Thermodynamic assessment of the Co-Mg binary system

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The RE-Mg-T (RE=rare earth and T=d-transition metals) alloys have attracted extensive attention due to their excellent properties, such as outstanding hydrogen storage capacity, high strength, good corrosion resistance and magnetic properties. As an important sub-system in RE-Mg-T alloys, the Co-Mg alloys can also be used as hydrogen storage materials because of their high theoretical capacity and high hydrogen volume density. To develop the hydrogen storage materials, a reliable knowledge of phase equilibria and thermodynamic properties for the Co-Mg system is of great interest.

4. Conclusion

Based on the reliable literature data, the Co-Mg binary system has been thermodynamically assessed with the aid of CALPHAD method and the following conclusions were drawn:

- A new set of self-consistent thermodynamic parameters has been obtained by critically evaluating literature data.
- The calculated phase diagram and the thermodynamic properties are in good agreement with the experimental values.

The step-by-step optimization procedure was utilized in the present work. Reliable experimental data for the Co-Mg system was employed in the optimization and each piece of experimental information was given a certain weight, which can be changed in view of the experimental errors. The thermodynamic optimization began with the MgCo\textsubscript{2} compound. Afterwards, the thermodynamic parameters of liquid phase were evaluated. Next, the parameters for the HCP\_A3 phase was introduced to describe the HCP\_A3 phase and fit the invariant equilibrium among liquid, (\(\alpha\)Co) and MgCo\textsubscript{2}. Finally, the thermodynamic parameters for all phases were adjusted simultaneously by considering all the phase diagram and thermodynamic data used in the optimization.

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1. Introduction

The Co-Mg binary system has been experimentally investigated and critically reviewed by Nayeb-Hashemi and Clark. However, only a few experimental studies were reported on the whole Co-Mg binary system. The tentative Co-Mg equilibrium phase diagram reported by Smith and Smith is shown in Fig. 1.

In the present work, the Co-Mg binary system has been investigated by means of CALPHAD (CALculation of PHAse Diagram) approach.

2. Thermodynamic models

<table>
<thead>
<tr>
<th>Phases</th>
<th>Thermodynamic models</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid phase</td>
<td>(Co\textsubscript{0.333}Mg\textsubscript{0.6667})</td>
</tr>
<tr>
<td>Stoichiometric compound MgCo\textsubscript{2}</td>
<td>(Mg\textsubscript{0.333}Co\textsubscript{0.6667})</td>
</tr>
<tr>
<td>Solution phase HCP_A3</td>
<td>(Co,Mg)\textsubscript{1}</td>
</tr>
</tbody>
</table>

3. Thermodynamic calculation

The assessed phase diagram of Co-Mg system reported by Smith and Smith is shown in Fig. 1.

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