中南大学 Central South University

相图、相变及材料智能设计与制备中心(中南大学)
Center for Phase Diagram, Phase Transition, Intelligent Materials Design and Preparation
中德“电化学存储系统的集成计算材料工程”联合实验室(中南大学 德国KIT)
Sino-German Cooperation Group "Integrated Computing Materials Enginnering for Electrochemical Storage System"
中德“微结构”联合实验室(中南大学 德国波鸿鲁尔大学)
Sino-German Cooperation Group "Microstructure"

Thermodynamic assessment of the Co-Mg binary system

Lianfeng Yang[a], Xudong Si[a], Huaqing Zhang[a], Yuling Liu[a]*, Yinping Zeng[a]*, Yong Du[a], Yaru Wang[b]

[a] State Key Laboratory of Powder Metallurgy ,Central South University, Changsha, Hunan 410083, China

[b] Hebei Key Laboratory of Advanced Materials for Transportation Engineering and Environment, School of materials science and Engineering, Shijiazhuang Tiedao University, Shijiazhuang, Hubei 050043, China

2021/4/27

1. Introduction

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.

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.

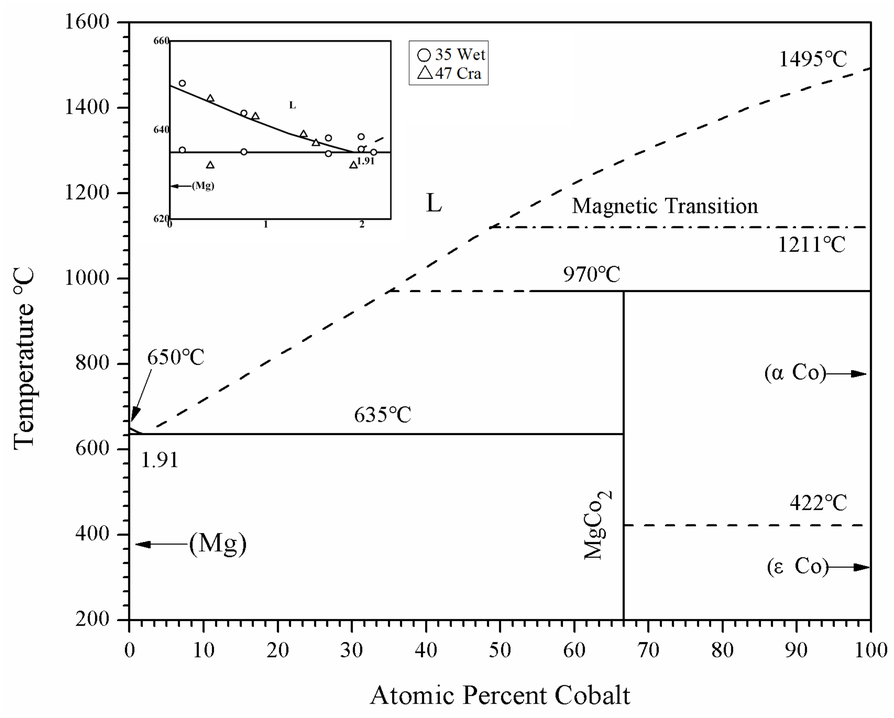

Figure 1. The assessed phase diagram of Co-Mg system reported by Smith and Smith.

2. Thermodynamic models

Phases	Thermodynamic models
Liquid phase	$(Co,Mg)_1$
Stoichiometric compound $MgCo_2$	$(Mg)_{0.3333}(Co)_{0.6667}$
Solution phase HCP_A3	$(Co,Mg)_1$

3. Thermodynamic calculation

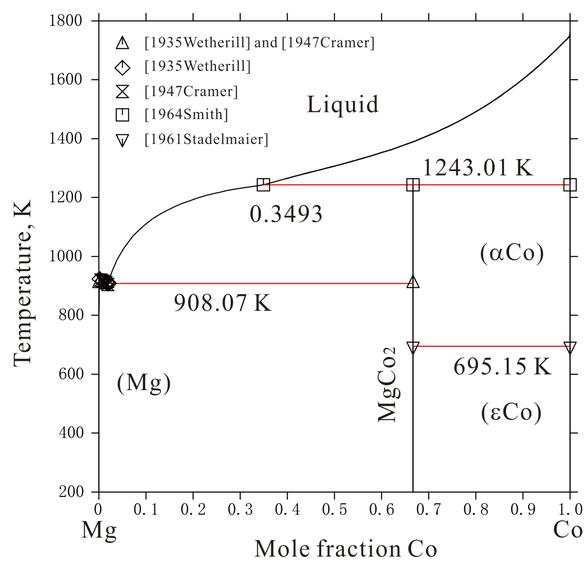

Figure 2. Calculated phase diagram of Co-Mg system compared with the experimental data

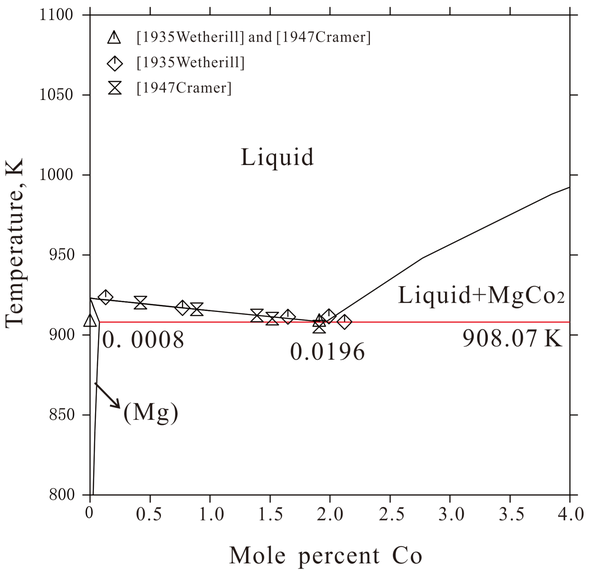

Figure 3. Calculated phase diagram of Co-Mg system: enlarged Mg-rich side

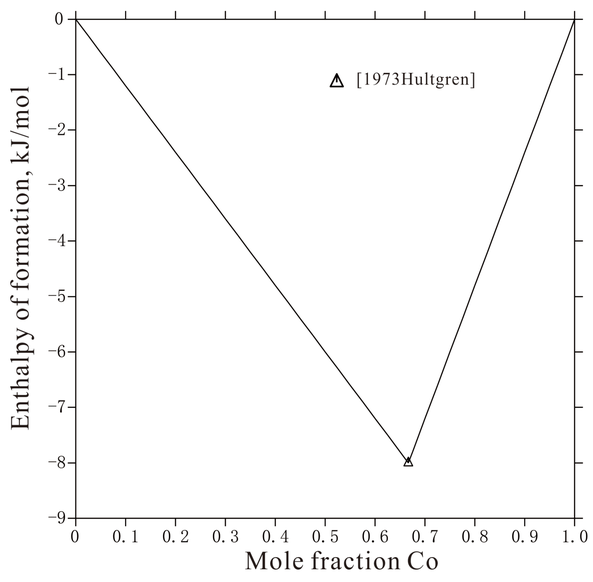

Figure 4. Enthalpy of formation of the solid phases at 800 K referred to hexagonal Co and Mg

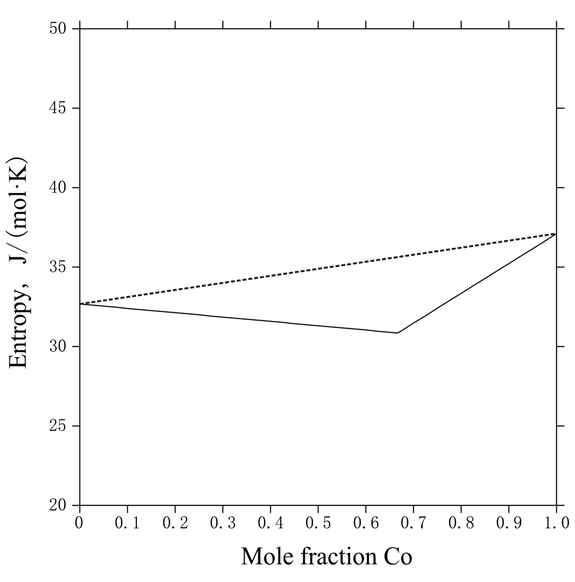

Figure 5. Calculated entropy at 298.15 K in the Co-Mg system

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 $MgCo_2$ 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, (αCo) and $MgCo_2$. Finally, the thermodynamic parameters for all phases were adjusted simultaneously by considering all the phase diagram and thermodynamic data used in the optimization.

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 financial supports form the following foundations are acknowledged:

- National Natural Science Foundation of China.

Your questions and suggestions are welcomed: Yanglf@csu.edu.cn

State Key Lab of Powder Metallurgy Central South University