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Letter to Editor

THERMODYNAMIC ASSESSMENT OF THE Co-Mg BINARY SYSTEM

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Abstract

No thermodynamic description was performed for the Co-Mg binary system according to literature review. Consequently, this binary system has been investigated by means of CALPHAD (CALculation of PHAse Diagrams) approach in the present work. The experimental phase diagram and thermodynamic data available in the literature were critically assessed. Based on the reliable literature data, a new set of self-consistent thermodynamic parameters for the Co-Mg system is obtained. The calculated results agree well with the experimental data from the literature, indicating the reasonability of the present thermodynamic optimization.

Keywords: *Co-Mg binary system; Phase diagram; Thermodynamic property; CALPHAD method*

1. Introduction

Recently, the RE-Mg-T (RE=rare earth metals and T=d-transition metals, such as Co, Ni and Cu) alloys have attracted extensive attention due to their excellent properties [1], such as outstanding hydrogen storage capacity [2, 3], high strength [4], good corrosion resistance, and magnetic properties [5]. As an important sub-system in RE-Mg-T alloys, the Co-Mg alloys can be used as hydrogen storage materials because of their high theoretical capacity and high hydrogen volume density [6]. Besides, the Co-Mg alloys can be utilized as magnetic recording materials [7], mechanical load sensors [8], and other magnetic properties applications [9] because of their unique magnetic properties. To expand the Co-Mg alloys' applications, reliable knowledge of phase equilibria and thermodynamic properties in the Co-Mg system is of great interest. The Co-Mg binary system has been experimentally investigated [10-14] and critically reviewed by Nayeb-Hashemi and Clark [15]. According to the literature review, the phase diagram of the Co-Mg system has been initially established, but so far no thermodynamic description is performed for the Co-Mg system. The CALPHAD method is a useful tool to establish thermodynamic databases [16]. Based on the thermodynamic databases, materials can be developed with lower costs and less time [17]. Besides, the CALPHAD method can also be used to predict interfacial energies for it is more accurate to find Gibbs energies through thermodynamic evaluations [18]. Therefore, the CALPHAD method was applied to investigate the Co-Mg system in the present work.

According to the experimental results from Wetherill [10], the eutectic reaction of Liquid ↔ (Mg) + $MgCo_2$ was determined to occur at 908.15 K with the eutectic composition of 2.12 at.% Co by using thermal analysis. Cramer et al. [11] also studied this eutectic reaction by means of thermal analysis and this eutectic point was placed at 1.91 at.% Co and 905.15 K, which is close to the eutectic point reported by Wetherill [10].

Besides, Smith and Smith [13] reported that the eutectic reaction temperature was 908.15 K, which agreed well with that reported by Wetherill [10] and Cramer et al. [11]. In the assessed Co-Mg binary phase diagram reported by Smith and Smith [13], which is shown in Fig. 1, the eutectic point was placed at 1.91 at.% Co and 908.15 K.

Nayeb-Hashemi and Clark [15] critically assessed the works of Wetherill [10], Cramer et al. [11], Raynor [12], and Smith and Smith [13]. They placed the eutectic point at 1.91 at% Co and 908.15 K, which was reliable and was considered in the present optimization.

Smith and Smith [13] also studied the peritectic reaction Liquid + (αCo) ↔ $MgCo_2$ by analyzing the heating and cooling curves of alloys with the compositions from 9 to 82.6 at.% Co and the peritectic temperature was determined to be 1243.15 K.

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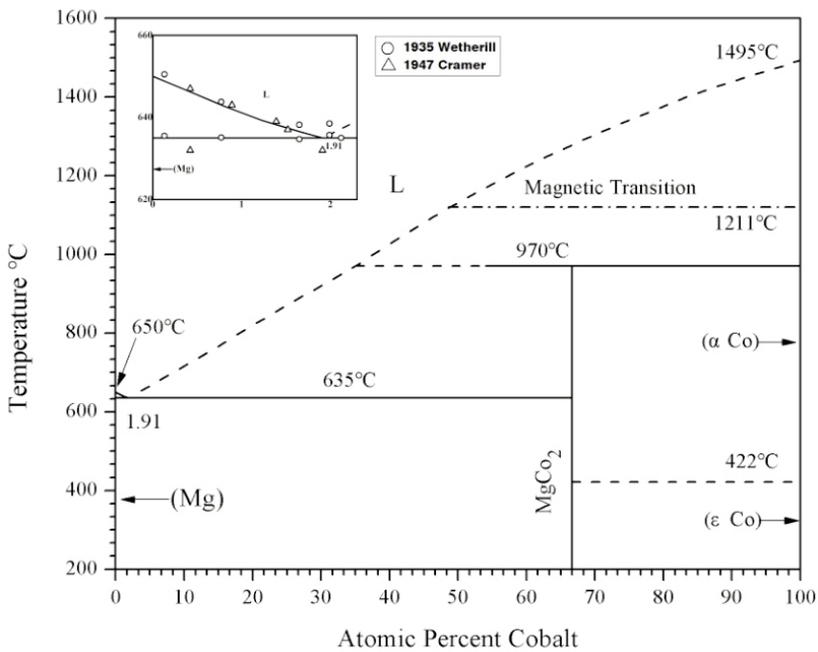

Figure 1. *The Co-Mg phase diagram assessed by Smith and Smith [13]*

Several researchers predicted the existence of following compounds: $MgCo_2$ [13, 14], Mg_2Co [11, 19, 20], MgCo [21-23], and Mg_2Co_3 [24]. Based on the diffusion couple with thermal analysis, metallography, and X-ray analyses, $MgCo_2$ compound was confirmed to be formed by the peritectic reaction of Liquid + (αCo) ↔ $MgCo_2$, and there is no evidence indicating the possible existence of Mg_2Co, MgCo, and Mg_2Co_3 phases according to Ref. [13]. Analyzing the lattice parameters, the authors [13] also found that the solid solubilities of Co in (Mg) and Mg in (Co) are all negligible. According to Hultgren et al. [25], the enthalpy of formation of $MgCo_2$ was determined to be -8 kJ/mole·atoms at 800 K by vapor-pressure measurement. Besides, the enthalpy of formation of $MgCo_2$ calculated by means of the first-principles calculations is -10 kJ/mole·atoms, which is included in the Materials Project [26]. In the present thermodynamic optimization, the enthalpy of formation of $MgCo_2$ from Hultgren et al. [25] was used because the experimental one is preferable.

As mentioned above, so far there is no thermodynamic optimization for the Co-Mg system in the literature. Thus, the purpose of the present work is to provide a consistent set of thermodynamic parameters for the Co-Mg system by means of the CALPHAD approach.

2. Thermodynamic model

2.1. Pure elements

Thermodynamic parameters for pure elements of Co and Mg are expressed as following:

$$G_i^{\varphi}(T) - H_i^{SER} = a + b \cdot T + c \cdot T \ln(T) + d \cdot T^2 + e \cdot T^3 + f \cdot T^{-1} + g \cdot T^7 + h \cdot T^9 \quad (1)$$

where H_i^{SER} is the mole enthalpy of pure element *i* (*i*=Co, Mg) at 298.15 K and 101325 Pa in its standard element reference (SER) state, and *T* is the absolute temperature. The thermodynamic coefficients *a* to *h* were taken from the Scientific Group Thermodata Europe (SGTE) database [27].

2.2. The stoichiometric compound $MgCo_2$

Since there is no solid solubility data for $MgCo_2$ compound, $MgCo_2$ is represented as a stoichiometric compound. Its Gibbs energy is expressed as following:

$$G^{MgCo_2} = \Delta^f G^{MgCo_2} + (1/3) \cdot {}^0G_{Mg}^{SER} + (2/3) \cdot {}^0G_{Co}^{SER} \quad (2)$$

${}^0G_{Mg}^{SER}$ and ${}^0G_{Co}^{SER}$ represent the mole Gibbs energy of the components Mg and Co with a stable crystal structure at 298.15 K and 101325 Pa, respectively. $\Delta^f G^{MgCo_2}$ is the Gibbs energy of formation for $MgCo_2$ compound, which can be expressed as $\Delta^f G^{MgCo_2} = a + b \cdot T$. The parameters *a* and *b* will be evaluated in this work according to experimental phase diagram and enthalpy of formation data.

2.3. Solution phases

In the Co-Mg binary system, there are three solution phases the liquid phase, the FCC_A1 phase and the HCP_A3 phase which are modeled as completely disordered solution phases. The Gibbs

energies of solution phases are described through Redlich-Kister polynomial [28]:

$$G^{\varphi} - H^{SER} = x_{Co}\,{}^{0}G^{\varphi}_{Co} + x_{Mg}\,{}^{0}G^{\varphi}_{Mg} + RT\left(x_{Co}\ln x_{Co} + x_{Mg}\ln x_{Mg}\right) + x_{Co}x_{Mg}\sum_{i=0}^{n}{}^{(i)}L^{\varphi}_{Co,Mg}\left(x_{Co}-x_{Mg}\right)^{i} \quad (3)$$

where H^{SER} is the abbreviation of $x_{Co}\cdot{}^{0}H^{SER}_{Co} + x_{Mg}\cdot{}^{0}H^{SER}_{Mg}$ x_{Co} and x_{Mg} represent the mole fractions of Co and Mg, respectively. ${}^{0}G^{\varphi}_{Co}$ and ${}^{0}G^{\varphi}_{Mg}$ are the Gibbs energies of Co and Mg in the φ phase, respectively. R is the gas constant (R=8.314 J/(mol·K)). The last term is the excess Gibbs energy and ${}^{(i)}L^{\varphi}_{Co,Mg}$ represents the interaction of Co and Mg in the φ phase and can be expressed as ${}^{(i)}L^{\varphi}_{Co,Mg}=a^{\varphi}_{i}+b^{\varphi}_{i}$, where a^{φ}_{i} and b^{φ}_{i} are the interaction parameters which will be evaluated based on the experimental phase diagram data [29].

3. Results and discussion

Table 1 summarizes the experimental phase diagram and thermodynamic data in the literature [10, 11, 13, 25]. Table 2 lists the thermodynamic parameters obtained in the present work by using the PARROT module of the Thermo-Calc software [30], which is based on minimizing the sum of squares of the differences between the experimental values and the computed ones [31, 32]. In the process of optimization, 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, and the parameter for a in $\Delta^{f}G^{MgCo_2}$ was adjusted to reproduce the experimental data of enthalpy of formation for $MgCo_2$ compound at 800 K. Afterwards, the thermodynamic parameters of liquid phase were evaluated. Considering the experimental, the eutectic reaction Liquid ↔ (Mg) + $MgCo_2$, the parameters of liquid phase, a_0^{liquid} and b_0^{liquid}, were introduced to describe the liquid phase and these parameters were still needed to be adjusted according to the experimental data of liquidus. If only these parameters were used, the peritectic reaction Liquid + (αCo) ↔ $MgCo_2$ in Co-Mg binary phase digram was described as a eutectic reaction Liquid ↔ (αCo) + $MgCo_2$. Consequently, a parameter of HCP_A3 phase, $a_0^{HCP\_A3}$, was introduced to describe the HCP_A3 phase and fit the invariant equilibrium among liquid, (αCo) and $MgCo_2$, which was determinded to be a peritectic reaction by Smith and Smith [13]. Finally, the thermodynamic parameters for all phases were adjusted simultaneously by considering all the phase diagram and thermodynamic data used in the optimization.

The calculated Co-Mg phase diagram using this set of thermodynamic parameters along with the experimental phase diagram data is presented in Fig. 2 and the enlarged Mg-rich side is demonstrated in Fig. 3. The calculated invariant reactions are given in Table 3 together with the experimental data. It can be seen that the calculated phase diagram is in good agreement with the experimental phase diagram data.

The calculated enthalpy of formation for $MgCo_2$ compound at 800 K together with the data from experiment and the first-principles calculations is shown in Fig. 4. Compared with the data from the first-principles calculations [26], the presently computed enthalpy of formation for $MgCo_2$ compound agrees better with the experimental data from Hultgren et al. [25].

In order to further check the reliability of the present thermodynamic parameters, the computed entropy at 298.15 K is presented in Fig. 5. It can be seen from the figure that the distance to the straight line which connects the entropies of the stable elements of Co and Mg is simply the entropy of formation (ΔS). And this entropy of formation is not excessively large, usually in the range of [-10 to 10 J/(mol-atoms·K)] [33]. This further verifies the

Table 1. *Summary of the experimental data used in the optimization*

Type of Experimental Data	References	Method
Liquidus: 0.13~2.12 at.% Co	[10]	Thermal analysis
Liquidus: 0.42~1.91 at.% Co	[11]	Thermal analysis
Composition of liquid phase for the eutectic reaction L ↔ (Mg) + $MgCo_2$	[11]	Metallography, thermal analysis
Temperature for the eutectic reaction L ↔ (Mg) + $MgCo_2$	[10]	Thermal analysis
Temperature for the peritectic reaction L + (αCo) ↔ $MgCo_2$	[13]	Metallography, thermal analysis X-ray diffraction (XRD)
$\Delta_f H(MgCo_2)$	[25]	Vapor-pressure measurement

Table 2. *Summary of the optimized thermodynamic parameters for the Co-Mg system in the present work*

Phase	Model	Parameters
Liquid	(Co, Mg)	${}^{0}L^{liquid}_{Co,Mg}=24444.11-7.199\cdot T$
$MgCo_2$	$(Mg)_{0.3333}(Co)_{0.6667}$	$\Delta_f G^{MgCo_2}=-8000+4.771\cdot T$
HCP_A3	(Co, Mg)	${}^{0}L^{HCP\_A3}_{Co,Mg}=48632.53$

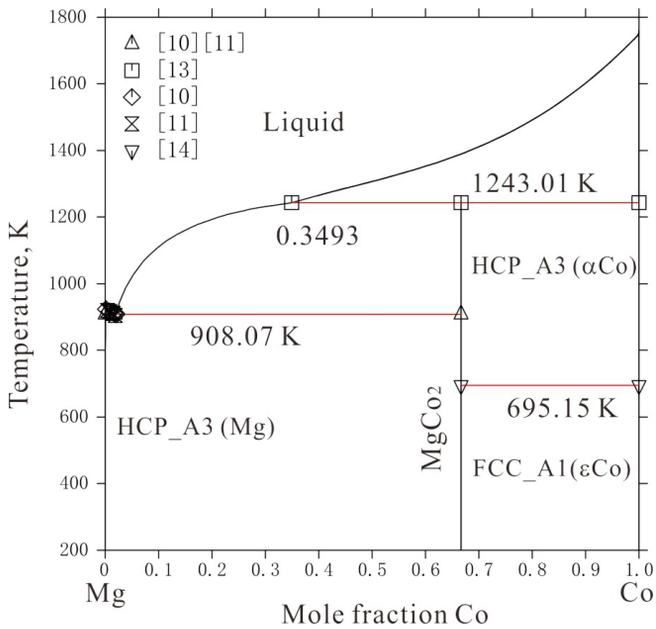

Figure 2. *Calculated phase diagram of Co-Mg system compared with the experimental data [10, 11, 13, 14]*

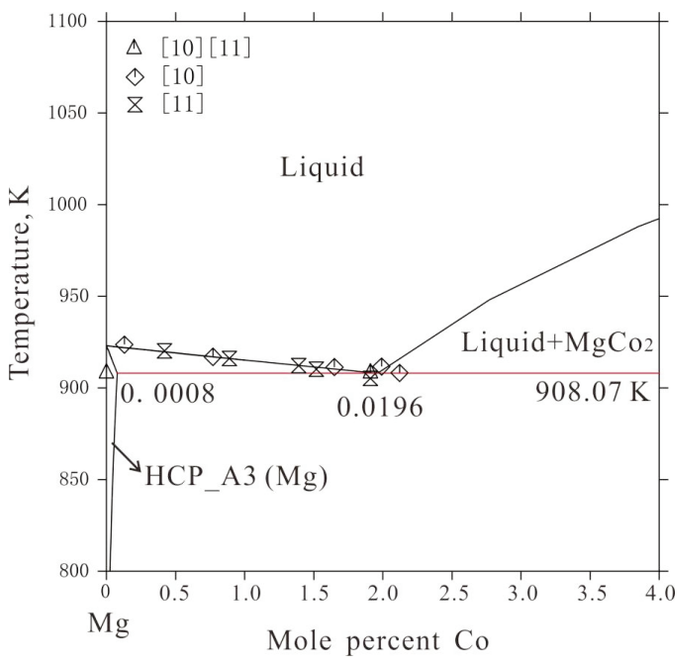

Figure 3. *Calculated phase diagram of Co-Mg system: enlarged Mg-rich side compared with the experimental data [10, 11]*

Table 3. *Calculated invariant reactions compared with the literature data in the Co-Mg system*

Invariant reactions	T/K	Composition/at.% Co			Reference
$L \leftrightarrow (Mg) + MgCo_2$	908.15	0.0212	0	0.6667	[10]
	906.15	0.0191	0	0.6667	[11]
	908.07	0.0196	0.0008	0.6667	This work
$L + (\alpha Co) \leftrightarrow MgCo_2$	1243.15	-	1	0.6667	[13]
	1243.01	0.3493	1	0.6667	This work

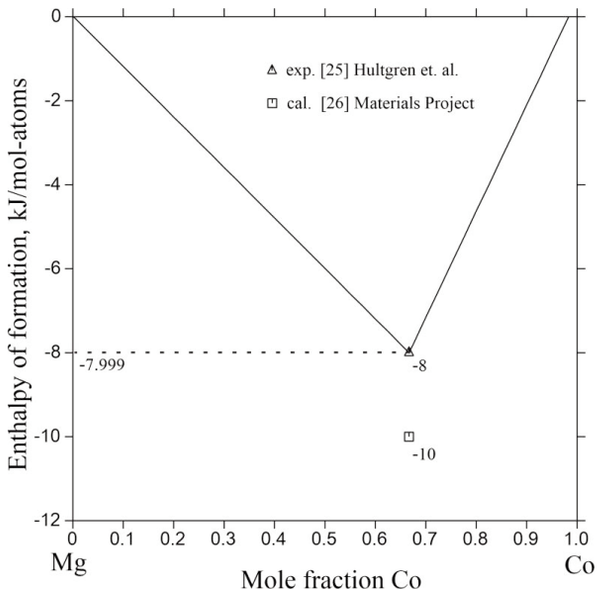

Figure 4. *Calculated enthalpy of formation of the solid phases at 800 K referred to hexagonal Co and Mg compared with the data from experiment and the first-principles calculations [25, 26]*

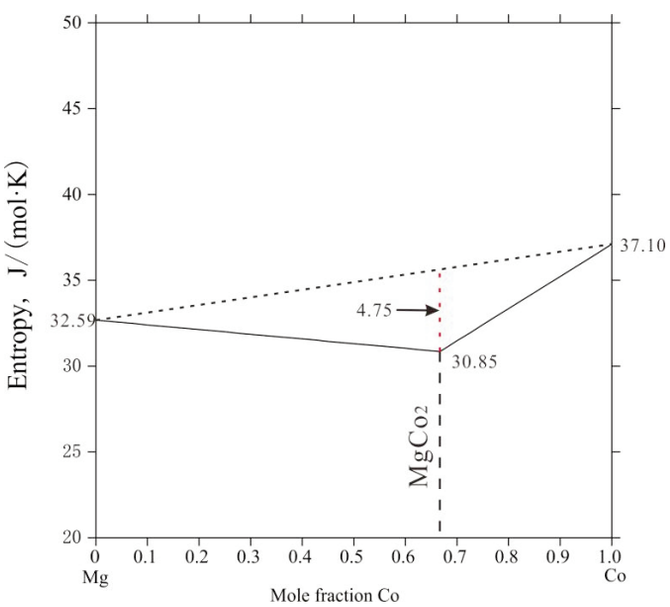

Figure 5. *Calculated entropy at 298.15 K in the Co-Mg system*

reliability of the presently obtained thermodynamic parameters.

The present assessment can be used as a key subsystem in the development of thermodynamic databases for multicomponent systems which contain Co-Mg system, such as La-Mg-T systems (T = metals belonging to the last transition groups). In fact, many phase diagrams in the La-Mg-T systems are still under exploring, and new compounds are continuously being detected, showing interesting structural and bonding peculiarities. Therefore, the thermodynamic description in the La-Mg-T systems is needed for expanding the application of these alloys.

4. Conclusions

Based on the reliable literature data, the Co-Mg binary system has been thermodynamically assessed with the aid of CALPHAD method. A new set of self-consistent thermodynamic parameters has been obtained by critically evaluating literature data. The calculated phase diagram and thermodynamic

properties are in good agreement with the experimental values, which confirms the reliability of this set of thermodynamic parameters. The thermodynamic description in the Co-Mg system is of interest to the development of the Co-Mg based alloys.

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Author contributions

Lianfeng Yang: Investigation, Writing-original draft, Writing-review & editing. Xudong Si: Methodology, Investigation. Huaqing Zhang: Methodology, Writing-review & editing. Fengyang Gao: Methodology, Investigation. Yinping Zeng: Methodology, Investigation, Writing-review & editing. Yuling Liu: Conceptualization, Methodology, Writing-review & editing. Yaru Wang: Writing-review & editing. Yong Du: Conceptualization, Supervision, Writing-review & editing.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflict of interest

The authors declare that they have no known conflict financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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TERMODINAMIČKA EVALUACIJA Co-Mg BINARNOG SISTEMA

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Apstrakt

Prema pregledu literature, za Co-Mg binarni sistem nije urađena termodinamička evaluacija. Zato je u ovom radu ovaj binarni sistem ispitivan uz pomoć CALPHAD (CALculation of PHAse Diagrams) metoda. Kritički su procenjeni fazni dijagram i termodinamički podaci koji su dostupni u literaturi. Na osnovu pouzdanih podataka iz literature, dobijen je novi skup samodoslednih termodinamičkih parametara za Co-Mg sistem. Izračunati rezultati su u saglasnosti sa eksperimentalnim podacima iz literature, što ukazuje na prihvatljivost predstavljene termodinamičke optimizacije.

Ključne reči: *Co-Mg binarni sistem; Fazni dijagram; Termodinamičke osobine; CALPHAD metod*