

A first-principles study on electronic structure and elastic properties of Al_4Sr , Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$ phases

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Abstract: The electronic structures and mechanical properties of Al_4Sr , Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$ phases were determined by the use of first-principles calculations. The calculated heat of formation and cohesive energy indicate that Al_4Sr has the strongest alloying ability as well as the highest structural stability. The elastic parameters were calculated, and then the bulk modulus, shear modulus, elastic modulus and Poisson ratio were derived. The ductility and plasticity were discussed. The results show that Al_4Sr and Mg_2Sr phases both are ductile, on the contrary, $\text{Mg}_{23}\text{Sr}_6$ is brittle, and among the three phases, Mg_2Sr is a phase with the best plasticity.

Key words: magnesium alloy; first-principles calculation; electronic structure; elastic property

1 Introduction

The interest in magnesium-based alloys is continuously increasing, especially because of their applications, e.g., automobile body materials, for weight reduction and higher fuel efficiency [1–2]. For the Mg–Al-based alloys, $\beta\text{-Mg}_{17}\text{Al}_{12}$ is an essential phase which plays an important role in strengthening crystal boundary and controlling high-temperature crystal running. However, the softening of the phase at the elevated temperature is detrimental to the creep property of the alloys. Therefore, the usage of these magnesium alloys in automobile industry is limited to non-critical parts. Calcium and strontium are two important additives used in magnesium alloys. However, Ca is detrimental since it results in the hot-cracking of the alloy [3]. On the other hand, Sr reduces the shrinkage and porosity of the alloy, and helps to abate the hot-cracking effect of Ca. Therefore, the Sr alloying magnesium alloys have drawn much attention in recent years.

Recent experiment investigations [4–6] have shown that strontium addition to the Mg–Al-based alloys improves greatly the heat resistance by forming Al_4Sr , Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$ phases. However, the alloying ability

and the structural stability of these compounds containing strontium in Mg–Al-based alloys have not been well studied yet. The reason is that these compounds are often brittle and it is very difficult to prepare the sample for the measurements of the mechanical properties. As a result, the investigations of the mechanical properties have been performed only for a few cubic and simple hexagonal Laves phases by dynamic measurements [7]. Recent first-principles investigations of the elastic constants of metals based on the density functional theory give quite satisfactory results for the evaluation of bulk modulus, shear modulus and other elastic constants [8–9]. However, to the best of our knowledge, no systematic theoretical study has been performed on the electronic structure and mechanical properties of Al_4Sr , Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$ phases from first-principles.

In this work, the electronic structure and mechanical properties of Al_4Sr , Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$ phases are investigated by the use of first-principles method. The structures are optimized by full relaxations of the lattice parameters and atomic positions. The heat of formation and cohesive energy are calculated and discussed. The densities of states (DOS) are calculated to study the mechanism of structural stability. The elastic parameters

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C_{ij} are calculated, the bulk modulus, shear modulus, elastic modulus and Poisson ratio are derived. The ductility, plasticity, and other mechanical properties of these compounds based on the calculated elastic properties are studied. The results give valuable estimation for the properties unavailable in experiments.

2 Method of computation

Cambridge serial total energy package (CASTEP) [10–11], a first-principles plane-wave pseudopotentials method based on density functional theory, was used in this work. CASTEP used a plane-wave basis set for the expansion of the single-particle Kohn-Sham wave-functions, and pseudopotentials to describe the computationally expensive electron-iron interaction, in which the exchange-correlation energy by the generalized gradient approximation (GGA) of Perdew was adopted for all elements in our models by adopting Perdew-Burke-Ernzerhof parameters [12–13]. Ultrasoft pseudopotentials [14–15] represented in reciprocal space was used. In the present calculations, the cutoff energy of wave functions (PWs), E_{cut} , was set at 330 eV. Sampling of the irreducible wedge of the Brillouin zone was performed with a $6 \times 6 \times 6$ regular Monkhorst-Pack grid of special k -point. The finite basis set correction [16] and the Pulay scheme of density mixing [17] were applied for

the evaluation of energy and stress. All lattice parameters and atomic positions in our model have been relaxed according to the total energy and force using the Broyden-Fletcher-Goldfarb-Shanno [18] scheme, based on the cell optimization criterion (RMs force of 5.0×10^{-6} eV/Å, stress of 0.01 GPa, and displacement of 5.0×10^{-4} Å). The SCF tolerance is set as 5.0×10^{-7} eV. In our calculations of elastic constants of Al_4Sr , Mg_2Sr , $\text{Mg}_{23}\text{Sr}_6$ compounds, the generalized gradient approximation (GGA) of Perdew was used by adopting PW91.

3 Results and discussion

3.1 Structures and lattice constants

The structure parameters of Al_4Sr , Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$ phases are listed in Table 1, and these structures are shown in Fig. 1. The lattice constants of these structures are estimated from the minimized total energy, and the results are listed in Table 2. It can be seen that the obtained results of lattice constants are close to the available theoretical and experimental values [4, 19]. The fairly good agreement between theoretical and experimental results show that the present calculations are highly reliable.

3.2 Heat of formation and cohesive energy

The heat of formation (ΔH) and the cohesive

Table 1 Structure parameters of Al_4Sr , Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$ phases

Phase	Structure type	Atom number in cell	Group (No.)	Atom site
Al_4Sr	DI_3	5	$I4/mmm(139)$	+1Sr: (0, 0, 0); +2Al(I): (0, 0, z), (0, 0, $-z$); $z=0.38+2\text{Al(II)}:(0, 1/2, 1/4), (1/2, 0, 1/4)$
Mg_2Sr	C14	12	$P6_3/mmc(194)$	+4Sr: $(1/3, 2/3, z), (-1/3, -2/3, -z), (1/3, 2/3, 1/2-z), (-1/3, -2/3, -1/2+z); z=0.062$; +2Mg(I): (0, 0, 0), (0, 0, 1/2); +6Mg(II): $(x, 2x, 1/4), (-x, -2x, -1/4), (-2x, -x, 1/4), (x, -x, 1/4); x=-0.170$
$\text{Mg}_{23}\text{Sr}_6$	$\text{Th}_6\text{Mn}_{23}$	29	$Fm3m(225)$	+1Mg(I): (0.5, 0.5, 0.5); +6 Mg(II): (0, 0.25, 0.25); +8Mg(III): (0.378, 0.378, 0.378); +8Mg(IV): (0.178, 0.178, 0.178); +6Sr: (0.203, 0, 0)

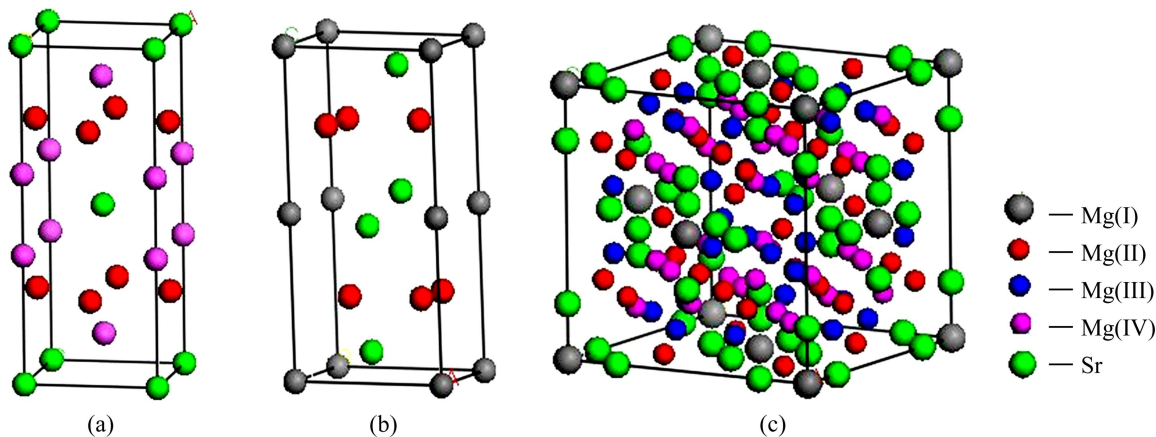


Fig. 1 Model of crystal cell of Al_4Sr (a), Mg_2Sr (b) and $\text{Mg}_{23}\text{Sr}_6$ (c)

Table 2 Lattice constants and formation heat of Al₄Sr, Mg₂Sr and Mg₂₃Sr₆ phases

Phase	Lattice constant/nm						Formation heat/(kJ·mol ⁻¹)	
	Present		Ref.		Exp.		Present	Ref.
	<i>a</i>	<i>c</i>	<i>a</i>	<i>c</i>	<i>a</i>	<i>c</i>		
Al ₄ Sr	0.440	1.113	—	1.107 [19]	—	1.108 [19]	-23.928	-23.7 [6], -24.2 [6], -22.8 [6], -25.6 [6], -26.2 [6]
Mg ₂ Sr	0.646	1.041	0.647 [4]	1.039 [4]	—	—	-11.057	-10.618 9 [4], -7.117 [20], -7.95 [5]
Mg ₂₃ Sr ₆	1.493	—	—	—	1.483	—	-8.278	—

energy (E_{coh}) of Al₄Sr, Mg₂Sr, Mg₂₃Sr₆ crystals are calculated by using the following expressions [21–22]:

$$\Delta H = E_{\text{tot}}^{\text{AB}} - [cE_{\text{form}}^{\text{A}} + (1-c)E_{\text{form}}^{\text{B}}] \quad (1)$$

$$E_{\text{coh}} = E_{\text{tot}}^{\text{AB}} - [cE_{\text{atom}}^{\text{A}} + (1-c)E_{\text{atom}}^{\text{B}}] \quad (2)$$

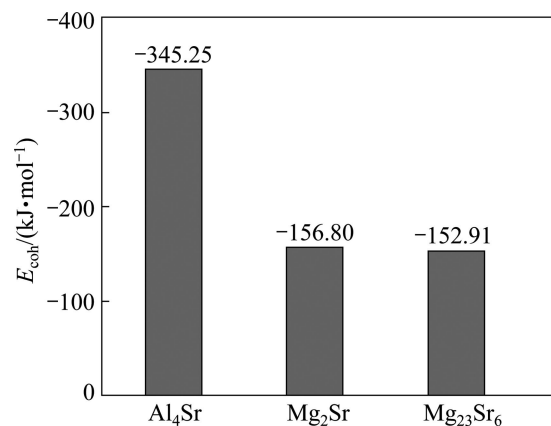
where $E_{\text{tot}}^{\text{AB}}$ refers to the total energy/atom of the intermetallic compound; $E_{\text{form}}^{\text{A}}$ and $E_{\text{form}}^{\text{B}}$ are the single atomic energies of pure constituents A and B in the elemental states; c refers to the atomic fraction of the constituent A; $E_{\text{atom}}^{\text{A}}$ and $E_{\text{atom}}^{\text{B}}$ are the total energies of isolated atoms A and B. The obtained ΔH calculated from Eq. (1) is also presented in Table 2.

From Table 2 we can see that, the formation heat of Al₄Sr is -23.928 kJ/mol, close to the corresponding calculation values of -23.7, -24.2, -22.8, -25.6 and -26.2 kJ/mol from Ref. [6]. The formation heat of Mg₂Sr is -11.057 kJ/mol, in good agreement with the theoretical values of -10.618 9 from Ref. [4], -7.117 kJ/mol from Ref. [20] and -7.95 kJ/mol from Ref. [5]. The heats of formation of Al₄Sr, Mg₂Sr and Mg₂₃Sr₆ are all negative, which means that these phases are energetically stable. The negative heat of formation decreases from Mg₂₃Sr₆ to Mg₂Sr to Al₄Sr, indicating that the alloying ability increases from Al₄Sr to Mg₂Sr to Mg₂₃Sr₆ [23]. Al₄Sr phase has the strongest alloying ability.

The stability of crystal is determined by its cohesive energy [24]. Generally, the cohesive energy can be defined as total energy released when isolated atoms combined into solid. Hence, the larger the absolute value is, the more stable the crystal structure is [24–25]. The obtained E_{coh} calculated from Eq. (2) is shown Fig. 2. It is found that the present calculated results are -345.25 kJ/mol for Al₄Sr, -156.80 kJ/mol for Mg₂Sr and -152.91 kJ/mol for Mg₂₃Sr₆, respectively. The obtained results show that the Al₄Sr phase is the most stable due to the highest E_{coh} , and Mg₂Sr is relatively stable, while the stability of Mg₂₃Sr₆ is the weakest due to the relatively lower E_{coh} .

3.3 Electronic structures

Usually, structural stability of intermetallic compounds depends on the bonding electron orbital characteristics. For example, the strength of covalent

**Fig. 2** Cohesive energy (E_{coh}) of Al₄Sr, Mg₂Sr and Mg₂₃Sr₆ phases

bond is related to covalent electron orbital hybridization, while ionic bonds are decided by transfer charge for different atoms [26–27]. In the present work, further analysis of total and partial densities of states (DOS) (see Fig. 3) of Al₄Sr, Mg₂Sr and Mg₂₃Sr₆ phases are performed to reveal the structural stability mechanism of these compounds. The total and partial DOSs of Al₄Sr, Mg₂Sr and Mg₂₃Sr₆ crystal cells are plotted in Figs. 3(a), (b) and (c), respectively. Here, we can see that the main bonding peaks for these compounds basically locate in energy range from 0 to -10 eV, and originate from the contribution of valence electron numbers of Al(s), Al(p), Sr(s) and Sr(p) orbits for Al₄Sr (see Fig. 3(a)), but for Mg₂Sr and Mg₂₃Sr₆, those are the result of the bonding Mg(s), Mg(p), Sr(s) and Sr(p) (see Figs. 3(b) and (c)). Further analysis was done. It is found that for Al₄Sr, covalent electron orbit hybridization takes place in 0–-2.5 eV energy range, which mainly is the weaker Sr(p)–Al(p) interaction, while for Mg₂Sr, hybridization is thought as the sp states of Sr and the sp states of Mg, in addition, some resonance phenomena happen between Sr(s), Mg(s) and Mg(p). But for Mg₂₃Sr₆, hybridization range becomes broader compared with those of Al₄Sr. Among three phases, there are most electronic states involved in hybridization and the strongest hybridization intensity for Mg₂₃Sr₆. Hence, from the perspective of covalent bond, the stability of Mg₂₃Sr₆ should be higher than that Mg₂Sr or Al₄Sr, which is not exactly the same

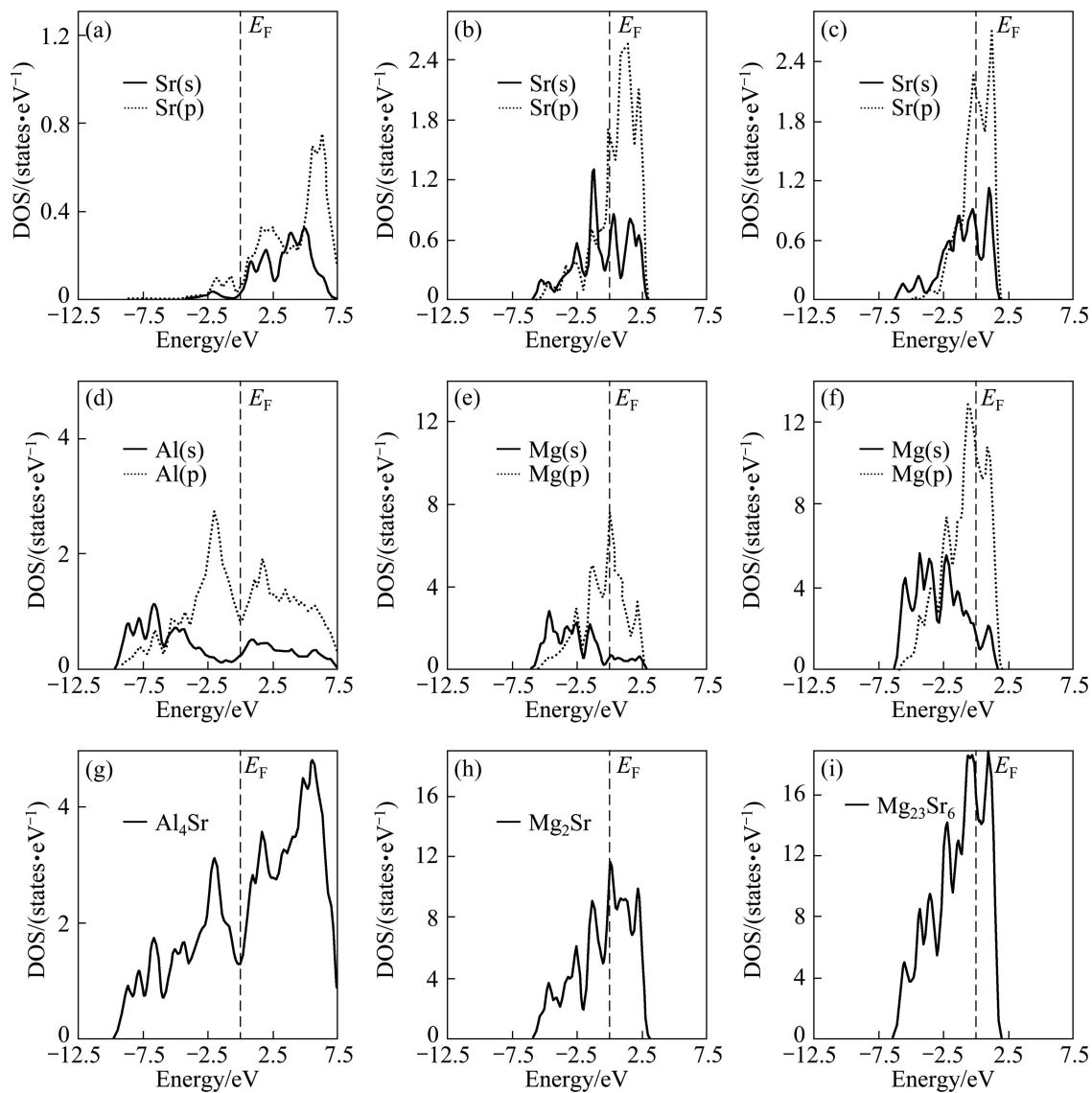


Fig. 3 Total and partial DOSs of Al_4Sr (a, d, g), Mg_2Sr (b, e, h) and $\text{Mg}_{23}\text{Sr}_6$ (c, f, i)

order compared with that of the calculated cohesive energy. Hence, characteristics of ionic bonds need be considered for three phases.

The calculated results of Mulliken electron occupation number for Al_4Sr , Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$ are listed in Table 3. It is found that the charge transfer phenomenon takes place from the Sr to Al atoms for Al_4Sr , and the total number of the system is about 2.10, but for Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$, the transfer charge from the Sr to Al atoms can be seen, the total number is about $3.88(0.97 \times 4)$, $6.72(1.12 \times 6)$, respectively. As far as Al_4Sr , Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$ are concerned, the system is not the same atomic number, which is 5, 12, 29 (see Table 1), respectively. If atom number of three phases is considered, the average transfer charge is approximately $0.420(2.10/5)$, $0.323(3.88/12)$, $0.232(6.72/29)$, indicating that the ionic bonds order from strong to weak is Al_4Sr , Mg_2Sr , $\text{Mg}_{23}\text{Sr}_6$, which is in good agreement with the

Table 3 Mulliken electronic populations of Al_4Sr , Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$

Phase	Atom	Electron orbit		Transfer charge
		s	p	
Al_4Sr	Al(I)	1.20	2.45	−0.66
	Al(II)	1.20	2.19	−0.39
	Sr	2.00	5.91	2.10
Mg_2Sr	Mg(I)	1.01	7.41	−0.42
	Mg(II)	1.07	7.44	−0.51
	Sr	2.54	6.49	0.97
$\text{Mg}_{23}\text{Sr}_6$	Mg(I)	0.87	7.39	−0.26
	Mg(II)	0.97	7.37	−0.34
	Mg(III)	1.00	7.26	−0.26
	Mg(IV)	1.00	7.30	−0.30
	Sr	2.40	6.48	1.12

cohesive energy calculations.

Calculations of the densities of states and Mulliken electronic populations for three phases show that the reason of Al₄Sr with the highest structural stability attributes to Al₄Sr phase having more the ionic bonds below Fermi level compared with those of Mg₂Sr and Mg₂₃Sr₆ phases, while the structural stability of Mg₂Sr is more than that of Mg₂₃Sr₆, which is the result of ionic and covalent bonds interaction.

3.4 Elastic properties

Elastic properties of Al₄Sr, Mg₂Sr and Mg₂₃Sr₆ phases, which are important for manufacturing Mg–Al-based alloys with strontium addition, are briefly discussed in this part. The calculated elastic constants for these intermetallics in the present work are listed in Table 4. As far as Mg₂₃Sr₆ phase, it is found that elastic constants satisfy the generalized elastic stability criteria for cubic crystals [7]: $(C_{11}+2C_{12})/3>0$, $C_{11}+2C_{12}>0$ and $C_{44}>0$. Hence, the computational elastic constants should be suitable. The bulk modulus B , shear modulus G and elastic modulus E are deduced according to the following formulae [28–29]:

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

$$E = \frac{(C_{11} - C_{12} + 3C_{44})(C_{11} + 2C_{12})}{2C_{11} + 3C_{12} + C_{44}} \quad (4)$$

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

Poisson ratio ν is obtained from [7]

$$\nu = \frac{3B - E}{6B} \quad (6)$$

Table 4 Calculated elastic constants of Al₄Sr, Mg₂Sr and Mg₂₃Sr₆

Phase	C_{11} /GPa	C_{12} /GPa	C_{13} /GPa
Al ₄ Sr	78.352	41.355	27.608
Mg ₂ Sr	48.40	22.667	12.459
Mg ₂₃ Sr ₆	49.449	14.678	–
Phase	C_{33} /GPa	C_{44} /GPa	C_{66} /GPa
Al ₄ Sr	114.579	28.612	35.805
Mg ₂ Sr	57.964	13.145	–
Mg ₂₃ Sr ₆	–	18.939	–

The obtained mechanical parameters of Al₄Sr, Mg₂Sr and Mg₂₃Sr₆ are listed in Table 5.

POUGH [30] introduced the ratio of the shear modulus to bulk modulus (G/B) of polycrystalline phases as prediction of the brittle and ductile behavior of materials. A high (low) G/B value is associated with

ductility (brittleness). The critical value which separates ductility from brittleness is about 0.5. From G/B calculated in Table 5, it is found that Al₄Sr and Mg₂Sr both are ductile, on the contrary, Mg₂₃Sr₆ is brittle. The G/B value of Mg₂Sr is the smallest, 0.417, indicating that Mg₂Sr has very good ductility among the three phases.

Table 5 Moduli of these phases derived by this work from elastic constants

Phase	B /GPa	G /GPa	E /GPa	G/B	Poisson ratio, ν
Al ₄ Sr	53.687	24.567	63.947	0.458	0.302
Mg ₂ Sr	31.258	13.041	34.347	0.417	0.317
Mg ₂₃ Sr ₆	26.269	18.317	44.588	0.697	0.217

Besides G/B , it is found that $C_{11}-C_{12}$ and elastic modulus E are also very significant for the mechanical properties of materials [31]. The smaller the values of $C_{11}-C_{12}$ and elastic modulus E are, the better the plasticity is. Figure 4 illustrates the value of $C_{11}-C_{12}$ and elastic modulus E for Al₄Sr, Mg₂Sr and Mg₂₃Sr₆. From Fig. 4 we can see that Mg₂Sr has lower values of elastic modulus E and $C_{11}-C_{12}$, implying better plasticity. On the contrary, Poisson ratio ν is used to quantify the stability of the crystal against shear, which usually ranges from -1 to 0.5 . The larger the Poisson ratio is, the better the plasticity is. Most of the calculated Poisson ratios are very close to 0.25 , which means that most of materials are with predominantly central interatomic forces [32]. Mg₂Sr has larger Poisson ratio, showing that Mg₂Sr is of good plasticity among the investigated compound. While for Mg₂₃Sr₆, the Poisson ratio is the smallest, corresponding to the poorest plasticity. All the results of the analysis on plasticity indicate that adding Sr to Mg–Al alloy can improve the ductility by forming Al₄Sr and Mg₂Sr phases.

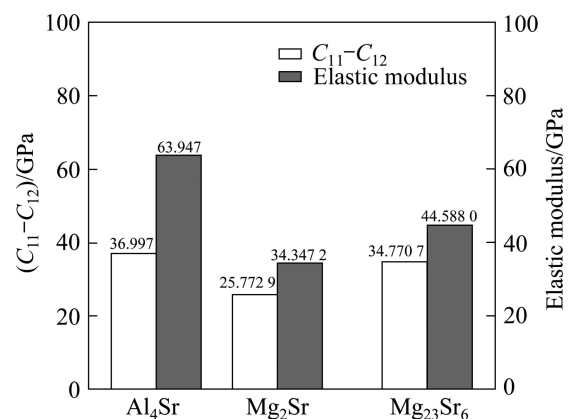


Fig. 4 Values of $C_{11}-C_{12}$ and elastic modulus E of Al₄Sr, Mg₂Sr and Mg₂₃Sr₆

4 Conclusions

1) The calculated heat of formation and cohesive energy show that Al_4Sr has the strongest alloying ability and the highest structural stability.

2) Calculations of the densities of states (DOS) and Mulliken electronic populations show that the reason of Al_4Sr with the highest structural stability attributes to Al_4Sr phase having more the ionic bonds below Fermi level compared with those of Mg_2Sr and $\text{Mg}_{23}\text{Sr}_6$ phases.

3) The calculated bulk modulus B , shear modulus G , elastic modulus E and Poisson ratio ν show that Al_4Sr and Mg_2Sr both are ductile, on the contrary, $\text{Mg}_{23}\text{Sr}_6$ is brittle, and among the three phases Mg_2Sr is a phase with the best plasticity.

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Al₄Sr, Mg₂Sr 和 Mg₂₃Sr₆ 相的电子结构与弹性性能的第一原理研究

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摘 要: 采用第一性原理计算 Al₄Sr, Mg₂Sr 和 Mg₂₃Sr₆ 相的电子结构与弹性性能。合金形成热与结合能的计算结果显示 Al₄Sr 具有最强的合金化形成能力和最高的结构稳定性。通过计算弹性常数、体模量、剪切模量、弹性模量和泊松比, 讨论了体系的韧性与塑性行为。结果表明, Al₄Sr 和 Mg₂Sr 为延性相, Mg₂₃Sr₆ 为脆性相, 在 3 种金属间化合物中, Mg₂Sr 的塑性最好。

关键词: 镁合金; 第一性原理计算; 电子结构; 弹性性能

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