RARE METALS
Vol. 25, No. 5, Oct 2006, p. 492

Thermodynamic modeling of the La-Mg-Y system and Mg-based alloys database

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(Received 2006-06-20)

Abstract: As an example of the La-Mg-Y system, the method how to set up the thermodynamic model of individual phases was introduced in the process of thermodynamic optimization. The solution phases (liquid, body-centered cubic, face-centered cubic, hexagonal close-packed and double hexagonal close-packed) were modeled with the Redlich-Kister equation. The compound energy model has been used to describe the thermodynamic functions of the intermetallic compounds in the La-Mg-Y systems. The compounds Mg_2Y, $Mg_{24}Y_5$, $Mg_{12}La$, $Mg_{17}La_2$, $Mg_{41}La_5$, Mg_3La and Mg_2La in the La-Mg-Y system were treated as the formulae $(Mg,Y)_2(La,Mg,Y)$, $Mg_{24}(La,Mg,Y)_4Y$, $Mg_{12}(La,Y)$, $Mg_{17}(La,Y)_2$, $Mg_{41}(La,Y)_5$, $Mg_3(La,Mg,Y)$ and $Mg_2(La,Y)$, respectively. A model $(La,Mg,Y)_{0.5}(La,Mg,Y)_{0.5}$ was applied to describe the compound MgM formed by MgLa and MgY in order to cope with the order-disorder transition between body-centered cubic solution (A2) and MgM with CsCl-type structure (B2) in the La-Mg-Y system. The Gibbs energies of individual phases were optimized in the La-Mg, La-Y and La-Mg-Y systems by CALPHAD technique. The projection of the liquidus surfaces for the La-Mg-Y system was predicted. The Mg-based alloys database including 36 binary and 15 ternary systems formed by Mg, Al, Cu, Ni, Mn, Zn and rare earth elements was set up in SGTE standard.

Key words: La-Mg-Y system; thermodynamic modeling; CALPHAD technique; order-disorder transition; Mg-based alloys database

[*This work was financially supported by the National Natural Science Foundation of China (Nos. 50471095 and 50271008).*]

1. Introduction

Magnesium and its alloys are becoming widely recognized as playing an increasingly important role in automotive and electronic products. The optimization of alloys composition and heat-treatment conditions is impossible without the knowledge of phase equilibria.

The isothermal sections of the Mg-rich side in the La-Mg-Y system at 773 K were determined by Giovannini *et al.* [1, 2]. Dobatkion *et al.* [3] investigated phase equilibria in the Mg corner up to 20 wt.% La and 20 wt.% Y at 500 and 300°C. Four vertical sections of the Mg-rich side in the La-Mg-Y system at $w(La) = 0.10$, $w(Y) = 0.22$, from Mg + 30 wt.% Y to Mg + 20 wt.% La and from Mg + 20 wt.% Y to Mg + 10 wt.% La were studied by Padezhnova *et al.* [4]. Based on these experimental results, the thermodynamic description of the La-Mg-Y system was obtained by means of CALPHAD (CALculation of PHAse Diagram) technique.

In order to obtain thermodynamic description of a multi-component system, a thermodynamic description of each lower-order system is necessary. The Mg-Y [5, 6] and La-Mg [7] systems have been optimized. In the present work, the La-Y and La-Mg systems were optimized in order to coincide exactly with the ternary phase equilibria in the La-Mg-Y system.

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2. Thermodynamic model

2.1. Solution phases

In the La-Mg-Y system, there are three solution phases: liquid, body-centered cubic (bcc), face-centered cubic (fcc), hexagonal close-packed (hcp) and double hexagonal close-packed (dhcp). Their Gibbs energies are described by the following expression:

$$G_{\mathrm{m}}^{\phi} = x_{\mathrm{La}}G_{\mathrm{La}}^{\phi}(T) + x_{\mathrm{Mg}}G_{\mathrm{Mg}}^{\phi}(T) + x_{\mathrm{Y}}G_{\mathrm{Y}}^{\phi}(T) + RT(x_{\mathrm{La}}\ln x_{\mathrm{La}} + x_{\mathrm{Mg}}\ln x_{\mathrm{Mg}} + x_{\mathrm{Y}}\ln x_{\mathrm{Y}}) + G_{\mathrm{m}}^{E,\phi} \tag{1}$$

where x_{La}, x_{Mg} and x_{Y} are the mole fractions of the pure elements La, Mg and Y, respectively; $G_{\mathrm{m}}^{E,\phi}$ is the excess Gibbs energy, expressed by the Redlich-Kister polynomial,

$$\begin{aligned} G_{\mathrm{m}}^{E,\phi} = {} & x_{\mathrm{La}}x_{\mathrm{Mg}}\sum_i {}^{i}L_{\mathrm{La,Mg}}^{\phi}(x_{\mathrm{La}} - x_{\mathrm{Mg}})^i + \\ & x_{\mathrm{La}}x_{\mathrm{Y}}\sum_i {}^{i}L_{\mathrm{La,Y}}^{\phi}(x_{\mathrm{La}} - x_{\mathrm{Y}})^i + \\ & x_{\mathrm{Mg}}x_{\mathrm{Y}}\sum_i {}^{i}L_{\mathrm{Mg,Y}}^{\phi}(x_{\mathrm{Mg}} - x_{\mathrm{Y}})^i + \\ & x_{\mathrm{La}}x_{\mathrm{Mg}}x_{\mathrm{Y}}L_{\mathrm{La,Mg,Y}}^{\phi} \end{aligned} \tag{2}$$

where ${}^{i}L_{\mathrm{La,Mg}}^{\phi}$, ${}^{i}L_{\mathrm{La,Y}}^{\phi}$ and ${}^{i}L_{\mathrm{Mg,Y}}^{\phi}$ are the interaction parameters between elements La and Mg, La and Y, and Mg and Y, respectively; $L_{\mathrm{La,Mg,Y}}^{\phi}$ is the ternary interaction parameter.

2.2. Line intermetallic compounds $\mathbf{Mg}_m\mathbf{(La,Y)}_n$

The intermetallic compounds Mg_2La, $Mg_{17}La_2$, $Mg_{12}La$ and $Mg_{41}La_5$ in the La-Mg system were treated as the stoichiometric compounds. In the La-Mg-Y system, these compounds extend into the ternary system with constant Mg content, i.e. they have partial solubility of other components with preferential substitution for one of the binary elements. In the present work, they are treated as the formula $Mg_m(La,Y)_n$ by a two-lattice model [8, 9] with La and Y on the second sublattice and Mg on the first one. The Gibbs energy per mole of formula unit Mg_mLa_n is expressed as follows:

$$\begin{aligned} G_{\mathrm{m}}^{\mathrm{Mg}_m\mathrm{La}_n} = {} & y_{\mathrm{La}}G_{\mathrm{Mg:La}}^{\mathrm{Mg}_m\mathrm{La}_n} + y_{\mathrm{Y}}G_{\mathrm{Mg:Y}}^{\mathrm{Mg}_m\mathrm{La}_n} + \\ & nRT(y_{\mathrm{La}}\ln y_{\mathrm{La}} + y_{\mathrm{Y}}\ln y_{\mathrm{Y}}) + \\ & y_{\mathrm{La}}y_{\mathrm{Y}}\sum_i {}^{i}L_{\mathrm{Mg:La,Y}}^{\mathrm{Mg}_m\mathrm{La}_n}(y_{\mathrm{La}} - y_{\mathrm{Y}})^i \end{aligned} \tag{3}$$

where y_{La} and y_{Y} are the site fractions of La or Y on the second sublattice; two parameters denoted $G_{\mathrm{Mg:La}}^{\mathrm{Mg}_m\mathrm{La}_n}$ and $G_{\mathrm{Mg:Y}}^{\mathrm{Mg}_m\mathrm{La}_n}$ represent the Gibbs energies of the compound Mg_mLa_n when the second sublattice is occupied by only one element La or Y ($y_{\mathrm{La}}=1$ or $y_{\mathrm{Y}}=1$), respectively, which are relative to the enthalpies of pure dhcp for La and hcp for Mg and Y in their SER state; ${}^{i}L_{\mathrm{Mg:La,Y}}^{\mathrm{Mg}_m\mathrm{La}_n}$ represents the *i*th interaction parameters between the elements La and Y on the second sublattice.

2.3. Non-Line intermetallic compounds

The intermetallic compound $Mg_{24}Y_5$ in the La-Mg-Y system is treated as $Mg_{24}(La,Mg,Y)_4Y$. The Gibbs energy per mole of formula unit $Mg_{24}Y_5$ is expressed as follows:

$$\begin{aligned} G^{\mathrm{Mg}_{24}\mathrm{Y}_5} = {} & y_{\mathrm{La}}G_{\mathrm{Mg:La:Y}}^{\mathrm{Mg}_{24}\mathrm{Y}_5} + y_{\mathrm{Mg}}G_{\mathrm{Mg:Mg:Y}}^{\mathrm{Mg}_{24}\mathrm{Y}_5} + y_{\mathrm{Y}}G_{\mathrm{Mg:Y:Y}}^{\mathrm{Mg}_{24}\mathrm{Y}_5} + 4RT(y_{\mathrm{La}}\ln y_{\mathrm{La}} + y_{\mathrm{Mg}}\ln y_{\mathrm{Mg}} + y_{\mathrm{Y}}\ln y_{\mathrm{Y}}) + \\ & y_{\mathrm{La}}y_{\mathrm{Mg}}\sum_i {}^{i}L_{\mathrm{Mg:La,Mg:Y}}^{\mathrm{Mg}_{24}\mathrm{Y}_5}(y_{\mathrm{La}} - y_{\mathrm{Mg}})^i + y_{\mathrm{La}}y_{\mathrm{Y}}\sum_i {}^{i}L_{\mathrm{Mg:La,Y:Y}}^{\mathrm{Mg}_{24}\mathrm{Y}_5}(y_{\mathrm{La}} - y_{\mathrm{Y}})^i + \\ & y_{\mathrm{Mg}}y_{\mathrm{Y}}\sum_i {}^{i}L_{\mathrm{Mg:Mg,Y:Y}}^{\mathrm{Mg}_{24}\mathrm{Y}_5}(y_{\mathrm{Mg}} - y_{\mathrm{Y}})^i + y_{\mathrm{La}}y_{\mathrm{Mg}}y_{\mathrm{Y}}L_{\mathrm{Mg:La,Mg,Y:Y}}^{\mathrm{Mg}_{24}\mathrm{Y}_5} \end{aligned} \tag{4}$$

where y_{La}, y_{Mg} and y_{Y} are the site fractions of La, Mg or Y on the second sublattice; the parameter denoted $G_{\mathrm{Mg:*:Y}}^{\mathrm{Mg}_{24}\mathrm{Y}_5}$ represent the Gibbs energies of the compound $Mg_{24}Y_5$ when the second sublattice is occupied by only one element La, Mg or Y ($y_{\mathrm{La}}=1$, $y_{\mathrm{Mg}}=1$ or $y_{\mathrm{Y}}=1$), respectively, which are relative to the enthalpies of pure dhcp for La and hcp for Mg and Y in their SER state; ${}^{i}L_{\mathrm{Mg:*,*:Y}}^{\mathrm{Mg}_{24}\mathrm{Y}_5}$ represents the *i*th interaction parameters between the elements La and Mg, La and Y and Mg and Y on the second sublattice; ${}^{i}L_{\mathrm{Mg:La,Mg,Y:Y}}^{\mathrm{Mg}_{24}\mathrm{Y}_5}$ is the ternary interaction parameter.

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