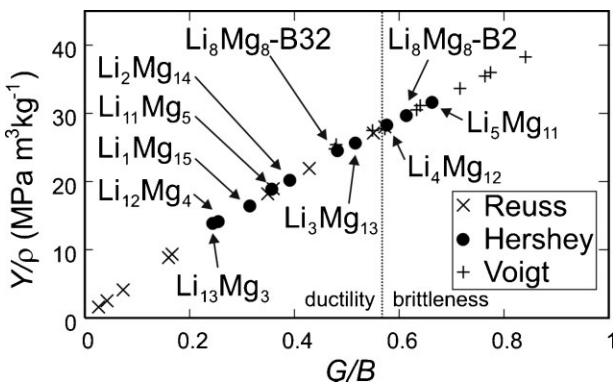


Fig. 1. Ashby map of  $Y/\rho$  versus  $G/B$  of bcc Mg–Li alloys. The vertical dotted line separates the ductile and brittle regions.<sup>[15]</sup> The map nicely shows that it is not possible to increase  $Y/\rho$  without increasing  $G/B$  (i.e., tendency toward the brittleness) by changing only the composition or distribution of atoms (see data points for  $\text{Mg}_8\text{Li}_8\text{-B2}$  and  $\text{Mg}_8\text{Li}_8\text{-B32}$  compounds with the same composition but different atomic distributions) over the lattice sites of the Mg–Li binary alloys.<sup>[13,14]</sup>

Table 1. Equilibrium bulk modulus  $B$ , self-consistently (Hershey) homogenized shear modulus  $G$ , Young’s modulus  $Y$ , their ratios, and the density  $\rho$  of calculated bcc MgLi–X ternaries ( $X = \text{Ca, Al, Si, Cu, Zn}$ ).

Compound	$B$ [GPa]	$G$ [GPa]	$Y$ [GPa]	$B/G$	$Y/G$	$\rho$ [ $\text{kg m}^{-3}$ ]
$\text{Mg}_8\text{Li}_8$	24.8	15.21	37.9	1.630	2.491	1276
$\text{Mg}_7\text{Li}_8\text{Al}$	26.2	19.03	45.9	1.374	2.414	1355
$\text{Mg}_7\text{Li}_8\text{Ca}$	23.1	14.21	35.4	1.624	2.489	1346
$\text{Mg}_7\text{Li}_8\text{Cu}$	25.7	15.50	38.7	1.661	2.498	1766
$\text{Mg}_7\text{Li}_8\text{Si}$	26.6	20.47	48.9	1.298	2.387	1400
$\text{Mg}_7\text{Li}_8\text{Zn}$	25.2	16.73	41.1	1.505	2.456	1804
$\text{Mg}_8\text{Li}_7\text{Al}$	27.4	20.73	49.7	1.321	2.396	1539
$\text{Mg}_8\text{Li}_7\text{Ca}$	23.5	12.42	31.7	1.895	2.551	1477
$\text{Mg}_8\text{Li}_7\text{Cu}$	26.8	20.37	48.8	1.315	2.393	1936
$\text{Mg}_8\text{Li}_7\text{Si}$	27.7	20.90	50.1	1.324	2.397	1589
$\text{Mg}_8\text{Li}_7\text{Zn}$	26.7	20.34	48.7	1.313	2.393	1989

improvement in the elastic properties is Si. For  $Mg_8Li_7X$  alloys, Si improves the bulk modulus by 2.9 GPa (12%), the Young's modulus by 12.2 GPa (32%), and the shear modulus by 5.7 GPa (37%). For  $Mg_7Li_8X$  alloys, Si improves the bulk modulus by 1.8 GPa (7%), the Young's modulus by 11 GPa (29%), and the shear modulus by 5.2 GPa (35%).

It is clear that the individual elastic properties of MgLi can be improved via alloying, in particular with Si or Al. What is not clear is whether the increase in the bulk, shear, and Young's moduli accompanies an increase in the brittleness of the MgLiX alloy. It would be ideal if alloying could improve the elastic properties with an increase in the ductility. The polycrystalline elastic constants in Table 1 have been plotted in an Ashby map of  $Y/\rho$  versus  $G/B$  in Figure 2. In this plot, the desired alloying element would simultaneously (i) increase  $Y/\rho$  and (ii) reduce  $G/B$  resulting in MgLiX data points lying in the upper left corner with respect to the MgLi master curve.

As can be seen in Figure 2, none of the MgLiX data points shows a simultaneous increase in specific modulus and ductility since all the MgLiX data points lie below the Mg-Li master curve. It is possible to increase the specific modulus by alloying with Al or Si, and it is possible to increase ductility by alloying with Ca and possibly Cu. It is interesting to note that alloying with Zn decreases both the specific modulus and ductility. This point illustrates that certain alloying elements provide no beneficial properties. The two best candidate alloys from this study are  $Mg_7Li_8Si$  and  $Mg_7Li_8Al$ . Both of these alloys lie close to the MgLi master curve suggesting that these alloys have properties comparable to binary MgLi.

The results in Figure 2 provide a combined perspective on the elastic properties of the MgLiX alloys. In contrast to studied individual elastic constants where alloying causes both positive and negative effects, the Ashby maps reveals that the improved bulk, Young's, and shear moduli values come at the expense of making the MgLi-X alloy more brittle. The predicted trends can be partly explained by the fact

that all the studied ternary elements have higher mass than either Li or Mg and so the selected solutes increase the density of the studied alloys. This increase of the density is unfortunately not compensated or, better, prevailed over by the change of the elastic moduli (and/or their ratios). The right choice of the alloying element, specifically with respect to an increasing density and its relation to the solid-solution strengthening, is clearly of paramount importance as elements in the periodic table that would be yet lighter than the constituents of the binary matrix, here Mg and Li, are lacking. As ab initio calculations can reliably predict changes of both density and elastic parameters, their use may shorten and optimize this search.

### Conclusions

In this paper, ab initio calculations are used to provide theoretical guidance in the design of bcc Mg-Li and MgLi-X ( $X = Ca, Al, Si, Cu, Zn$ ) alloys. Basic mechanical and physical properties, like crystal structure and single-crystal elastic constants, are calculated at zero temperature using DFT. The single-crystal elastic constants are used to calculate bounds and an estimate of isotropic polycrystalline elastic constants using various homogenization techniques. The homogenized polycrystalline elastic constants are then used to calculate two essential engineering parameters: the shear modulus/bulk modulus ratio (a measure of ductility) and the Young's modulus/mass density ratio (a measure of stiffness per weight). Using the DFT calculated data, an Ashby map containing  $Y/\rho$  versus  $G/B$  was constructed and the existence of a universal master curve is predicted. The existence of such a universal curve indicates that there is a fundamental materials-design limitation, i.e., it is not possible to increase both  $Y/\rho$  and ductility by changing only the composition or local order of a binary alloy. In an attempt to bypass this limitation, stoichiometric MgLi was chosen as initial point for studying ternary alloys, specifically MgLi-X ( $X = Ca, Al, Si, Cu, Zn$ ). It is shown that none of the studied solute additions simultaneously improves both specific Young's modulus and ductility.

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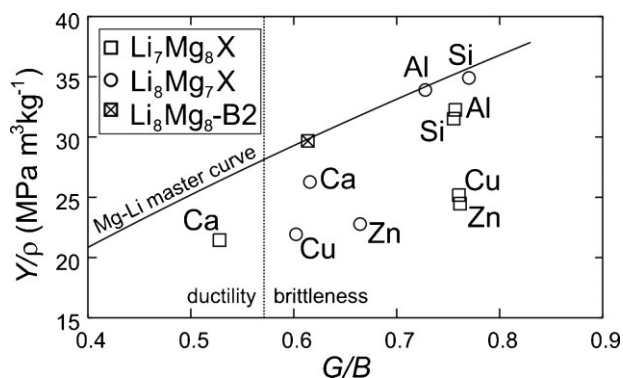


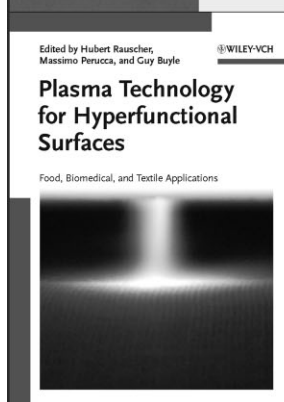
Fig. 2. Ashby map of  $Y/\rho$  versus  $G/B$  for bcc MgLi-based ternaries with the master curve of Mg-Li binary system (third-order polynomial fit, solid line) where every data point is accompanied with the name of ternary solute  $X$  ( $X = Ca, Al, Si, Cu, Zn$ ) in MgLi-X compounds. Data points for two different substitutions are shown: open squares correspond to states with one Li atom (out of eight in the supercell) replaced by one of the studied solute atoms; open circles represent the replacement of one Mg atom. The data point for MgLi-B2 is shown by a crossed square. The dotted vertical line (for  $G/B = 0.57$ ) is the threshold separating the brittle and ductile regions.

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