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Transactions of Nonferrous Metals Society of China

www.tnmsc.cn



Trans. Nonferrous Met. Soc. China 34(2024) 1091-1109

Phase equilibria and solidification behavior of Mg-Al-Gd casting alloys

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Received 7 November 2022; accepted 5 May 2023

Abstract: The Mg–Al–Gd ternary system was re-assessed by the CALPHAD (CALculation of PHAse Diagrams) method and a set of self-consistent thermodynamic parameters of the system were obtained. The long-period stacking ordered (LPSO) phases, 14H and 18R, were described by thermodynamic model of Mg_x(TM,Mg)₆(RE,Mg)₈ (TM=Transition Metal, RE=Rare Earth). Representative isothermal sections, vertical sections, liquidus projections and the related invariant reactions were calculated and compared with the experimental data, showing the reliability of the obtained thermodynamic parameters. Reaction scheme for the whole ternary system was also presented. The Scheil solidification paths and the phase fractions of several Mg–Al–Gd alloys were calculated and analyzed. The phase formation during solidification and the phase content of γ and LPSO phases are clearly described with the increase of Gd content, which is crucial to the microhardness, ultimate tensile strength and yield strength of Mg–Al–Gd casting alloys.

Key words: thermodynamic modeling; CALPHAD; Mg-Al-Gd system; LPSO; Scheil solidification

1 Introduction

As lightweight structural material, magnesium alloys have great potential in automotive, aerospace and electronics industries because of their high specific strength [1-7]. Mg-Al serial alloys are the most commonly used magnesium alloys due to their excellent castability, corrosion resistance, and strength at room temperature [8-11]. With increasing Al content, main structure of the alloys will change from hcp(Mg) solid solution to the eutectic mixture of hcp(Mg) + γ . The occurrence of γ then becomes the main reason for the poor heat resistance of the Mg-Al alloys [12]. Alloying is one of the most effective ways to suppress the formation of γ and improve the high-temperature properties of Mg-Al alloys. CHEN et al [13] and ATHUL et al [14] reported that the addition of Gd to the Mg-Al alloys facilitates the formation of Al2Gd and

inhibits the precipitation of γ and the as-cast Mg-7.5Al-7.5Gd and Mg-9.0Al-2.0Gd (wt.%) alloys have the highest microhardness, ultimate tensile strength and yield strength at both room and high temperature in their work [13,14]. It is primary to obtain the phase equilibria and solidification behavior of the alloys to understand the thermodynamic reasons for the microstructure and mechanical properties of the alloys. During the past decade, the LPSO structures were reported in magnesium alloys containing transition metals and rare earth, which can improve the strength, stiffness and creep resistance of Mg alloys for their superior hardness, elastic modulus, excellent thermal stability as well as strong inhibition effect on the grain boundary migration [15-19]. It was reported that 14H and 18R are thermodynamically stable in the Mg-Al-Gd system [20-24].

It is necessary to clarify the thermodynamic stability and phase equilibria of the LPSO structures.

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Based on the first-principles calculations and thermodynamic modelling, the LPSO phases in the Mg-Al-Gd system were thermodynamically described by (Mg)_{68+24x}(Mg,Gd,Al)₁₆(Mg,Gd,Al)₁₂- $(Mg,Gd,Al,Va)_2$ ($x_{14H}=3$, $x_{18R}=2$) by KIM et al [25]. However, a rigorous literature evaluation revealed that KIM et al [25] omitted some key data [26-28] in their work and the model is complex so that it is not conducive on the construction of a multicomponent thermodynamic database. Recently, thermodynamic model of the LPSO phases in Mg-Ni-Y using stoichiometric compounds was developed by LIU et al [29]. However, the TM₆RE₈-type L1₂ cluster structure was not fully considered. In our previous work [30], a general thermodynamic model for LPSO phases was proposed and successfully applied to describing the Mg-Y-Zn system, which can not only reflect the crystal structures of the LPSO phases, but also describe their homogeneity ranges reasonably.

The purposes of the present work are to: (1) Describe the LPSO phases in the Mg–Al–Gd system with the model of Mg_x(TM,Mg)₆(RE,Mg)₈ ($x_{14H}=71$, $x_{18R}=59$) and obtain a set of accurate thermodynamic parameters of the system by means of the CALPHAD approach; (2) Obtain the phase

Table 1 Notations of phases in Mg-Al-Gd system

equilibria of the system by calculating isothermal sections, vertical sections, liquidus projection as well as the Scheil reaction scheme; (3) Perform Scheil solidification calculations to analyze the thermodynamic reasons for the mechanical properties of the Mg–xAl-yGd alloys and predict the candidate alloys composition.

2 Literature review

The Mg–Al–Gd ternary system contains three binary systems (i.e. Mg–Al, Mg–Gd and Al–Gd). The thermodynamic descriptions for all the three binary systems are available in literature. Phases notation with the crystal structures information in the Mg–Al–Gd system are listed in Table 1.

2.1 Binary systems

The Mg–Al binary system was first thermodynamically evaluated by SAUNDERS [31], and ZUO and CHANG [32]. Subsequent experiments by SU et al [33] and DONNADIEU et al [34] showed that the obtained experimental data are deviated from the calculated results. In order to obtain a more reliable thermodynamic description of the system, the Mg–Al phase diagram was

Phase	Prototype/Clusters	Personal system	Space group	Phase description		
fcc(Al)	Cu	cF4	$Fm\overline{3}m$	Solid solution based on fcc_A1 Al		
hcp(Gd)	Mg	hP2	$P6_3/mmc$	Solid solution based on hcp_A3 Gd		
hcp(Mg)	Mg	hP2	$P6_3/mmc$	Solid solution based on hcp_A3 Mg		
bcc(Gd)	W	cI2	$Im \overline{3}m$	Solid solution based on bcc_A2 Gd		
Al ₃ Gd	Ni ₃ Sn	hP8	$P6_3/mmc$	Binary phase on Al ₃ Gd		
Al ₂ Gd	MgCu ₂	cF4	$Fd\overline{3}m$	Solid solution based on Laves phase_C15		
AlGd	DyAl	oP16	Pmma	Binary phase on AlGd		
Al_2Gd_3	Zr_3Al_2	<i>tP</i> 20	$P4_2/mnm$	Binary phase Al ₂ Gd ₃		
AlGd ₂	Co ₂ Si	oP12	Pnma	Solid solution based on AlGd ₂		
Mg5Gd	GdMg ₅	<i>cF</i> 448	$F\overline{4}3m$	Solid solution based on Mg5Gd		
Mg ₃ Gd	BiF ₃	<i>cF</i> 16	$Fm\overline{3}m$	Solid solution based on Mg3Gd		
Mg ₂ Gd	MgCu ₂	<i>cF</i> 24	$Fd\overline{3}m$	Solid solution based on Laves phase_C15		
MgGd	CsCl	cP2	$Pm\overline{3}m$	Ordered phase related to A2		
β	Mg ₂ Al ₃	<i>cF</i> 1832	$Fd\overline{3}m$	Binary phase Al ₁₄₀ Mg ₈₉		
γ	α-Mn	<i>cl</i> 58	$I\overline{4}3m$	Solid solution based on Al ₁₂ Mg ₁₇		
3	Co ₅ Cr ₂ Mo ₃	hR159	$R\overline{3}$	Binary phase Al ₃₀ Mg ₂₃		
τ	MgZn ₂	<i>hP</i> 24	P6 ₃ /mmc	Ternary compound based on Al ₄ GdMg		
14H	Al_6Gd_8	_	<i>P</i> 6 ₃ 22	Long-period stacking ordered phase 14H		
18R	Zn_6Gd_8	_	C2/c	Long-period stacking ordered phase 18R		

experimentally re-investigated and re-optimized by LIANG et al [35] and the obtained thermodynamic parameters are widely used in the related systems. Although the Mg-Al system was later re-optimized by ZHONG et al [36] using a combination of first-principles calculations and the CALPHAD method, the results did not change much. Later, REN et al [37] and SHI et al [38] experimentally measured the phase equilibria of the Mg-Al binary system at 250-400 °C and then adjusted the thermodynamic parameters on the α , β and γ phases and solidus boundaries. Considering complexity of the reported thermodynamic parameters by SHI et al [38] and consistency of the developed thermodynamic database of Mg-based alloys [39], thermo- dynamic parameters of the binary Mg-Al system in this work was adopted from LIANG et al [35], as shown in Fig. 1(a).

The Mg–Gd binary system has been optimized by many researchers [40–45]. The existence of several intermediate phases, Mg₅Gd, Mg₃Gd and Mg₂Gd, order-disorder transition and the metastable phase in the system makes the phase diagram very complex and it is challenge to obtain a reliable thermodynamic description. Based on the thermodynamic properties and phase diagram data available in literature, WU et al [45] recently provided a set of thermodynamic parameters for both stable and metastable phases in the Mg–Gd binary system. The calculated Mg–Gd phase diagram is shown in Fig. 1(b) based on the thermodynamic parameters from WU et al [45].

The Al–Gd binary system was first thermodynamically assessed by GROBNER et al [28]. Subsequently, the Al-rich region of this system was reassessed by HACKENBERG et al [46] when they calculated the Al–Fe–Gd phase diagram. Recently, CACCIAMANI et al [43] reassessed the system and the reported thermodynamic parameters can reproduce the experimental phase diagram reasonably. Therefore, the parameters from CACCIAMANI et al [43] are used in this work, and the calculated phase diagram is shown in Fig. 1(c).

2.2 Mg-Al-Gd ternary system

With XRD (X-ray diffraction), OM (Optical microscopy), SEM (Scanning electron microscopy) and DTA (Differential thermal analysis), phase equilibrium for the Mg–Al–Gd system was firstly experimentally investigated by ROKHLIN et al in



Fig. 1 Calculated Mg–Al (a), Mg–Gd (b), and Al–Gd (c) phase diagrams using thermodynamic parameters from LIANG et al [35], WU et al [45] and CACCIAMANI et al [43], respectively

the range of Al–Mg–Mg₅Gd–Al₂Gd [26,27]. In their work, the isothermal section at 400 °C, three vertical sections, i.e., 50 wt.% Al, 70 wt.% Al and Mg–Al₂Gd, as well as partial liquidus surface of the Mg–Al–Gd system were constructed. A ternary compound τ (Al₄GdMg) with MgZn₂ Laves

structure was reported. The vertical section of Mg-Al₂Gd was reported as a pseudobinary section with a maximum eutectic temperature of 636 °C. The melting temperature of the ternary phase τ was not measured but assumed to be about 800 °C with the peritectic reaction of Liquid+Al₂Gd+ Al₃Gd $\rightarrow \tau$. Subsequently, GROBNER et al [28,47] carried out a thermodynamic assessment of the Mg-Al-Gd system mainly based on the experimental data of ROKHLIN et al [26,27] and prepared three alloys by arc melting to check the calculated phase equilibria and to provide the missing high temperature data by XRD and DTA. Their works confirmed the existence of the ternary compound τ and the ternary peritectic reaction temperature of formation of τ was measured to be 752 °C. Other two three-phase regions of Al₂Gd+ Mg2Gd+MgGd and AlGd+Mg5Gd+Mg3Gd were observed, but no ternary solid solubilities were detected. Both results of ROKHLIN et al [27] and GROBNER et al [28] showed an invariant reaction at about 450 °C.

Later, de NEGRI et al [48] prepared five ternary alloys to investigate the phase equilibria of the Mg-Al-Gd system at 400 °C and the formation temperature of the ternary compound τ by XRD, electronic probe microscopy analysis (EPMA) and DTA. DTA showed a very large thermal effect at about 450 °C, which was interpreted as the formation of τ but different from the reported invariant reaction by ROKHLIN et al [27] and GROBNER et al [28]. In addition, the solid solubility of Al in MgGd and Mg in Al₂Gd was respectively measured to be about 33-34 at.% Al and about 9 at.% Mg at 400 °C. A three-phase region of (Al,Mg)₂Gd+(Mg,Al)Gd+Mg₃Gd was observed. These results are not in agreement with the three-phase region of Al2Gd+Mg2Gd+MgGd reported by GROBNER et al [28], who did not detect the ternary solubilities of the Al2Gd and MgGd phases. Subsequently, CACCIAMANI et al [43] performed thermodynamic assessment on the Mg-Al-Gd system using the CALPHAD approach mainly based on the experimental data from de NEGRI et al [48].

In recent years, many scholars have observed the LPSO phases at Mg-rich corner of the Mg-Al-Gd system, which can improve the mechanical properties and corrosion behavior of the alloys. KINOSHITA et al [49] prepared a nominal Mg-3.5at.%Al-5.0at.%Gd alloy by high-frequency induction-melting in an argon atmosphere. The ingots were homogenized at 550 °C for 2 h and then heat-treated at 400 °C for 10 h. The hcp(Mg)+ Mg5Gd+14H+18R phase constituent was observed and the ideal composition of 14H was measured to be about Mg-7.1at.%Al-9.5at.%Gd by means of scanning transmission electron microscopy (STEM). Subsequently, KISHIDA et al [50,51] produced an as-solidified Mg-Al-Gd ingot by high-frequency induction-melting mixture of high-purity Mg, Al and Gd amounting in a carbon crucible with a lid in vacuum. The as-solidified ingot exhibits inhomogeneous microstructure depending on ingot position. The lower and upper parts of the ingot have average chemical composition of Mg-10at.%Al-9at.%Gd and Mg-1at.%Al-5at.%Gd, respectively. The lower part is composed of hcp(Mg)+Mg5Gd+Al2Gd, while the upper part exhibits 18R+Al₂Gd+ hcp(Mg)+Mg₅Gd. When the upper part was annealed at 525 °C for 4 and 64 h successively, the volume fraction of 18R increased slightly, while that for Al₂Gd and Mg₅Gd decreased significantly and as a result, the alloy was basically composed of 18R+hcp(Mg)+Al₂Gd after annealing at 525 °C for 64 h.

LU et al [52] prepared a nominal Mg-3.5at.%Al-5.0at.%Gd alloy by melting commercially pure Mg and Al (99.9 wt.%) ingots, and Mg-30Gd (wt.%) master alloys under the protection of a mixed SF6 (1 vol.%) and CO₂ (99 vol.%) atmosphere in an electric resistance furnace. After mixing at 730 °C for 1 h, the melt was poured into a steel mold preheated at 200 °C and naturally cooled to room temperature with the mold. According to the XRD and SEM results, the as-cast alloy mainly consists hcp(Mg)+Al2Gd+Mg5Gd+Mg50.97Al29.13Gd19.9. of When the obtained as-cast sample was cut into several pieces, heated in the furnace from 25 to 565 °C at the rate of 10 °C/min, kept at 565 °C for 24 h and then taken out of the furnace and quenched in 80 °C water, Mg5Gd and Mg50.97Al29.13-Gd_{19.9} dissolved into the matrix, while Al₂Gd remained original large size and a certain amount of rod-like Mg_{90,91}Al_{4,38}Gd_{4,72} phase emerged, which are similar to the fine LPSO lamellae in Mg-Zn-RE alloys [53-55]. Subsequently, the 18R-LPSO phase was detected by means of TEM when the sample was heated again from 25 to 565 °C at the rate

of 10 °C/min, kept at 300 °C for 20 h and then quenched in 80 °C water. Based on experimental phenomena, it can be inferred that the phase region of Mg-3.5at.%Al-5.0at.%Gd alloy at 565 °C may be hcp(Mg)+ Al₂Gd+18R.

GU et al [56] speculated that the composition point of 18R at 500 °C was about 9.5-13 at.% Gd and 7-10 at.% Al. Based on the experimental equilibria data, KIM et al [25] reassessed the Mg-Al-Gd system by combining first-principles calculations and thermodynamic modelling. The LPSO phases 14H and 18R were described by $(Mg)_{68+24x}(Mg,Gd,Al)_{16}(Mg,Gd,Al)_{12}(Mg,Gd,Al,Va)_2$ $(x_{18R}=2, x_{14H}=3)$ model. Same as CACCIAMANI et al [43], KIM et al [25] did not consider the experimental data of ROKHLIN et al [26,27] and GROBNER et al [28]. The four vertical sections obtained by ROKHLIN et al [27] and GROBNER et al [28] are of great significance to evaluate the phase diagram and are considered in the present optimization to obtain more comprehensive thermodynamic parameters. The experimental data on phase equilibria of the Mg-Al-Gd system are summarized in Table 2.

3 Thermodynamic models

Gibbs energy functions of the pure elements, Mg, Al and Gd, were taken from the SGTE database compiled by DINSDALE [57]. Based on the critical review, the thermodynamic parameters for binary Mg–Al, Mg–Gd and Al–Gd systems were adopted from LIANG et al [35], WU et al [45] and CACCIAMANI et al [43], respectively, in the present work.

3.1 Solution phases

The solution phases, i.e., liquid, fcc(Al) and hcp(Mg), were described by the substitutional solution model. Taking the fcc phase as an example, its molar Gibbs energy can be expressed by the Redlich-Kister-Muggianu polynomial [58]:

$$G^{\text{fcc}} = x_{\text{Al}}G_{\text{Al}}^{0,\text{fcc}} + x_{\text{Gd}}G_{\text{Gd}}^{0,\text{fcc}} + x_{\text{Mg}}G_{\text{Mg}}^{0,\text{fcc}} + RT \cdot (x_{\text{Al}}\ln x_{\text{Al}} + x_{\text{Gd}}\ln x_{\text{Gd}} + x_{\text{Mg}}\ln x_{\text{Mg}}) + x_{\text{Al}}x_{\text{Gd}}L_{\text{Al,Gd}}^{\text{fcc}} + x_{\text{Gd}}x_{\text{Mg}}L_{\text{Gd,Mg}}^{\text{fcc}} + x_{\text{Al}}x_{\text{Mg}}L_{\text{Al,Mg}}^{\text{fcc}} + x_{\text{Al}}x_{\text{Gd}}x_{\text{Mg}}(x_{\text{Al}}^{0}L_{\text{Al,Gd,Mg}}^{\text{fcc}} + x_{\text{Gd}}^{1}L_{\text{Al,Gd,Mg}}^{\text{fcc}} + x_{\text{Mg}}^{2}L_{\text{Al,Gd,Mg}}^{\text{fcc}})$$
(1)

Technique ^(a)	Type of data	Quoted mode ^(b)	Ref.
	Isothermal section at 400 °C		[26]
VDD SEM	Vertical sections at 50 wt.% Al	0	[27]
ARD, SEM	Vertical sections at 70 wt.% Al	0	[27]
	Vertical sections at Mg-Al ₂ Gd	0	[27]
VPD DTA	Vertical section at 9 wt.% Mg		[28]
AKD, DIA	τ formed below 752 °C		[28]
XRD, DTA, SEM,	Isothermal section at 400 °C		[48]
EPMA, LOM	τ formed below 450 °C		[48]
STEM	hcp(Mg)+Al ₂ Gd+14H+18R phase at 400 °C		[49]
STEM	Ideal composition of 14H phase is Mg ₃₅ Al ₃ Gd ₄ at 400 °C		[49]
STEM	Ideal composition of 18R phase is 9.5–13 at.% Gd and 7–10 at.% Al at 500 $^{\circ}\mathrm{C}$		[56]
SEM, STEM	Three-phase regions of hcp(Mg)+Mg ₅ Gd+18R and hcp(Mg)+Mg ₅ Gd+18R at 525 $^\circ$ C		[50]
SEM, EBSD, STEM	Three-phase region of hcp(Mg)+Al ₂ Gd+18R at 525 °C		[51]
STEM	Three-phase region of hcp(Mg)+Al ₂ Gd+18R at 565 °C	•	[52]

Table 2 Experimental phase equilibria data for Mg-Al- Gd system available in literature

^(a)XRD–X-ray diffraction; LOM–Light optical metallography; SEM–Scanning electron microscopy; EMPA–Electron probe micro-analyzer; DTA–Differential thermal analysis; STEM–Scanning transmission electron microscopy; TEM–Transmission electron microscopy; EBSD–Electron back-scatter diffraction; EDX–Energy dispersive X-ray detector; ^(b) \blacksquare Used; \Box Not used; \circ Not used but estimated to be reliable data for checking the modeling

where *R* represents the molar gas constant, *T* represents the thermodynamic temperature, and x_{Al} , x_{Gd} , and x_{Mg} represent the molar fractions of the elements Al, Gd, and Mg, respectively. The ternary interaction parameters $L_{Al,Gd,Mg}^{0,fec}$, $L_{Al,Gd,Mg}^{1,fec}$ and $L_{Al,Gd,Mg}^{2,fec}$ are linearly temperature-dependent, which can be expressed as $L_{Al,Gd,Mg}^{fec} = A + BT$. The coefficients *A* and *B* will be optimized according to the experimental data available in present work.

3.2 Binary phases extending into ternary system

According to the experimental data from the literature [26–28,48], the binary phases, Al₂Gd, Mg₂Gd and γ , exhibit extended solubilities of the third elements in corresponding ternary systems. Sublattice models [59,60] were used to describe these binary phases, as listed in Table 1. Taking the Al₂Gd phase, modeled as (Al,Gd,Mg)₂(Al,Gd,Mg)₁ (the boldfaces mean the major atoms in the sublattices), as an example, its Gibbs energy can be expressed as

$$G^{Al_{2}Gd} = y'_{Al}y''_{Al}G^{Al_{2}Gd}_{Al:Al} + y'_{Al}y''_{Gd}G^{Al_{2}Gd}_{Al:Gd} + y'_{Al}y''_{Gd}G^{Al_{2}Gd}_{Al:Mg} + y'_{Gd}y''_{Al}G^{Al_{2}Gd}_{Gd:Al} + y'_{Gd}y''_{Gd}G^{Al_{2}Gd}_{Gd:Gd} + y'_{Gd}y''_{Gd}G^{Al_{2}Gd}_{Gd:Mg} + y'_{Mg}y''_{Al}G^{Al_{2}Gd}_{Mg:Al} + y'_{Mg}y''_{Gd}G^{Al_{2}Gd}_{Mg:Gd} + y'_{Mg}y''_{Gd}G^{Al_{2}Gd}_{Mg:Mg} + 2RT(y'_{Al}\ln y'_{Al} + y'_{Gd}\ln y'_{Gd} + y'_{Mg}\ln y'_{Mg}) + RT \cdot (y''_{Al}\ln y''_{Al} + y''_{Gd}\ln y''_{Gd} + y''_{Mg}\ln y''_{Mg}) + y'_{Al}y'_{Gd}(y''_{Al}L^{Al_{2}Gd}_{Al,Gd:Al} + y''_{Gd}L^{Al_{2}Gd}_{Al,Gd:Gd} + y''_{Mg}L^{Al_{2}Gd}_{Al,Gd:Mg}) + y''_{Al}y''_{Gd}(y'_{Al}L^{Al_{2}Gd}_{Al,Gd:Gd} + y''_{Gd}L^{Al_{2}Gd}_{Al;Al,Gd} + y''_{Mg}L^{Al_{2}Gd}_{Al;Al,Gd}) + \cdots$$
(2)

where y'_i and y''_i represent the site fractions of *i* (*i*=Al, Gd, Mg) in the first and second sublattices for model (Al,Gd,Mg)₂(Al,Gd,Mg)₁, respectively. The parameters denoted as $G_{i:j}^{Al_2Gd}$ (*i*, *j*=Al, Gd, Mg) represent the Gibbs energies of hypothetic end-members. The ternary interaction parameters $L_{i,j:k}^{Al_2Gd}$ and $L_{i:j,k}^{Al_2Gd}$ (*i*, *j*, *k*=Al, Gd, Mg) are also linearly temperature-dependent, which can be expressed as $L_{i,j:k}^{Al_2Gd} = a + bT$. The coefficients *a* and *b* were optimized according to the experimental data available in the literature. The analogous expressions similar to Eq. (2) were applied to describing the Gibbs energies of the Mg₂Gd and γ phases.

3.3 Ordered and disordered phases

Ordered bcc_B2 (MgGd) phase is modeled as (Al,Gd,Mg)_{0.75}(Al,Gd,Mg)_{0.75}Va₃. In order to use a single function to represent the Gibbs energy of both the ordered and disordered phases, the disordered bcc_A2 (bcc(Gd)) is described with (Al,Gd,Mg)₁Va₃. DUPIN et al [61] and ANSARA et al [62] have derived an equation resolving Gibbs energy into three terms so that the thermodynamic properties of the disordered and ordered phases can be evaluated independently. Thus, the Gibbs energy of both the bcc_A2 and bcc_B2 phases is given by a single function of the following form:

$$G_{\rm m}^{\theta} = G_{\rm m}^{\rm bcc-A2}(x_i) + G_{\rm m}^{\rm bcc-B2}(y'_i, y''_i) - G_{\rm m}^{\rm bcc-B2}(x_i)$$
(3)

where θ represents both the bcc_A2 and bcc_B2 phases. y'_i (*i*=Al, Gd, Mg) is the site fraction of Al, Gd and Mg in the first sublattice, and y''_i is that in the second one. $G_m^{bcc-A2}(x_i)$ is the Gibbs energy of the disordered bcc_A2 phase. The second term $G_m^{bcc-B2}(y'_i, y''_i)$ is described by the sublattice model and implicitly contains a contribution from the disordered state. The last term $G_m^{bcc-B2}(x_i)$ represents the contribution from the disordered state to the ordered one. When the site fractions are equal, i.e. $y'_i = y''_i$, the last two terms cancel out. In this case, Eq. (3) corresponds to the disordered state. Hence, the parameters of the ordered and disordered phases can be evaluated independently.

3.4 Ternary compounds

The ternary phase τ was described by the sublattice model (Al,Gd,Mg)₂(Al,Gd,Mg) according to the prototype "hP12-MgZn₂". Analogous Eq. (2) can also be written for the Gibbs energy of the τ phase.

The crystal structure of LPSO phases is characterized by (1) enrichment of TM and RE atoms in two consecutive close-packed atomic planes in each structural block, and (2) introduction of a stacking fault between two consecutive atomic planes with TM and RE enrichment that breaks the hexagonal close-packed (hcp) stacking of the AB type. KISHIDA et al [49–51] and YOKOBAYASHI et al [63,64] showed that the LPSO phases in the Mg–Al–Gd system were found to form by stacking structural blocks, each consisting of six closepacked atomic planes. In each structural block, long-range ordering of the constituent Mg, Al and

Gd atoms occurs with the enrichment of Gd atoms in four consecutive atomic planes. The in-plane long-range ordering in the four consecutive atomic planes occurs to form Al₆Gd₈ clusters in a periodic manner. The ideal chemical composition of the structural block is determined to be Mg₂₉Al₃Gd₄. However, the stacking of structural blocks is basically disordered, while the constituent atoms in each structural block in Mg-Al-Gd system are long-range ordered. Hence, the LPSO phases in Mg-Al-Gd system are special ordered-disordered structures. In our previous work [30], a general thermodynamic model for LPSO phases was proposed based on two key factors: the TM₆RE₈type $L1_2$ clusters and the variation of chemical compositions, which can not only reflect the crystal structures of LPSO phases, but also describe their homogeneity ranges reasonably. It has been successfully applied to describing the Mg-Y-Zn system. In the present work, the three-sublattice model of the LPSO phases is expressed as $Mgx(Al,Mg)_{6}(Gd,Mg)_{8}$ and Gibbs energy is described as follows:

$$G_{\rm m}^{\rm LPSO} = y_{\rm Mg}'' y_{\rm Mg}'' G_{\rm Mg:Mg:Mg}^{\rm LPSO} + y_{\rm Mg}'' y_{\rm Gd}' G_{\rm Mg:Mg:Gd}^{\rm LPSO} + y_{\rm Al}' y_{\rm Mg}'' G_{\rm Mg:Al:Gd}^{\rm LPSO} + \frac{6}{x+14} RT(y_{\rm Al}' \ln y_{\rm Al}' + y_{\rm Mg}'' \ln y_{\rm Mg}') + \frac{8}{x+14} RT(y_{\rm Gd}'' \ln y_{\rm Gd}'' + y_{\rm Mg}'' \ln y_{\rm Mg}'') + \cdots$$
(4)

where y_i'' and y_i''' represent the site fractions of *i* (*i*=Al, Gd, Mg) in the second and third sublattices for the model Mg_x(Al,Mg)₆(Gd,Mg)₈, respectively. The parameters denoted as $G_{Mg:Mg:Gd}^{LPSO}$, $G_{Mg:Mg:Gd}^{LPSO}$, $G_{Mg:Al:Mg}^{LPSO}$ and $G_{Mg:Al:Gd}^{LPSO}$ represent Gibbs energy of the end-members.

4 Results and discussion

4.1 Thermodynamic calculations on phase equilibria

Based on the experimental data available in literature, the Mg–Al–Gd system was evaluated by the optimization module PARROT [65] of the program Thermo-Calc, which works by minimizing the square sum of the differences between measured and calculated values. The presently obtained thermodynamic parameters of Mg–Al–Gd system

are listed in Table 3. Some representative phase diagrams of the Mg–Al–Gd system are calculated.

Figure 2(a) shows the calculated isothermal section of Mg-Al-Gd system at 400 °C compared with the experimental data from de NEGRI et al [48]. It can be seen that the calculated isothermal section is in good agreement with the measured one except the two-phase region, AlGd₂+MgGd. The present calculation on AlGd₂+ MgGd is consistent with the calculation results by CACCIAMANI et al [43] and KIM et al [25]. As seen in Fig. 2(a), there are 17 three-phase regions at 400 °C. The phase regions with green tie lines are the two-phase regions. The composition of τ was reported to be about Mg-16.6at.%Gd-66.7at.%Al and Mg-17.5at.%Gd-66.9at.%Al by de NEGRI et al [48] and ROKHLIN et al [26], respectively. the calculated composition range However, of τ in this work is about 16.0–17.3 at.% Mg and 66.6 at.% Al, which includes the composition of Al₄GdMg. The presently calculated maximum solubilities of Mg in Al2Gd and Al in MgGd at 400 °C are 7.5 at.% Mg and 34.2 at.% Al, respectively, which agree well with the reported data of about 9 at.% Mg and 33-34 at.% A1 [48]. The calculated isothermal section at 400 °C of the Mg-Al-Gd system along with the experimental data from ROKHLIN et al [26] are shown in Fig. 2(b). Comparisons between the calculated results and experimental data show that almost all the reliable experimental data can be satisfactorily reproduced by the present modeling.

The calculated vertical sections at 50 and 70 wt.% Al in comparison with the experimental data [27] are shown in Figs. 3(a, b), respectively. It can be seen that the calculated liquidus temperatures are much higher than the measured ones and many phase equilibria below 400 °C are predicted, which indicates that the reported vertical sections at 50 and 70 wt.% Al by ROKHLIN et al [27] are incomplete. Therefore, the reported DTA signals in ROKHLIN et al [27] are considered only and well reproduced by the present work, which is similar to the calculation results of GROBNER et al [28]. Figures 4(a, b) present the calculated vertical sections at Mg-Al2Gd and 9 wt.% Mg in comparison with the experimental data from ROKHLIN et al [27] and GROBNER et al [28]. As seen from Fig. 4(a), the present work predicts an extremely narrow three-phase region of

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Phases model	Thermodynamic parameter			
Liquid: (Al,Gd,Mg) ₁	$L_{Al,Gd,Mg}^{0,\text{liquid}} = 50000 , L_{Al,Gd,Mg}^{1,\text{liquid}} = -180000 , L_{Al,Gd,Mg}^{2,\text{liquid}} = -90000$			
Al ₂ Gd: (Al,Gd,Mg) ₂ (Al,Gd,Mg)	$\begin{split} G^{\rm Al_2Gd}_{\rm Al:Mg} &= 15000 + 2G^{0,\rm fcc}_{\rm Al} + G^{0,\rm hcp}_{\rm Mg} , G^{\rm Al_2Gd}_{\rm Mg:Mg} = 15000 + 3G^{0,\rm hcp}_{\rm Mg} , \\ G^{\rm Al_2Gd}_{\rm Mg:Al} &= 15000 + G^{0,\rm fcc}_{\rm Al} + 2G^{0,\rm hcp}_{\rm Mg} , G^{\rm Al_2Gd}_{\rm Gd:Mg} = G^{0,\rm hcp}_{\rm Mg} + 2G^{0,\rm hcp}_{\rm Gd} , \\ G^{\rm Al_2Gd}_{\rm Mg:Gd} &= -49865 + 39.92T + 2G^{0,\rm hcp}_{\rm Mg} + G^{0,\rm hcp}_{\rm Gd} \end{split}$			
MgGd: (Al,Gd,Mg) _{0.5} (Al,Gd,Mg) _{0.5} Va ₃	$\begin{split} L^{0,\mathrm{MgGd}}_{\mathrm{Al},\mathrm{Gd}:\mathrm{Va}} &= -69875 + 19.84T, \ L^{0,\mathrm{MgGd}}_{\mathrm{Gd},\mathrm{Al}:\mathrm{Va}} = -69875 + 19.84T, \\ L^{0,\mathrm{MgGd}}_{\mathrm{Al},\mathrm{Mg}:\mathrm{Va}} &= 60124 - 30.11T, \ L^{0,\mathrm{MgGd}}_{\mathrm{Mg},\mathrm{Al}:\mathrm{Va}} = 60124 - 30.11T \end{split}$			
Mg2Gd: (Al,Gd,Mg)2(Al,Gd,Mg)	$\begin{split} G^{\rm Mg_2Gd}_{\rm Al:Al} &= 60000 + G^{0,\rm fcc}_{\rm Al} \ , \ G^{\rm Mg_2Gd}_{\rm Al:Gd} = 2G^{0,\rm fcc}_{\rm Al} + G^{0,\rm hcp}_{\rm Gd} , \\ G^{\rm Mg_2Gd}_{\rm Al:Mg} &= 2G^{0,\rm fcc}_{\rm Al} + G^{0,\rm hcp}_{\rm Mg} , \ G^{\rm Mg_2Gd}_{\rm Gd;Al} = 2G^{0,\rm hcp}_{\rm Gd} + G^{0,\rm fcc}_{\rm Al} , \\ G^{\rm Mg_2Gd}_{\rm Mg:Al} &= 2G^{0,\rm hcp}_{\rm Mg} + G^{0,\rm fcc}_{\rm Al} \end{split}$			
τ: (Al,Gd,Mg)2(Al,Gd,Mg)	$\begin{split} G_{\rm Al:Gd}^{\tau} &= -116120 + 22.7273T + 2G_{\rm Al}^{0,\rm fcc} + G_{\rm Gd}^{0,\rm hcp}, \\ G_{\rm Al:Mg}^{\tau} &= 30000 + 2G_{\rm Al}^{0,\rm fcc} + G_{\rm Mg}^{0,\rm hcp}, \\ G_{\rm Mg:Al}^{\tau} &= G_{\rm Al}^{0,\rm fcc} + 2G_{\rm Mg}^{0,\rm hcp}, G_{\rm Gd:Al}^{\tau} &= G_{\rm Al}^{0,\rm fcc} + 2G_{\rm Gd}^{0,\rm hcp}, \\ G_{\rm Gd:Mg}^{\tau} &= G_{\rm Mg}^{0,\rm hcp} + 2G_{\rm Gd}^{0,\rm hcp}, G_{\rm Mg:Gd}^{\tau} &= 2G_{\rm Mg}^{0,\rm hcp} + G_{\rm Gd}^{0,\rm hcp}, \\ G_{\rm Al:Al}^{\tau} &= 15000 + 3G_{\rm Al}^{0,\rm fcc}, G_{\rm Mg:Mg}^{\tau} &= 15000 + 3G_{\rm Mg}^{0,\rm hcp}, \\ G_{\rm Gd:Gd}^{\tau} &= 3G_{\rm Gd}^{0,\rm hcp}, L_{\rm Al:Gd:Mg}^{0,\tau} &= -148550 \end{split}$			
14H: (Mg) ₇₁ (Al,Mg) ₆ (Gd,Mg) ₈	$\begin{split} G^{14\mathrm{H}}_{\mathrm{Mg:Al:Gd}} &= -850988 + 199.85T + 71G^{0,\mathrm{hcp}}_{\mathrm{Mg}} + 6G^{0,\mathrm{fcc}}_{\mathrm{Al}} + 8G^{0,\mathrm{hcp}}_{\mathrm{Gd}}, \\ G^{14\mathrm{H}}_{\mathrm{Mg:Al:Mg}} &= 35000 + 79G^{0,\mathrm{hcp}}_{\mathrm{Mg}} + 6G^{0,\mathrm{fcc}}_{\mathrm{Al}}, \\ G^{14\mathrm{H}}_{\mathrm{Mg:Mg:Gd}} &= 35000 + 77G^{0,\mathrm{hcp}}_{\mathrm{Mg}} + 8G^{0,\mathrm{hcp}}_{\mathrm{Gd}}, \\ G^{14\mathrm{H}}_{\mathrm{Mg:Mg:Mg}} &= 35000 + 85G^{0,\mathrm{hcp}}_{\mathrm{Mg}}, L^{0,14\mathrm{H}}_{\mathrm{Mg:Al,Mg:Gd,Mg}} = 35000 \end{split}$			
18R: (Mg) ₅₉ (Al,Mg) ₆ (Gd,Mg) ₈	$G_{Mg;Al:Gd}^{18R} = -704003 + 59G_{Mg}^{0,hcp} + 6G_{Al}^{0,fcc} + 8G_{Gd}^{0,hcp},$ $G_{Mg;Al:Mg}^{18R} = 35000 + 67G_{Mg}^{0,hcp} + 6G_{Al}^{0,fcc},$ $G_{Mg:Mg;Gd}^{18R} = 35000 + 65G_{Mg}^{0,hcp} + 8G_{Gd}^{0,hcp},$ $G_{Mg;Mg;Mg}^{18R} = 35000 + 73G_{Mg}^{hcp}$			

Table 3 Presently optimized thermodynamic parameters in Mg-Al-Gd system

Temperature (T) is in Kelvin and Gibbs energy is in J/mol; The Gibbs energies for the pure elements are taken from the compilation of DINSDALE [57]; The thermodynamic parameters for the binary Mg–Al, Mg–Gd and Al–Gd systems are adopted from LIANG et al [35], WU et al [45] and CACCIAMANI et al [43], respectively

Liquid+Al₂Gd+hcp(Mg) at around 610 °C at the section of Mg–Al₂Gd instead of the reported eutectic reaction at 636 °C by ROKHLIN et al [27]. Based on the thermodynamic parameters optimized by CACCIAMANI et al [43] and KIM et al [25], the calculation of the vertical section at Mg–Al₂Gd is consistent with the present calculated results. The parameters in the present work are acceptable since

the calculated phase region of liquid+Al₂Gd+ hcp(Mg) is so narrow that the DTA measurement is probably hard to detect accurately. It can be seen in Fig. 4(b) that three thermal signals measured by GROBNER et al [28] are mostly reproduced by the present work. The present calculation confirms that the τ phase is formed via a peritectic reaction of Liquid+Al₂Gd+Al₃Gd $\Rightarrow \tau$ at 751 °C.

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Fig. 2 Calculated isothermal sections of Mg–Al–Gd system at 400 °C along with experimental data: (a) de NEGRI et al [48]; (b) ROKHLIN et al [26]



Fig. 3 Calculated vertical sections compared with experimental data [27]: (a) 50 wt.% Al; (b) 70 wt.% Al



Fig. 4 Calculated vertical sections compared with experimental data [27,28]: (a) Mg-Al₂Gd; (b) 9 wt.% Mg

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Figure 5 shows the calculated liquidus projection of the Mg-Al-Gd system over the whole composition using the presently obtained thermodynamic parameters. Figures 5(b, c) show the enlargements of rich Mg-corner and Mg-Gd binary side of Fig. 5(a), respectively. A comparison between the calculated and experimentally measured invariant reactions is listed in Table 4. Figure 6 shows the constructed reaction scheme for the Mg-Al-Gd system according to the liquidus projection in Fig. 5 and invariant reactions in Table 4. A general agreement is obtained between the calculations and the experiments except for some invariant reactions by ROKHLIN et al [27]. The reported invariant reactions, i.e., Liquid+ $Al_3Gd=\tau+fcc(Al)$, Liquid=Mg₅Gd+hcp(Mg)+Al₂Gd, Liquid+ $\varepsilon = \beta + \tau$, Liquid+ $\tau = Al_2Gd + \gamma$, and Liquid= γ +hcp(Mg)+Al₂Gd at the measured temperatures were replaced by Liquid+Al₂Gd=hcp(Mg)+18R, Liquid = Mg₅Gd + hcp(Mg) + 18R, Liquid = $\tau + \beta + \gamma$, Liquid + Al₂Gd = hcp(Mg) + τ , and Liquid = $\tau + \gamma +$ hcp(Mg) with the present calculations, respectively. Considering the 14H and 18R phases that were not considered in the invariant reactions reported by ROKHLIN et al [27], their reported vertical sections at 50 and 70 wt.% Al were incomplete. It is comprehensible that the invariant reactions reported by ROKHLIN et al [27] are different from the calculated ones in this work. According to the present calculations, the τ phase is formed via the peritectic reaction Liquid + $Al_2Gd + Al_3Gd = \tau$ at 751 °C and decomposed into Al₃Gd + ε + γ phases at 296 °C, as can be seen from Figs. 5 and 6 as well as Table 4.

The calculated isothermal sections in the Mg-rich corner at 400, 450, 500, 525, 550 and 565 °C of the Mg–Al–Gd system along with the experimental data [49–52,56] are shown in Figs. 7(a–f), respectively. As can be seen from these figures, three-phase regions $18R+hcp(Mg)+Al_2Gd$ and $18R+hcp(Mg)+Mg_5Gd$ determined by KISHIDA et al [50,51] and LU et al [52] can be reproduced well by the present modeling. The presently calculated composition of the 14H and 18R phases are Mg_{83.5}Gd_{9.4}Al_{7.1} and Mg_{81.6}Gd_{10.2}Al_{8.2}, respectively, corresponding to the reported composition of 14H and 18R phase: Mg–7.1at.%Al–9.5at.%Gd and Mg–(9.5–13)at.%Gd–(7–10)at.%Al by KISHIDA et al [49] and GU et al [56].

Figure 8 shows the calculated vertical section of Al₇Gd₁₀–Mg (at.%) in comparison with the experimental data [52]. The three-phase region of



Fig. 5 Calculated liquidus projection of Mg–Al–Gd system: (a) Whole composition; (b) Enlargement of rich Mg–Al binary side in (a); (c) Enlargement of rich Mg-corner in (a)



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Table 4 Calculated invariant reactions in Mg-Al-Gd system compared with experimental data

Туре	Invariant Reaction	Temperature/°C	<i>x</i> (Gd)/at.%	<i>x</i> (Al)/at.%	Method	Source
U	Liquid+AlGd=Al2Gd+MgGd	861.26	46.32	27.22	Calculated	This work
U	Liquid+AlGd=MgGd+Al2Gd3	858.67	54.33	28.62	Calculated	This work
U	Liquid+Al2Gd3=MgGd+AlGd2	809.04	62.16	23.31	Calculated	This work
U	Liquid+bcc(Gd)=MgGd+hcp(Gd)	798.54	66.08	11.48	Calculated	This work
		751.00	1.59	51.85	Calculated	This work
Р	Liquid+Al ₂ Gd+Al ₃ Gd=τ	761.00			Calculated	[28]
	-	≈800.00 752.00			Measured	[27]
E	Liquid=MgGd+AlGd2+hcp(Gd)	738.43	69 93	17 27	Calculated	This work
U	Liquid+Mg ₂ Gd=Mg ₂ Gd+MgGd	713.06	24 82	1 64	Calculated	This work
U	Liquid+MgGd=Al ₂ Gd+Mg ₂ Gd	669.44	19.88	4.5	Calculated	This work
U	Liquid+Mg2Gd=Al2Gd+Mg2Gd	623.01	13.08	23	Calculated	This work
U	L_{1}	623.91	0.22	2.5	Calculated	
0	Liquid+Al ₂ Od=18K+Mg ₅ Od	5/4.1/	9.22	1.44		This work
TT	L1qu1d+Al ₂ Gd=hcp(Mg)+18R	566.90	0.05	1.39	Calculated	This work
U	$Liquid=Mg_5Gd=ncp(Mg)+Al_2Gd$ $Liquid=Al_2Gd=\tau+fcc(Al)$	565.00			Measured	[28] [27]
	$\frac{1}{10000000000000000000000000000000000$	547.50	7 52	0.76	Calculated	This work
Е	Liquid+Al ₃ Gd= τ +fcc(Al)	515.00	1.52	0.70	Calculated	[28]
	Liquid=Mg5Gd+hcp(Mg)+Al2Gd	≈548.00			Measured	[27]
U	$Liquid+Al_3Gd=\tau+fcc(Al)$	485.66	0.06	68.63	Calculated	This work
U	Al ₂ Gd+hcp(Mg)+18R=14H	451.35	10.93	8.22	Calculated	This work
U	Al2Gd+hcp(Mg)=14H+Mg5Gd	450.36	10.93	8.22	Calculated	This work
		450.34	0.02	63.79	Calculated	This work
E	Liquid= τ +fcc(Al)+ β	450.00			Calculated	[28]
- L		450.00			Measured	[28]
	L1qu1d+fcc(Al)= $\tau + \beta$	≈448.00	0.02	67 (1	Measured	[27]
Б	Liquid= $\tau + \beta + \gamma$	449.39	0.02	57.61	Calculated	This work
Е <u>–</u>	$I_{iauid+\epsilon=\beta+\tau}$	449.00			Measured	[20]
E	18R=Al2Gd+Mg5Gd+14H	447 51	10.94	8 22	Calculated	$\frac{\lfloor 2 / \rfloor}{\text{This work}}$
		441.89	0.06	30.40	Calculated	This work
U	Liquid+Al ₂ Gd=hcp(Mg)+ τ	439.00			Calculated	[28]
	Liquid+ τ =Al ₂ Gd+ γ	440.00			Measured	[27]
E	Liquid= $\tau + \gamma + hcp(Mg)$	435.95	0.05	31.05	Calculated	This work
	Liquid+ $\tau = \gamma + hcp(Mg)$	436.00			Calculated	[28]
	$L_1qu_1d=\gamma+hcp(Mg)+Al_2Gd$	432.00			Measured	[27]
U	$eta{+}\gamma{=} au{+}arepsilon$	409.78	16.17	66.63	Calculated	This work
U	$hcp(Mg)+\tau=\gamma+Al_2Gd$	397.75	17.45	66.53	Calculated	This work
U	τ +Al ₂ Gd=Al ₃ Gd+ γ	372.60	17.37	66.57	Calculated	This work
U	τ +fcc(Al)=Al ₃ Gd+ β	369.31	16.03	66.65	Calculated	This work
U	$\tau + \beta = Al_3Gd + \varepsilon$	298.69	16.13	66.66	Calculated	This work
Е	$\tau = Al_3Gd + \varepsilon + \gamma$	296.33	16.14	66.66	Calculated	This work
U	γ +Al ₂ Gd=Al ₃ Gd+hcp(Mg)	243.55	33.28	66.68	Calculated	This work
Е	14H=Al ₂ Gd+Mg ₅ Gd+hcp(Mg)	230.00	0.46	0.01	Calculated	This work
p_{max1}	Liquid+AlGd=MgGd	865.62	49.65	28.03	Calculated	This work
p_{max2}	Liquid+Al ₂ Gd=hcp(Mg)	605.94	2.13	5.02	Calculated	This work
p_{max3}	Liquid+Al ₂ Gd=18R	578.80	7.52	1.55	Calculated	This work
e _{max1}	Liquid= $\tau + \gamma$	463.12	0.03	47.06	Calculated	This work
e _{max2}	Liquid= $\tau + \beta$	451.55	0.02	60.81	Calculated	This work



Fig. 7 Calculated isothermal sections in Mg-rich corner of Mg–Al–Gd system with experimental data [49–52,56]: (a) 400 °C; (b) 450 °C; (c) 500 °C; (d) 525 °C; (e) 550 °C; (f) 565 °C

 $18R + hcp(Mg) + Al_2Gd$ is reproduced in Mg-3.5at.%Al-5.0at.%Gd observed by LU et al [52]. As can be seen from Fig. 8 and Table 4, the 14H phase is formed via the peritectic reaction $Al_2Gd + hcp(Mg) + 18R = 14H$ at 451 °C and decomposed by $14H = Al_2Gd+Mg_5Gd+hcp(Mg)$ at 230 °C, and the 18R phase is formed via the transition of Liquid+Al₂Gd=18R+Mg₅Gd at 574 °C and decomposed by $18R=Al_2Gd+Mg_5Gd+14H$ at 447 °C. Therefore, it can be concluded that the 14H and 18R phases are stable at 230–451 °C and 447–574 °C, respectively.

4.2 Simulation of microstructure evolution of ascast alloys

Mg-7.5Al-xGd (x=0, 2.5, 5.0 and 7.5, wt.%) and Mg-9.0Al-xGd (x=0.5, 1.0, and 2.0, wt.%) coatings were prepared by CHEN et al [13] and ATHUL et al [14] when they investigated the effect of Gd addition on the microstructure and properties of Mg-Al alloys. The results show that the addition of Gd leads to the formation of the cubic Al2Gd phase and inhibits the precipitation of the eutectic phase. The laser-fused coatings nominally γ containing 7.5 and 2.0 wt.% Gd exhibited the highest microhardness, ultimate tensile strength, and yield strength at both room temperature and high temperature. Thermodynamic calculations on the Mg-7.5Al-xGd (x=0, 2.5, 5.0 and 7.5, wt.%) and Mg-9Al-xGd (x=0, 0.5, 1.0, and 2.0, wt.%) alloys based on the presently obtained thermodynamic parameters are shown in Figs. 9–12. Figures 9(a, b) show the phase fractions of Mg–7.5Al–xGd (x=2.5, 5.0 and 7.5, wt.%) and Mg–9.0Al–xGd (x=0.5, 1.0, and 2.0, wt.%) under Scheil condition. It can be seen that the fraction of the Al₂Gd, Al₃Gd and hcp(Mg) phases gradually increases and that of the γ phase decreases with the increase of Gd content. The change in phase fraction is consistent with the conclusions of CHEN et al [13] and ATHUL et al [14].

Figure 10 shows the variation of phase fraction in Mg–7.5Al–xGd and Mg–9.0Al–xGd alloys at room temperature as the Gd content increases under Scheil conditions. It can be seen that the fraction of γ gradually decreases to zero with the addition of Gd from 0 to about 20 wt.%. According to the reported results [13,14], the poor properties of Mg–Al–Gd alloys are mainly attributed to the



Fig. 8 Calculated vertical sections compared with experimental data [52]: (a) Al₇Gd₁₀-Mg; (b) Enlargement of Mg-rich region in (a)



Fig. 9 Calculated phase fractions of representative alloys under Scheil conditions: (a) Mg-7.5Al-xGd (x=2.5, 5.0 and 7.5, wt.%); (b) Mg-9.0Al-xGd (x=0.5, 1.0 and 2.0, wt.%)



Fig. 10. Phase fraction variation of Mg-7.5Al-*x*Gd and Mg-9.0Al-*x*Gd alloys at room temperature under Scheil condition

Fig. 11 Calculated solidified path of representative alloys of Mg-7.5Al-xGd (x=2.5, 5.0 and 7.5, wt.%) and Mg-9Al-xGd (x=0.5, 1.0, and 2.0, wt.%) under Scheil solidification condition

existence of the eutectic γ phase. From this point, it can be seen that the variation of phase fractions can provide theoretical guidance for designing Mg-Al-Gd alloys with high-performance. Further, in order to provide more details on the solidification behavior to obtain the desired solidification microstructure according to the relationship between microstructure and properties, the solidification behaviors of Mg-7.5Al-xGd (x=0, 2.5, 5.0 and 7.5, wt.%) and Mg-9.0Al-xGd (x=0.5, 1.0, and 2.0, wt.%) alloys simulated under the Gulliver-Scheil non-equilibrium condition using the present thermodynamic parameters are performed and shown in Fig. 11. It can be seen that the calculated

solidification paths of Mg-7.5Al-*x*Gd (*x*=2.5, 5.0 and 7.5, wt.%) and Mg-9.0Al-*x*Gd (*x*=0.5, 1.0, and 2.0, wt.%) alloys are Liquid \rightarrow Liquid+hcp(Mg) \rightarrow Liquid+hcp(Mg)+Al₂Gd \rightarrow Liquid+hcp(Mg)+ $\tau \rightarrow$ Liquid+hcp(Mg)+ $\tau+\gamma$.

In order to design the Mg–Al–Gd alloys containing LPSO phases, simulated solidification paths and phase fractions of the as-cast Mg–xAl–10Gd (x=1.0, 2.0, and 3.0, wt.%) and Mg–1Al–xGd (x=2.5, 5.0, and 7.5, wt.%) alloys under Scheil solidification condition are shown in Figs. 12(a, b), which clearly predicts that the phase fraction of 18R gradually increases with the increase of Gd content but decreases with the increase of Al content. As shown in Fig. 12(a), the 14H phase is not present in the calculated solidification paths of Mg–xAl–10Gd (x=1.0, 2.0, and 3.0, wt.%) and Mg–1.0Al–xGd (x=2.5, 5.0, and 7.5, wt.%) alloys,

Fig. 12 Calculated solidified path (a) and 18R phase fractions (b) of representative alloys of Mg–xAl–10Gd (x=1.0, 2.0, and 3.0, wt.%) and Mg–1.0Al–xGd (x=2.5, 5.0, and 7.5, wt.%) under Scheil solidification conditions

Fig. 13 Calculated vertical sections based on thermodynamic parameters of this work: (a) 10 wt.% Gd; (b) 1 wt.% Al

which agrees with the report in literature. The calculated vertical sections of 10 wt.% Gd and 1 wt.% Al are shown in Fig. 13, which can predict that the 14H phase will appear in the Mg–xAl–10Gd alloy after heat treatment at 230–398 °C when the content of Al is less than 1 wt.%, and in the Mg–1Al–xGd alloy after heat treatment from 230 to 346 °C when the content of Gd is higher than 5 wt.%.

5 Conclusions

(1) The experimental phase equilibria data for the Mg-Al-Gd system available in literature were critically evaluated. Based on the experimental data in literature, the Mg-Al-Gd system was assessed by means of the CALPHAD method. A set of self-consistent thermodynamic parameters of the Mg-Al-Gd system was obtained. Mg_x(TM,Mg)₆-(RE,Mg)₈ model can be applied to describing the LPSO phases in the Mg-Al-Gd system. Some representative isothermal sections, vertical sections, liquidus surface projections and the solubilities of the third element in the binary compounds were calculated. The calculated composition range of the τ phase is 16.0–17.3 at.% Mg and 66.6 at.% Al, which is stable between approximately 296 and 751 °C. The reaction scheme for the Mg-Al-Gd system was also constructed. Most of the reliable experimental data can be well reproduced by the present thermodynamic modeling.

(2) The calculated isothermal sections in the Mg-rich corner at 400, 450, 500, 525, 550 and 565 $^{\circ}$ C of the Mg–Al–Gd system and the phase

relationship of the LPSO phases were determined. The ideal composition of the 14H and 18R phases were calculated to be $Mg_{83.5}Gd_{9.4}Al_{7.1}$ and $Mg_{80.9}Gd_{10.9}Al_{8.2}$, respectively. According to the calculations, 14H is formed via the peritectic reaction: Al₂Gd+hcp(Mg)+18R=14H at 451 °C and decomposed by 14H=Al₂Gd+Mg₅Gd+hcp(Mg) at 230 °C, and 18R is formed via the transition: Liquid + Al₂Gd = 18R + Mg₅Gd at 574 °C and decomposed by 18R=Al₂Gd+Mg₅Gd+14H at 447 °C. Therefore, it can be concluded that 14H and 18R are stable between 230 and 451 °C and between 447 and 574 °C, respectively.

(3) Based on the obtained thermodynamic parameters in the present work, the Scheil solidification paths and the phase fractions of as-cast alloys were calculated and simulated. The variation of phase composition and phase fraction is clearly described, which provides quantitative theoretical guidance for the design of high-performance Mg–Al–Gd alloys.

CRediT authorship contribution statement

Cheng-liang QIU: Experimental determination, Optimization, Writing – Original draft; **Shu-hong LIU:** Funding acquisition, Revised manuscript; **Jin-hui HUANG:** Crystal structure analysis; **Yong DU:** Contributed reagents and analysis tools.

Declaration of competing interest

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

Acknowledgments

The financial supports from the National Key Laboratory of Science and Technology on High-strength Structural Materials and the National Natural Science Foundation of China (No. 51771235) are greatly acknowledged.

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Mg-Al-Gd 铸造合金的相平衡及凝固行为

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摘 要:采用 CALPHAD (CALculation of PHAse Diagrams)方法重新对 Mg-Al-Gd 三元系进行评估,获得一套自 洽的热力学参数。用 Mgx(TM,Mg)6(RE,Mg)8 热力学模型(TM=过渡金属,RE=稀土金属)描述长周期堆积有序相 14H 和 18R。计算代表性的等温截面、垂直截面、液相线投影图和相关的零变量反应,与实验数据进行比较,表明所 得热力学参数的可靠性。绘制了整个三元体系的反应图,并对几种 Mg-Al-Gd 合金的 Scheil 凝固路径和相分数进 行计算和分析,清楚地描述了凝固过程中各相的形成以及 y 和 LPSO 相的相分数随 Gd 成分的变化,这些是影响 Mg-Al-Gd 合金的显微硬度、极限抗拉强度和屈服强度的重要因素。

关键词:热力学模型;CALPHAD;Mg-Al-Gd体系;LPSO;希尔凝固

(Edited by Bing YANG)