I: Electronic structure calculations of ordered cubic-based Mg-Li alloys

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II: Microstructural evolution of α+β

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Mg alloys have, in the past decade, received revolutionary attention which emanated from the need of lightweight materials in transportation and allied industries, wherein intrinsic strength to weight ratio is of paramount importance.

Al, Li, Zn, Mn, etc., identified as suitable main alloying elements candidates.

Due to atomic size, mobility, solute solubility.

Due to their properties, with lightness and recyclability in the forefront, they are potential candidates to replace steel and aluminium alloys in many structural and mechanical applications.

Lithium at a density of 0.53 g/cm³ not only enjoys superiority lightness, but also a useful phase change to bcc when alloyed at about 11wt% concentration and increase in ductility.

High amount of experiment work been carried out on Mg-Li alloys, few investigations has been done through theoretical ab initio techniques.
Mg & Mg alloys: Properties

Advantages
- Availability (8th most abundant 2.7% earth crust)
- Extremely light
- High strength: weight ratio
- Excellent machinability
- Good castability
- Inherent recyclability
- High dumping capacity
- Good creep resistance

Disadvantages
- High cost
- Poor wear & corrosion resistance
- Low elastic modulus
- Limited cold workability
- High chemical reactivity
- Limited strength at elevated T

Need: Weight reduction in transport without sacrificing structural strength

Applications: automotive & aerospace components, computer parts, mobile phones, sporting goods, handheld tools, household equipments
Other possible Appl.: implants due to low weight & inherent biocompatibility
Applications

Mordike et al.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Motor/Gear friction</th>
<th>Motor/Gear management</th>
<th>Estimated potential</th>
</tr>
</thead>
<tbody>
<tr>
<td>variable compression</td>
<td>&lt; 1%</td>
<td>&lt; 10%</td>
<td>Measures are not additive</td>
</tr>
<tr>
<td>variable valve control throttle choke losses</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fuel quality</td>
<td></td>
<td>Weight light materials</td>
<td>&lt; 30%</td>
</tr>
<tr>
<td>1-3%</td>
<td></td>
<td>c_w-value</td>
<td>&lt; 1%</td>
</tr>
<tr>
<td>Diesel direct injection turbo-engine</td>
<td>Motor-preheating</td>
<td>Efficiency and performance of ancillary aggregates</td>
<td>Tyre/road</td>
</tr>
<tr>
<td>&lt; 15%</td>
<td>2-8%</td>
<td>&lt; 2%</td>
<td>&lt; 1%</td>
</tr>
</tbody>
</table>
Hierarchies of length scales
I: Methodology

- Total energy code, CASTEP, based on DFT within GGA-PBE.

- Vanderbilt ultrasoft pseudopotentials - using plane wave

- Monkhorst-Pack scheme

- Energy cut-off & k-points were converged
Results

Heats of formation

![Graph showing heats of formation with Mg and Li concentration (atomic%) on the x-axis and E_form (meV/atom) on the y-axis. The graph includes various points labeled with structures like Mg<sub>15</sub>Li, Mg<sub>7</sub>Li, MgLi<sub>15</sub>, MgLi<sub>7</sub>, and Mg<sub>L</sub>Li<sub>2</sub>, among others. The graph also shows different states of matter represented by symbols like fcc and bcc.]
Bulk Modulus

![Graph showing the bulk modulus (B) in GPa as a function of Li at%.

- **P-V fcc**
- **Cij fcc**
- **P-V bcc**
- **Cij bcc**
- **Skriver fcc**
- **Skriver bcc**
- **Exp bcc**

The graph depicts the changes in bulk modulus with varying lithium concentrations in different crystallographic structures. The X-axis represents Li at%, while the Y-axis shows the bulk modulus (B) in GPa. The data points are color-coded and labeled according to the different phases (fcc, bcc), with experimental (Exp) and theoretical (P-V, Cij, Skriver) contributions.
Shear, Energy correlation

Craievich et al 1996
Bulk moduli decrease monotonically with increase in Li concentration.

Predicted heats of formation for all the different ground state superstructures result in a representative stability profile, which shows that the \( \text{DO}_3 \), B2 and \( \text{DO}_{22} \) structures are the most stable amongst various phases having \( \text{Mg}_3\text{Li} \), \( \text{MgLi} \) and \( \text{MgLi}_3 \) compositions, respectively. The similar stability is also being investigated by the use of density of states (DOS).

Stability profile hcp-bcc-fcc-hcp is predicted

Elasticity studies predicts stability of \( \text{DO}_3 \) structure in the \( \alpha + \beta \) region

Correlation \( C' \ vs \ e/a \ & \ \Delta E \ vs \ e/a \), region where bcc is very stable compared to fcc, the shear modulus is positive for bcc but negative for fcc (i.e. the fcc lattice is the mechanically unstable) and vice versa.
From ab initio predictions, experiments were conducted as follows:

- Preparations of Mg-Li samples
- Heat treatments
- Microstructural phase observations
- Mechanical tests
- Structure evolution (OOFEM)
Sample Preparation Conditions

- Arc Melting furnace
- Argon - protecting atmosphere
## Composition of samples

<table>
<thead>
<tr>
<th>Sample</th>
<th>Li content (wt.%)</th>
<th>Relative $\rho$ g/cm$^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg-9Li</td>
<td>8.69</td>
<td>1.44</td>
</tr>
<tr>
<td>Mg-10Li</td>
<td>10.03</td>
<td>1.40</td>
</tr>
<tr>
<td>Mg-11Li</td>
<td>10.99</td>
<td>1.37</td>
</tr>
<tr>
<td>Mg-12Li</td>
<td>12.01</td>
<td>1.35</td>
</tr>
</tbody>
</table>
SEM Observations: RT

(a) Mg-9Li alloy
(b) Mg-10Li alloy
(c) Mg-11Li alloy
(d) Mg-12Li alloy
# Microstructure Analysis

<table>
<thead>
<tr>
<th>Sample</th>
<th>Phases present</th>
<th>Observation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg-9Li</td>
<td>$\alpha+\beta$ (hcp+bcc)</td>
<td>Evenly distributed dual phase alloy</td>
</tr>
<tr>
<td>Mg-10Li</td>
<td>$\alpha+\beta$ (hcp+bcc)</td>
<td>Dominant $\beta$ phase with $\alpha$ precipitates</td>
</tr>
<tr>
<td>Mg-11Li</td>
<td>$\beta$ (bcc)</td>
<td>Single phase with slight oxidation</td>
</tr>
<tr>
<td>Mg-12Li</td>
<td>$\beta$ (bcc)</td>
<td>Single phase</td>
</tr>
</tbody>
</table>
Heat treatments
Heat treatment Results

Mg9Li 300 °C

Mg9Li 500 °C

Mg10Li 300 °C

Mg10Li 500 °C
Heat treatment Results

Mg11Li 300 °C

Mg11Li 500 °C

Mg12Li 300 °C

Mg12Li 500 °C
Compression Tests

Instron machine – cylindrical specimens
  \( d = 3.87 \text{ mm} \quad l = 6.80 \text{ mm} \)

Compression/deformation speed = 0.001 mm/s
Compression Tests

RT Compression Tests A

Stress (MPa) vs. Strain (%)

- Mg-10Li
- Mg-11Li
- Mg-12Li
- Mg-9Li
III: Future work - Bridging length-scales

- Binaries Mg-X (X = Al, Zn, Si,)
- Ternaries MgLi-X (X = Al, Zn, Cd, Ti, Ca, Pb, Mn)
  MgZn-X, MgAl-X (X = Li, Zn, Cd, Ti, Mn, RE)
- Solid phase transformation
  Phase diagram predictions

**Multiscale Materials Design**

**Ab initio Calculations**
(CASTEP, VASP)

**Thermodynamic Calculations**
(CALPHAD, Thermo-Calc)

**Phase-field Model (Microstructure)**

**Microstructure Evolution (OOF)***
Integrated set of Comp tools for Multicomponent Materials Design

First principles calculations and experiments

- Thermodynamic data of unary, binary and ternary systems
- Lattice parameters and interphase boundary energy
- Kinetic data of unary, binary and ternary systems

CALPHAD approach to data optimization

- Thermodynamic database for multicomponent systems
- Database for lattice parameters, elastic constants, and interfacial energies
- Kinetic database for multicomponent systems

A multicomponent phase-field model

- Simulated microstructure in 1, 2, and 3 dimensions
- Elastic constants of individual phases

OOF: Object-oriented finite element analysis of material microstructures

Mechanical response of simulated microstructure
Directions of Mg alloy development

Mordike et al - Germany
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