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ARTICLE

First-principles Calculation of Electronic Structure and Mechanical Properties of Binary Phases in Mg-Zn-Y-La Alloy

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Abstract: In order to investigate the effect of rare earth elements on the properties of Mg-Zn magnesium alloys, the structural stability, electronic structure and mechanical properties of Mg_2Y, Mg_2La and Mg_3La compounds were calculated and analyzed by using the plane wave pseudo-potential method based on the first principles calculation. The results show that Mg_3La has the strongest forming ability, Mg_2La has the most stable structure by comparing the heat of formation and cohesive energy among the three compounds. The stabilization mechanism of the structure was analyzed based on the calculation of electron densities of states (DOS), electron occupation number and electron density difference. The bulk modulus *B*, shear modulus *G*, Young's modulus *E*, and Poisson's ratio *v* were further calculated by the elastic constants. The calculated results indicate that Mg_2Y has the strongest ability of resisting deformation, Mg_3La has the strongest stiffness and resistance to shear deformation, Mg_2La has the strongest plasticity, Mg_2Y and Mg_2La are ductile phases while Mg_3La is a brittle phase. In addition, the calculated results of hardness and melting temperature show that Mg_3La has the largest hardness and Mg_2Y has the highest melting temperature among the three compounds.

Key words: magnesium alloy; first principles calculation; structural stability; electronic structure; elastic properties

Magnesium alloy is the lightest metal material in industrial application and it has been intensively used in the automobile, aerospace and 3C industries due to its advantages of high specific strength and high rigidity, good shock resistance and machinability[1-3]. However, the inferior mechanical properties of magnesium alloys at high temperature restricted its further development. Research results show that an effective way to improve the mechanical properties of magnesium alloys was alloying magnesium alloys using rear earth elements[4]. Mg-Zn-Y ternary alloy has attracted much attention due to its excellent mechanical properties and unique crystal structure[5]. The addition of Y to the Mg-Zn alloy can not only improve the ambient mechanical properties by improving the casting properties and the formation of the stable quasicrystal strengthening phase but also improve the high temperature strength and creep resistance of magnesium alloys[6, 7]. However, the improvement of the properties of the alloys was limited by only one type of rear earth element addition. The research results show that the addition of multiple rare earth elements could significantly improve the properties of the magnesium alloys through the mutual influence of several elements[8]. Many researches has focused on the high cost heavy rear earth elements, such as Gd and Dy, while only little attention has been paid to low cost light rare earth elements, such as La and Ce. The structural stability and electronic structure of Mg-La intermetallic compounds were investigated[9,10]. It was found that Mg_3La had the strongest forming ability and MgLa had the most stable structure. The elastic properties and electronic structure of Mg_2Y and Mg_2La compounds were investigated by Chen et al[11]. It was found that Mg_2Y was a ductile phase, while Mg_2La was a brittle phase. The calculated results of elastic and thermodynamic properties of Mg_3La phase showed that

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it was a brittle phase which is dynamically stable[12]. Irrespective of the above mentioned theoretical investigation on the Mg_2Y, Mg_2La and Mg_3La compounds, no systematic theoretical investigation has been reported on structural stability, electronic structure and mechanical properties of Mg_2Y, Mg_2La and Mg_3La laves phases in La alloying Mg-Zn-Y alloys by first principles calculations.

In order to study the stability, electronic structure and mechanical properties of Mg_2Y, Mg_2La and Mg_3La compounds, the heat of formation, cohesive energy, density of state, Mulliken electron occupation numbers, electron density difference, elastic constants, hardness and melting temperature of Mg_2Y, Mg_2La and Mg_3La were calculated and analyzed by using the first-principle method in the present work. The calculated results have good consistency with other theoretical and experimental values of relevant documents. We hope that the research results can serve as a theoretical guidance of the development of Mg-Zn-Y series alloys.

1 Computational Methods

This study was carried out by the first principle method, which is based on density functional theory (DFT)[13], using the Cambridge Serial Total Energy Package (CASTEP) code. Through the plane wave pseudo-potentials method[14], the exchange-correlation terms in the electron-electron interaction was treated with the Perdew-Bruke-Ernzerhof (PBE)[15] version of generalized gradient approximation (GGA). The cut-off energy of plane wave was set to 380 eV, in order to keep the total energy and function on the atomic force convergence. The total energy convergence value is 5.0×10^{-8} eV/atom, and the force on all atoms is less than 0.001 eV/nm. The k-points of Monkhost-Pack scheme is 6×6×6.

2 Results and Discussion

2.1 Crystal structure and stability

The crystal structures of Mg_2Y, Mg_2La and Mg_3La are shown in Fig.1. The structure parameters are listed in Table 1. The calculated crystal constants of Mg_2Y, Mg_2La and Mg_3La are listed in Table 2. For the reference the calculated results by other authors using the same calculation method are also shown in Table 2. It can be seen that the present optimized results are in good agreement with other computational results, suggesting that the calculated results in this work are highly reliable. In order to compare the forming and thermodynamic stability, the heats of formation and cohesive energies of Mg_2Y, Mg_2La and Mg_3La are calculated in the present paper by the following equations:

$$\Delta H = \frac{E_{\text{tot}}^{\text{AB}} - N_{\text{A}}E_{\text{solid}}^{\text{A}} - N_{\text{B}}E_{\text{solid}}^{\text{B}}}{N_{\text{A}} + N_{\text{B}}} \quad (1)$$

$$E_{\text{coh}} = \frac{E_{\text{tot}}^{\text{AB}} - N_{\text{A}}E_{\text{atom}}^{\text{A}} - N_{\text{B}}E_{\text{atom}}^{\text{B}}}{N_{\text{A}} + N_{\text{B}}} \quad (2)$$

where ΔH and E_{coh} are the heats of formation and cohesive energies of intermetallic compound, respectively, $E_{\text{tot}}^{\text{AB}}$ is the total energy of alloy, $E_{\text{solid}}^{\text{A}}$ and $E_{\text{solid}}^{\text{B}}$ are the energy per atom of pure elements A and B, respectively. $E_{\text{atom}}^{\text{A}}$ and $E_{\text{atom}}^{\text{B}}$ are the energies of A and B atoms in the free state, respectively, N_{A} and N_{B} are the atom numbers in the unit cell.

The heats of formation and cohesive energies of three kinds of crystal structure are shown in Table 3. The easiness of formation of intermetallic compounds can be expressed by heats of formation. The lower the heats of formation are, the better the forming ability are. The negative values of the heats of formation of the three crystalline structures imply that all the three compounds can be formed by exothermic reaction in Mg-Zn-Y-La alloys. By comparison it can be seen that Mg_3La is the easiest to form, followed by Mg_2La and Mg_2Y.

The stability of the crystal structure is decided by the cohesive energy. The definition of cohesive energy is that if the crystal is split into a single atom, the lower the cohesive energy is, the more stable the crystal structure is[19]. It is shown that Mg_2La has the strongest alloying ability, followed by Mg_2Y and Mg_3La. For the other important structure of $MgZn_2$ in Mg-Zn-Y-La alloy, the cohesive energy has been already calculated by our research group[3], and the value is -134.22 kJ/mol. The cohesive energies of Mg_2Y, Mg_2La and Mg_3La are found to be much higher than that of $MgZn_2$ by comparison. Therefore, the addition of Y and La elements play a very important role in improving the stability of Mg-Zn alloy structure.

2.2 Electronic structures

The stability and mechanical properties of intermetallic compounds are determined by their electronic structures [23]. In order to further understand the bonding characteristics,

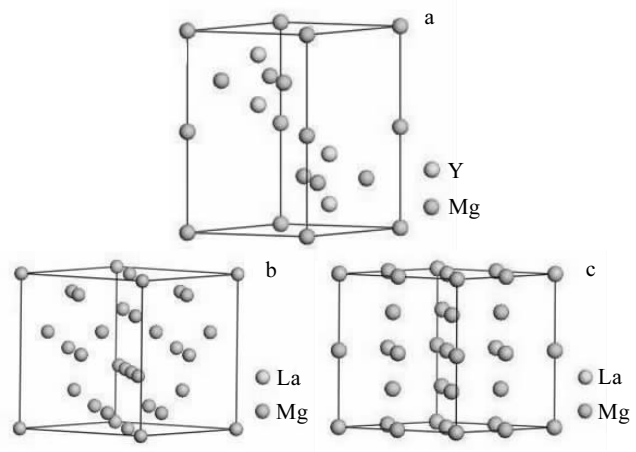

Fig.1 Crystal structures of Mg_2Y (a), Mg_2La (b), and Mg_3La (c)

Table 1 Structure parameters of Mg_2Y, Mg_2La and Mg_3La

Phase	Atom number in cell	Space group	Structure type	Pearson sign	Atomic coordinate
Mg_2Y	12	P63/MMC	C14	hP12	Mg: (0,0,0), Mg: (0.84,0.68,0.25) Y: (0.33,0.67,0.62)
Mg_2La	24	FD-3M	C15	cF24	Mg: (0.625,0.625,0.625), La: (0,0,0)
Mg_3La	16	FM-3M	C15	cF16	Mg: (0.5,0.5,0.5) Mg: (0.25,0.25,0.25), La: (0,0,0)

Table 2 Crystal constant of Mg_2Y, Mg_2La and Mg_3La

Phase	a_0/×0.1 nm		c_0/×0.1 nm		V_0/×10^{-3} nm^3	ρ/g·cm^{-3}
	Present	Ref.	Present	Ref.		
Mg_2Y	6.032	6.037 [16], 6.064 [17]	9.960	9.752 [16], 9.786 [17]	317.393	2.968
Mg_2La	8.827	8.769 [9], 8.817 [17]	8.827	8.769 [9], 8.817 [17]	687.671	3.622
Mg_3La	7.537	7.495 [9], 7.507 [18]	7.537	7.495 [9], 7.507 [18]	428.165	3.286

Table 3 Calculated heat of formation (ΔH) and cohesive energy (E_{coh}) of Mg_2Y, Mg_2La and Mg_3La

Phase	ΔH/kJ·mol^{-1}			E_{coh}/kJ·mol^{-1}		
	Present	Exp.	Cal.	Present	Exp.	Cal.
Mg_2Y	-10.74	-10.37 [17]	-11.99 [17], -9.17 [20]	-243.69	-	-
Mg_2La	-11.77	-12.30 [21]	-11.66 [21], -12.55 [22]	-251.78	-	-253.11 [9]
Mg_3La	-12.49	-13.50, -13.30 [18]	-13.36 [18], -9.00 [9]	-225.82	-	-229.66 [9]

the electronic structures of Mg_2Y, Mg_2La and Mg_3La compounds were calculated and analyzed. The total and partial density of states are shown in Fig.2, and the Fermi level E_F are indicated by the dotted line in the figures. It can be seen from Fig.2 that the peak density of states near the Fermi level for Mg_2Y, Mg_2La and Mg_3La are all concentrated between -7 and 0 eV, implying that, Mg_2Y, Mg_2La and Mg_3La all exhibit metallic properties. The contribution of Mg_2Y bonding electrons mainly come from the orbital electrons of Mg(3s), Mg(2p), Y(5s), Y(4p) and Y(4d). The binding electrons of Mg_2La and Mg_3La are mainly originated from Mg(3s), Mg(2p), La(6s), La(5p), La(5d) orbital. The total density of states at the Fermi level are also shown in Fig.2. It is found that the states density of the Mg_2Y, Mg_2La and Mg_3La compounds at the Fermi level are 13.70, 24.678 and 8.96, respectively. From this, it can be concluded that Mg_2La has the highest conductivity in the three compounds.

The stability of the crystal structure is also closely related to the number of bonding electrons. The more electrons are bonded, the stronger the interaction between the charges and the more stable of the structure is[24]. The number of bonded electrons between -7 and 0 eV for Mg_2Y is 75.98, Mg_2La is 215.92 and Mg_3La is 35.09. It can be seen from the interaction between the charge available that Mg_2La has the highest stability, followed by Mg_2Y, and then Mg_3La. Considering the combination of cohesive energy and electronic structure, it can be deduced that Mg_2La has the highest stability among the three compounds.

The bonding strength between atoms can be analyzed by electron occupation number[25]. The calculated results of the electron occupation numbers of Mg_2Y, Mg_2La and Mg_3La are shown in Table 4. From the table it can be seen that for Mg_2Y, the electrons transfer not only takes place from Y to Mg atoms, but also between Mg and Mg atoms. As for Mg_2La electrons transfer from La to Mg atoms. Whereas for Mg_3La electrons transfer from Mg to La atoms. Considering the atoms number, the average charge transfer between different types of atoms in the three compounds is 0.043 for Mg_2Y, 0.19 for Mg_2La, and 0.047 for Mg_3La. In the three kinds of crystal structures, the order of the ionic bond is Mg_2La>Mg_3La >Mg_2Y, which is in agreement with the results of bonding electron number analysis. Based on the above analysis, it can be found that although Mg_3La has the strongest formation ability, the stability of Mg_3La is weaker than that of Mg_2La.

The bonding characteristics of the intermetallic compounds can also be visualized by the electron density difference. In this paper, the electron density difference of Mg_2Y, Mg_2La and Mg_3La crystal structures is calculated and analyzed, as shown in Fig.3. The contour lines are drawn within the following ranges: Mg_2Y: -4.232×10^{-2} to 7.631×10^{-2} v/nm^3, Mg_2La: -4.423×10^{-2} to 1.367×10^{-1} v/nm^3, Mg_3La: -4.647×10^{-2} to 1.875×10^{-1} v/nm^3. The spacings are: Mg_2Y, 0.423×10^{-2} v/nm^3, Mg_2La, 4.524×10^{-2} v/nm^3 and Mg_3La, 5.423×10^{-2} v/nm^3. From the electron density difference, it can be inferred that Mg-Y atoms in Mg_2Y are ionic bonds , Mg-Mg atoms are covalent bonds and Y-Y atoms are metallic bonds. Mg-La atoms in Mg_2La and Mg_3La are ionic bonds, Mg-Mg atoms are covalent bonds, and the La-La atoms are metallic bonds. Based on the

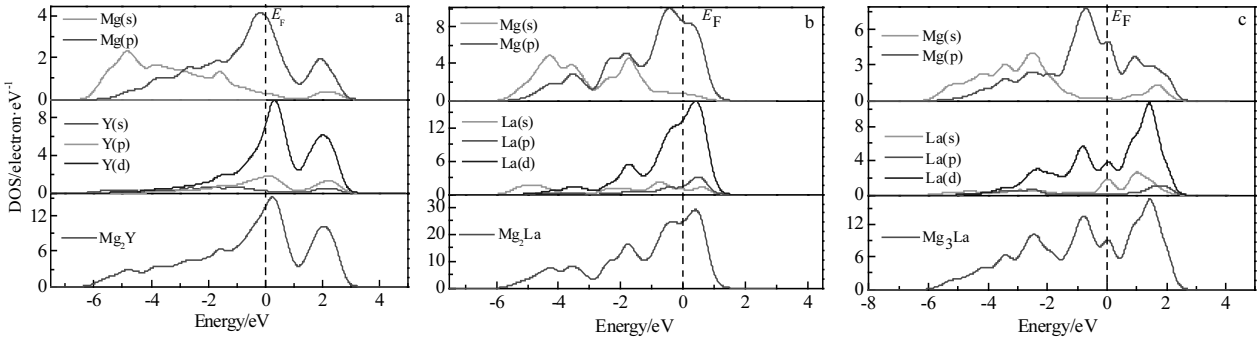

Fig.2 Total (Partial) density of states of Mg_2Y(a), Mg_2La (b), and Mg_3La (c)

Table 4 Electron occupation numbers of Mg_2Y, Mg_2La, and Mg_3La

Phase	Atom	s	p	d	Total	Charge, e
Mg_2Y	Mg (Ⅰ)	0.94	7.02	0.00	7.97	0.03
	Mg (Ⅱ)	0.96	7.08	0.00	8.04	-0.04
	Y	0.59	0.53	1.82	2.95	0.05
Mg_2La	Mg	0.87	7.23	0.00	8.09	-0.09
	La	2.60	6.05	2.16	10.81	0.19
Mg_3La	Mg (Ⅰ)	0.75	7.15	0.00	7.90	0.10
	Mg (Ⅱ)	0.87	7.12	0.00	7.98	0.02
	La	2.29	6.32	2.52	11.14	-0.14

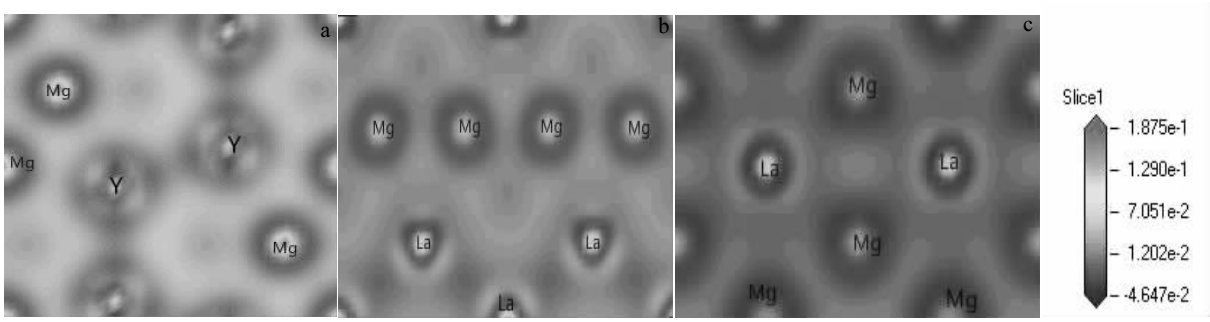

Fig.3 Electron density difference of Mg_2Y (a), Mg_2La (b), and Mg_3La (c)

above analysis, it can be found that the stability of Mg_2Y, Mg_2La and Mg_3La crystal structures is based on the interaction of ionic bond, covalent bond and metallic bond.

2.3 Elastic properties

The ability of a material to resist external forces is generally analyzed by elastic constants. Mg_2Y has a hexagonal crystal structure with five independent elastic constants C_{11}, C_{12}, C_{13}, C_{33} and C_{44}, satisfying the following stability criteria[25, 26]: $C_{11}>0$, $C_{11}-C_{12}>0$, $C_{44}>0$, $(C_{11}+C_{12})C_{33}-2C_{33}^2>0$. Mg_2La and Mg_3La are cubic crystal structures with three independent elastic constants C_{11}, C_{12} and C_{44}, satisfying the following stability criteria[27]: $(C_{11}+2C_{12})/3>0$, $C_{11}-C_{12}>0$, $C_{44}>0$. The calculated elastic constants of Mg_2Y, Mg_2La and Mg_3La are shown in Table 5. All the three crystal structures meet the stability criteria, indicating that they all have a stable structure, which is consistent with the conclusion obtained by the cohesive energy analysis.

The elastic modulus of the polycrystals can be obtained from the results of the elastic constants of the single crystals. For Mg_2La and Mg_3La with cubic crystal structures, the bulk modulus B and shear modulus G can be obtained by the following equation [28].

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{3}$$

$$G = \frac{1}{5}(3C_{44} + C_{11} - C_{12}) \tag{4}$$

For hexagonal Mg_2Y, the bulk modulus B and the shear modulus G are calculated based on the VRH approximation[10, 29]. Voigt approximation equation is as follows:

$$B_V = \frac{1}{9}\left[2(C_{11} + C_{12}) + C_{33} + 4C_{13}\right] \tag{5}$$

$$G_V = \frac{1}{30}(7C_{11} - 5C_{12} + 12C_{44} + 2C_{33} - 4C_{13}) \tag{6}$$

Table 5 Elastic constants of Mg_2Y, Mg_2La and Mg_3La

Phase		Elastic constants/GPa				
		C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
Mg_2Y	Present	79.18	25.44	27.84	81.84	19.11
	Cal. [11]	76.83	25.41	21.11	83.96	17.78
	Cal. [8]	62.86	39.91	27.16	77.07	17.42
Mg_2La	Present	52.24	25.65	-	-	20.80
	Cal. [21]	58.00	25.00	-	-	22.20
	Cal. [27]	58.17	25.03	-	-	20.32
Mg_3La	Present	60.96	29.65	-	-	34.24
	Cal. [18]	57.91	27.10	-	-	36.18
	Cal. [9]	56.47	26.83	-	-	22.08

Reuss approximation formula is as follows:

$$B_R = \frac{c^2}{C_{11} + C_{12} + 2C_{33} - 4C_{13}} \quad (7)$$

$$G_R = \frac{5}{2}\left\{\frac{c^2 C_{44} C_{66}}{3B_V C_{44} C_{66} + c^2 (C_{44} + C_{66})}\right\} \quad (8)$$

Hill approximation formula is as follows:

$$B = \frac{1}{2}(B_V + B_R) \quad (9)$$

$$G = \frac{1}{2}(G_V + G_R) \quad (10)$$

The Young's modulus E, the Poisson's ratio ν and the elastic anisotropy coefficient A can be obtained from the results of the bulk modulus and the shear modulus, by using the following equation [8, 17]:

$$E = \frac{9BG}{3B + G} \quad (11)$$

$$\nu = \frac{1}{2}\left[\frac{B - (2/3)G}{B + (1/3)G}\right] \quad (12)$$

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \quad (13)$$

The calculated results of the elastic modulus and the Poisson's ratio of Mg_2Y, Mg_2La and Mg_3La are shown in Table 6. It can be seen that the calculated results are consistent with the results listed in other literatures, indicating that the calculation method is reliable. It is found that the bulk modulus B of the three crystal structures is larger than the shear modulus G, indicating that the stability of the structure is mainly affected by the shear modulus G.

Modulus B is usually used to characterize the ability of a material to resist deformation under applied stress[31]. The greater the value of the bulk modulus B, the stronger the resistance to deformation. It can be seen from Table 6 that the resistance ability of the three kinds of compounds to extend force deform is: $Mg_2Y > Mg_3La > Mg_2La$. Similarly, the shear modulus G can be used to characterize the ability of a material to resist shear deformation under shear stress[31]. The larger the value of shear modulus, the stronger the resistance to shear deformation. It can be seen from Table 6 that the resistance ability of the three kinds of compounds to shear deformation is $Mg_3La > Mg_2Y > Mg_2La$. Young's modulus E can be used as a measure of solid stiffness. The greater the Young's modulus E, the greater the stiffness of the material[31, 32]. The stiffness of the three compounds is $Mg_3La > Mg_2Y > Mg_2La$. Poisson's ratio is a measure of the resistance of a crystal to shear, usually the value is between -1 and 0.5. The greater the Poisson's ratio, the better the plasticity of a material[31]. The Poisson's ratio result in Table 6 indicates that plasticity order from strong to weak is $Mg_2La > Mg_2Y > Mg_3La$. The Poisson's ratio between 0.25 and 0.5 means that the binding force among the atoms in the material is the central atomic force. The Poisson's ratio of Mg_2Y and Mg_2La is between 0.25 and 0.5, indicating that their interatomic binding energies are all central atomic forces.

The ratio of shear modulus to bulk modulus can be used to evaluate the material ductility. If the G/B ratio is less than 0.57, then the material shows ductility, otherwise the material is brittle. The G/B values of Mg_2Y, Mg_2La and Mg_3La are 0.522, 0.504 and 0.624, respectively, indicating that Mg_2Y and Mg_2La are ductile phases and Mg_3La is a brittle phase. In addition, the ductility and brittleness of a material also can be estimate by the values of the elastic constants $C_{12} - C_{44}$[33]. If $C_{12} - C_{44} < 0$, the material is brittle, whereas the material is ductile. As can be seen from Table 6 that the C_{12}-C_{44} values of Mg_2Y and Mg_2La are positive, implying that they are ductile material. Whereas the C_{12}-C_{44} value of Mg_3La is negative implying that it is a brittle material, which is in agreement with the result estimated by G/B value.

2.4 Melting temperature and hardness

It is well known that the properties of materials are closely associated with the hardness and melting temperature. The hardness and melting temperature are important indicators to evaluate the abrasive resistance and heat resistance of materials[34]. Here, the hardness and melting temperature of Mg_2Y, Mg_2La and Mg_3La are further studied. The hardness H can be calculated based on the following semi-empirical equation [35]:

$$H = \frac{(1 - 2\nu)E}{6(1 + \nu)} \quad (14)$$

Table 6 Calculated bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson ratio (v), anisotropic coefficient (A) and G/B of Mg_2Y, Mg_2La and Mg_3La

Phase		B/GPa	G/GPa	E/GPa	v	A	G/B	$(C_{12}-C_{44})$/GPa
Mg_2Y	Present	44.70	23.32	59.60	0.2778	0.710	0.522	6.33
	Cal. [17]	41.43	23.59	59.48	0.2607	0.69	0.569	7.63
	Cal. [30]	42.00	23.00	59.00	0.2640	-	0.548	-
Mg_2La	Present	34.51	17.38	44.65	0.2844	1.56	0.504	4.85
	Cal. [21]	36.00	19.80	49.90	-	-	0.550	2.80
	Cal. [27]	36.08	16.57	47.90	-	1.23	0.459	4.71
Mg_3La	Present	40.09	25.01	62.11	0.2418	2.19	0.624	-4.59
	Cal. [18]	37.37	25.69	62.70	0.2200	2.34	0.687	-9.08
	Cal. [21]	37.40	26.50	64.30	-	-	0.709	-10.1

For metal materials, the melting temperature T_m can also be estimated using the C_{11} elastic constant in intermetallic compounds, as given below [36]:

$$T_m = 553\ \mathrm{K} + (5.91\ \mathrm{K/GPa})C_{11} \pm 300\ \mathrm{K} \quad (15)$$

The calculated results of hardness and melting temperature are shown in Table 7. It can be seen that Mg_3La has the highest hardness in the three phases followed by Mg_2Y and Mg_2La. It can also be seen that Mg_2Y has the highest melting temperature in the three phases followed by Mg_3La and Mg_2La. These calculated results indicate that Mg_3La has the best abrasive resistance while Mg_2Y has the best heat resistance among the three compounds.

Table 7 Hardness and melting temperature parameters of Mg_2Y, Mg_2La and Mg_3La

Phase	H/GPa	T_m/K
Mg_2Y	5.64	1021
Mg_2La	4.12	862
Mg_3La	6.64	913

3 Conclusions

1) The calculated crystal structures of Mg_2Y, Mg_2La and Mg_3La are in good agreement with literature values. The analysis of formation and cohesive energy show that the Mg_3La has stronger alloying ability and Mg_2La has stronger structural stability. The addition of Y and La can improve the stability of Mg-Zn alloy.

2) The analysis of the electronic structure show that Mg_2La has the strongest conductivity and stability, followed by Mg_2Y and Mg_3La. The stability of Mg_2Y, Mg_2La and Mg_3La crystal structures are determined by the interaction of ionic bond, covalent bond and metal bond.

3) The elastic constants show that three phases are mechanically stable. The analyses of bulk modulus B, shear modulus G, Young's modulus E and Poisson's ratio v show that Mg_2Y has the strongest resistance to deformation, Mg_3La has the strongest resistance to shear deformation and stiffness, Mg_2Y and Mg_2La are ductile phase, Mg_3La is a brittle phase.

4) The calculated results of hardness and melting temperature show that Mg_3La has the largest hardness and Mg_2Y has the highest melting temperature.

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Mg-Zn-Y-La 合金中二元相的电子结构和力学性质的第一性原理计算

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摘　要：为了研究稀土元素对镁锌合金性能的影响，利用基于第一性原理计算的平面波赝势方法，对 Mg_2Y、Mg_2La 和 Mg_3La 的结构稳定性、电子结构和力学性能进行了计算和分析。形成热和结合能的计算结果表明，Mg_3La 具有最强合金化能力，而 Mg_2La 具有最强的结构稳定性。通过电子态密度（DOS），电子占据数和差分电荷密度分析了结构的稳定机制。计算了 3 种结构的弹性常数，并进一步得到了体模量 B，剪切模量 G，杨氏模量 E 和泊松比 γ 等。计算结果表明：Mg_2Y 具有最强的抵抗变形能力，Mg_3La 具有最强的刚度和抵抗剪切变形能力，而 Mg_2La 塑性最强。进一步分析表明 Mg_2Y 和 Mg_2La 为延性相，而 Mg_3La 为脆性相。此外，硬度和熔点的计算结果表明，3 种金属间化合物中，Mg_3La 的硬度最大，Mg_2Y 的熔点最高。

关键词：镁合金；第一性原理计算；结构稳定性；电子结构；弹性性质

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