ABSTRACT

Mg alloys are promising materials for the automotive industry. The two-phase region of the Mg-Li system is of particular interest since the presence of both HCP and BCC phases exhibit better formability than the HCP phase alone. Al-Li alloys are of great interest for aeronautic applications because of their low specific weight, high stiffness and high strength. The chemical reactivity of lithium in the fabrication of the alloys influences the production techniques and the cost of the final product. Another concern is the thermal stability of certain phases when subjected to a temperature gradient induced upon heating or cooling during use of these products. Thermodynamic models describing the Gibbs free energy of the different phases of the Mg-Al-Li-Si are crucial for a better understanding of the various chemical phenomena observed in Mg-Al-Li-Si alloy production, shaping and application.

THERMODYNAMIC MODELING

Stoichiometric Compounds

<table>
<thead>
<tr>
<th>Stoichiometric Compounds</th>
<th>Binary Compounds</th>
<th>Ternary Compounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li$_2$Si</td>
<td>Li$_2$Mg</td>
<td>Li$_2$MgSi</td>
</tr>
<tr>
<td>Li$_2$Al</td>
<td>Li$_2$MgAl</td>
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<tr>
<td>Al$_4$Li$_4$</td>
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<tr>
<td>Al$_4$Li$_2$Mg</td>
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<td>Al$_4$Li$_2$Si</td>
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<td>Al$_4$Li$_2$MgSi</td>
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</tbody>
</table>

**Stoichiometric Compound Model**

$$G^*(T) = \Delta H^0 + T \Delta S^0 + TS^0$$

**Phases**

**THERMODYNAMIC DATA**

**Phases**

**Solid Solutions**

- Mg-HCP
- Li-BCC
- Al-FCC
- Si-Diaryon
- MgSi dissolving Li
- γ phases (Mg$_2$Al, Mg$_2$Li)
- ALi

**Liquid Solution**

In multicomponent liquid metallic solutions, some near-neighbour interactions can be strong enough to modify the configuration of the liquid (short-range-ordering).

The thermodynamic model must take this effect into account in the configurational entropy expression of the liquid phase.

**Modified Quasichemical Model – Pair Approximation**

$$G = \sum_{i,j,k \geq 0} n_i n_j n_k \ln \frac{X_{ij,k} X_{ji,k} X_{ki,j}}{X_{ij,k} X_{ji,k} X_{ki,j}}$$

**VALIDATION OF THE TERNARY MODEL**

**APPLICATION OF THE DATABASE**

I) Mg-Li Alloy Design

Moderate strength
Low formability
Good creep resistance

Good ductility
Low strength
Low creep resistance

II) Mg-Li-Al Alloy Elaboration

Casting of Mg-Li-Al alloys in sand molds (SiO$_2$

Reaction between the liquid and SiO$_2$

Evolution of the Composition of the Liquid Alloy

Effect of Si in Mg-Li-Al Alloys during Equilibrium Cooling

Scheil Cooling of a Mg-Li-Al Alloy

Heat of formation
Heat capacity
EMF
ab initio calculations
Phase diagram data (liquidus, eutectic, XRD)

Heat of mixing
EMF
Defect concentrations
XRD analysis
Microprobe analysis
Phase diagram data
Vapor pressure