First principles studies on the structural, elastic, electronic properties and heats of formation of Mg–AE (AE = Ca, Sr, Ba) intermetallics

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ABSTRACT

First principles calculations have been performed to study the structural, heats of formation, elastic properties, and densities of states of eight Mg–AE (AE = Ca, Sr, Ba) intermetallic compounds. The obtained results indicate that with increasing atom weight and concentration of AE, the bulk moduli decrease monotonously, and the larger the electronegativity difference is, the smaller the elastic modulus would be. Based on the ratios of shear moduli to bulk moduli, it has been found that Mg_2Ca, $Mg_{38}Sr_9$, Mg_2Sr, $Mg_{17}Ba_2$ and $Mg_{23}Ba_6$ behave in a brittle manner, and $Mg_{17}Sr_2$, $Mg_{23}Sr_6$ and Mg_2Ba behave in a ductile manner. Our calculations of the densities of states, heats of formation, and elastic constants of all the eight Mg compounds indicate that they are all conductors, thermodynamically and mechanically stable.

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1. Introduction

The study of Mg intermetallics has been attracting much attention because of their important applications in the automobile and aerospace industries [1–3]. Among the Mg based intermetallics, Mg–AE (AE = Ca, Sr, Ba) systems intermetallic compounds have generated significant interests over the past few decades [4–7]. The phase diagrams of Mg–Ca, Mg–Sr, and Mg–Ba systems have been investigated, and eight stable intermetallics, such as Mg_2Ca, $Mg_{17}Sr_2$, $Mg_{38}Sr_9$, $Mg_{23}Sr_6$, Mg_2Sr, $Mg_{17}Ba_2$, $Mg_{23}Ba_6$ and Mg_2Ba, have been found [8–10], and these intermetallics can be emerged as promising candidate materials for transportation, aeronautical and helicopters [11,12]. Due to their importance, various studies have been undertaken of crystal structures and lattice parameters [10,11,13–17], as well as thermodynamic properties [2–9] for the eight Mg intermetallic compounds. Moreover, investigations focused on the elastic properties for Mg_2Ca, $Mg_{23}Ba_6$ and Mg_2Ba, and electronic properties for Mg_2Ca have also been reported by Ganeshan et al. [1], Sumer et al. [18] and Jaswal et al. [19]. Although tremendous experimental and theoretical efforts have been devoted to these systems, additional work is still necessary. For instance, elastic properties for other five Mg intermetallics have not

been reported. The results on electronic properties of other seven Mg intermetallic compounds, considered in this work, have still been lacking. In the present paper, by means of first principles computational method based on density functional theory, we have systematically studied the structural, heats of formation, elastic properties, as well as electronic properties of all the eight Mg intermetallic compounds.

2. Computational method

In this work, eight Mg–AE intermetallic compounds have been investigated by using first principles calculations based on the density functional theory and plane-wave pseudopotential techniques as incorporated in the CASTEP package [20,21] and the Vienna ab initio simulation package (VASP) [22]. In CASTEP calculations, the ultrasoft pseudopotentials (UP) have been employed for the $2p^63s^2$, $3p^64s^2$, $4s^24p^65s^2$, and $5s^25p^66s^2$ atom configurations of Mg, Ca, Sr, and Ba, respectively [23]. Exchange–correlation interaction was described by using the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerh of parameterization [24]. The **k** point separation in the Brillouin zone of the reciprocal space is 0.04 nm^{-1}, that is, $5 \times 5 \times 2$, $3 \times 3 \times 2$, $3 \times 3 \times 2$, $3 \times 3 \times 3$, $4 \times 4 \times 2$, $3 \times 3 \times 3$, $3 \times 3 \times 3$, $4 \times 4 \times 2$ for Mg_2Ca, $Mg_{17}Sr_2$, $Mg_{38}Sr_9$, $Mg_{23}Sr_6$, Mg_2Sr, $Mg_{17}Ba_2$, $Mg_{23}Ba_6$, and

Mg$_2$Ba, respectively. An energy cut-off of 400 eV was used. The reliability of this method was demonstrated in our previous works [25—28]. For VASP calculations, the ion—electron interaction has been described by the projector-augmented wave (PAW) potentials [29]. A plane-wave basis energy cut-off of 500 eV was used, and the Brillouin zone of the cells has been sampled by $4 \times 4 \times 4$ **k**-point mesh for Mg$_2$Ca, Mg$_{17}$Sr$_2$, Mg$_{23}$Sr$_6$, Mg$_2$Sr, Mg$_{17}$Ba$_2$, Mg$_{23}$Ba$_6$, Mg$_2$Ba and $3 \times 3 \times 2$ **k**-point mesh for Mg$_{38}$Sr$_9$.

3. Results and discussion

3.1. Structural properties

The initial crystal structures of the eight Mg intermetallic compounds have been built based on the experimental crystallographic data [8—10,13—15]. Using both GGA-UP (CASTEP) method and GGA-PAW (VASP) method, their lattice parameters and internal coordinates were optimized. Calculated lattice parameters in comparison with the available experimental data and their corresponding crystal structures are given in Table 1. It can be seen that the calculated data are in a good agreement with the available experimental data. As well as the comparison of the calculated results from GGA-UP (CASTEP) method and GGA-PAW (VASP) method shows that the lattice constants are very close to each other. These results pointing that the computational scheme utilized in this work is reasonable. Fig. 1 depicts the calculated mass densities using GGA-UP (CASTEP) method and experimental values of the eight Mg intermetallic compounds. As can be seen from Fig. 1, all the data points lie close to the center dot line.

3.2. Thermodynamic stability and heats of formation

By using Formula (1) below, heats of formation of Mg—AE (AE = Ca, Sr, Ba) systems intermetallic compounds can be calculated by using the ground state total energies of the eight Mg compounds and pure Mg, Ca, Sr and Ba:
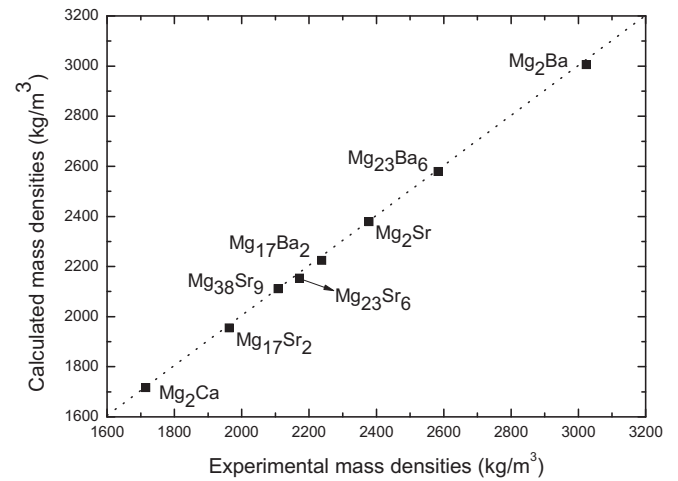

Fig. 1. Calculated and experimental mass densities of Mg—AE system intermetallic compounds.

$$E_{\text{form}}^{\text{Mg}_m\text{AE}_n} = \frac{E_{\text{tot}}^{\text{Mg}_m\text{AE}_n} - \left(mE_{\text{solid}}^{\text{Mg}} + nE_{\text{solid}}^{\text{AE}} \right)}{m + n}, \quad (1)$$

where $E_{\text{tot}}^{\text{Mg}_m\text{AE}_n}$ is the total energy of a Mg$_m$AE$_n$ primitive cell that includes m Mg atoms and n AE atoms with equilibrium lattice parameters, $E_{\text{solid}}^{\text{Mg}}$ and $E_{\text{solid}}^{\text{AE}}$ are the total energy of a Mg atom and an AE (AE = Ca, Sr, Ba) atoms in their stable structures.

Table 2 presents the calculated heats of formation of the eight Mg intermetallic compounds using both GGA-UP (CASTEP) method and GGA-PAW (VASP) method together with their available theoretical and experimental data [30—37]. These results have also been depicted in Fig. 2. It can be seen that the difference between the CASTEP calculated data and the VASP calculated data for Mg$_2$Ca, Mg$_{17}$Sr$_2$, Mg$_{38}$Sr$_9$, Mg$_{23}$Sr$_6$, Mg$_2$Sr, Mg$_{17}$Ba$_2$, Mg$_{23}$Ba$_6$, and Mg$_2$Ba is less than 0.5—8.7%, which presents a good agreement between calculated data by using CASTEP and VASP. It

Table 1
Calculated and experimental lattice parameters for Mg—AE system intermetallic compounds.

Phase	At.% AE	Pearson symbol	Space group	Prototype	Lattice parameters (Å)		Mass density (kg/m^3)	Reference
					a	c		
Mg$_2$Ca	33.3	hP12	P6$_3$/mmc	MgZn$_2$	6.261	10.105	1716.94	GGA-UP(CASTEP)
					6.239	10.009		GGA-PAW (VASP)
					6.253	10.144	1715.21	[10]
Mg$_{17}$Sr$_2$	10.5	hP38	P6$_3$/mmc	Ni$_{17}$Th$_2$	10.597	10.284	1954.96	GGA-UP(CASTEP)
					10.514	10.274		GGA-PAW (VASP)
					10.535	10.356	1963.26	[13]
Mg$_{38}$Sr$_9$	19.1	hP94	P6$_3$/mmc	Mg$_{38}$Sr$_9$	10.542	27.978	2111.46	GGA-UP(CASTEP)
					10.446	27.919		GGA-PAW (VASP)
					10.500	28.251	2107.96	[14]
Mg$_{23}$Sr$_6$	20.7	cF116	Fm$\bar{3}$m	Mn$_{23}$Th$_6$	14.956		2153.66	GGA-UP(CASTEP)
					14.890			GGA-PAW (VASP)
					14.914		2171.89	[15]
Mg$_2$Sr	33.3	hP12	P6$_3$/mmc	MgZn$_2$	6.474	10.479	2378.83	GGA-UP(CASTEP)
					6.460	10.390		GGA-PAW (VASP)
					6.475	10.451	2378.03	[16]
Mg$_{17}$Ba$_2$	10.5	hR57	R$\bar{3}$m	Zn$_{17}$Th$_2$	10.683	15.583	2224.69	GGA-UP(CASTEP)
					10.497	15.517		GGA-PAW (VASP)
					10.650	15.587	2238.05	[13]
Mg$_{23}$Ba$_6$	20.7	cF116	Fm$\bar{3}$m	Mn$_{23}$Th$_6$	15.271		2579.63	GGA-UP(CASTEP)
					15.213			GGA-PAW (VASP)
					15.263		2583.51	[13]
Mg$_2$Ba	33.3	hP12	P6$_3$/mmc	MgZn$_2$	6.678	10.638	3005.90	GGA-UP(CASTEP)
					6.660	10.564		GGA-PAW (VASP)
					6.670	10.602	3023.47	[17]

Table 2
Calculated and experimental heats of formation for Mg–AE system intermetallic compounds.

| Phase	Heats of formation (kJ/mol atoms)			
	GGA-UP (CASTEP)	GGA-PAW (VASP)	Experiment	Other theories
Mg₂Ca	−13.03	−12.85	−12.23 [31,32], −13.38 [33], −13.04 [34], −11.29 [35], −14.59 [36], −20.97 [37]	−12.14 [2], −11.72 [4,5], −13.47 [6], −13.80 [30]
Mg₁₇Sr₂	−5.72	−5.60		−4.80 [4]
Mg₃₈Sr₉	−6.86	−6.74		−6.27 [4]
Mg₂₃Sr₆	−7.84	−8.52		−7.74 [4]
Mg₂Sr	−11.02	−11.34	−7.12 [33]	−10.62 [4], −7.95 [6]
Mg₁₇Ba₂	−6.80	−6.76		−6.60 [2]
Mg₂₃Ba₆	−8.36	−8.02		−7.50 [2]
Mg₂Ba	−9.50	−9.00		−8.50 [2]

further confirms that the computational scheme utilized in this work is credible. Thus, we just compare the CASTEP calculated data with the experimental data. For the Mg₂Ca compound, the calculated heat of formation is −13.03 kJ/mol atoms, which is in a better agreement with most of the reported results but different from Pyagai et al. [37] value of −20.97 kJ/mol atoms. It was demonstrated that the result obtained by Pyagai et al. may not be reliable. For Mg–Sr system compounds, the calculated heats of formation of Mg₁₇Sr₂, Mg₃₈Sr₉, Mg₂₃Sr₆ and Mg₂Sr are −5.72, 6.86, 7.84 and −11.02 kJ/mol atoms, which is in accordance with the heats of formation calculated by Zhong et al. [4]. For Mg–Ba system compounds, the calculated heats of formation of Mg₁₇Ba₂, Mg₂₃Ba₆ and Mg₂Ba are −6.80, −8.36 and −9.50 kJ/mol atoms. The results are consistent with the calculated heats of formation for Mg–Ba system compounds made by Zhang et al. [2]. For the eight Mg intermetallic compounds considered in this work, the calculated heats of formation are all negative, indicating that they are all thermodynamically stable. Moreover, it can be observed from Tables 2 and 4 that, the Mg₂Ca compound has the most negative heat of formation and the largest bulk modulus. This complies with the fact that the more negative heat of formation is, the larger value of bulk modulus would be, as pointed out by Zhang et al. [2].

3.3. Elastic properties and mechanical stability

Table 3 shows the GGA-UP (CASTEP) method calculated elastic constants C_{ij} (GPa) and bulk moduli of the eight Mg intermetallic compounds, together with their available experimental and theoretical data. It can be seen that, for Mg₂Ca, Mg₂₃Ba₆, and Mg₂Ca, the calculated elastic constants are in a better agreement with the previous experimental and theoretical data [1,18]. No elastic constants have been reported for other five Mg intermetallics. Based on the calculated elastic constants, mechanical stability of the eight intermetallics has been analyzed. For the eight Mg intermetallic compounds, it was found that Mg₂₃Sr₆ and Mg₂₃Ba₆ have cubic structures, Mg₂Ca, Mg₁₇Sr₂, Mg₃₈Sr₉, Mg₂Sr, and Mg₂Ba have hexagonal structures, and Mg₁₇Ba₂ has a trigonal structure.

For Mg₂₃Sr₆ and Mg₂₃Ba₆ compounds, all elastics constants are larger than zero, namely, $C_{11} > 0$, $C_{44} > 0$, $C_{11}-C_{12} > 0$, $C_{11} + 2C_{12} > 0$, which is consistent with the stability condition for cubic structure [38], indicating that the two intermetallic compounds are elastically stable. For Mg₂Ca, Mg₁₇Sr₂, Mg₃₈Sr₉, Mg₂Sr, and Mg₂Ba compounds, the mechanical stability restrictions

for hexagonal structures are as follows [39,40]: $C_{11} > 0$, $C_{44} > 0$, $C_{11}-C_{12} > 0$, $(C_{11} + C_{12}) C_{33}-2C_{13}^2 > 0$. As shown in Table 3, the elastic constants of all the five hexagonal structures can comply with the stability criteria, and these results imply that all the five intermetallics are mechanically stable. As for Mg₁₇Ba₂, the
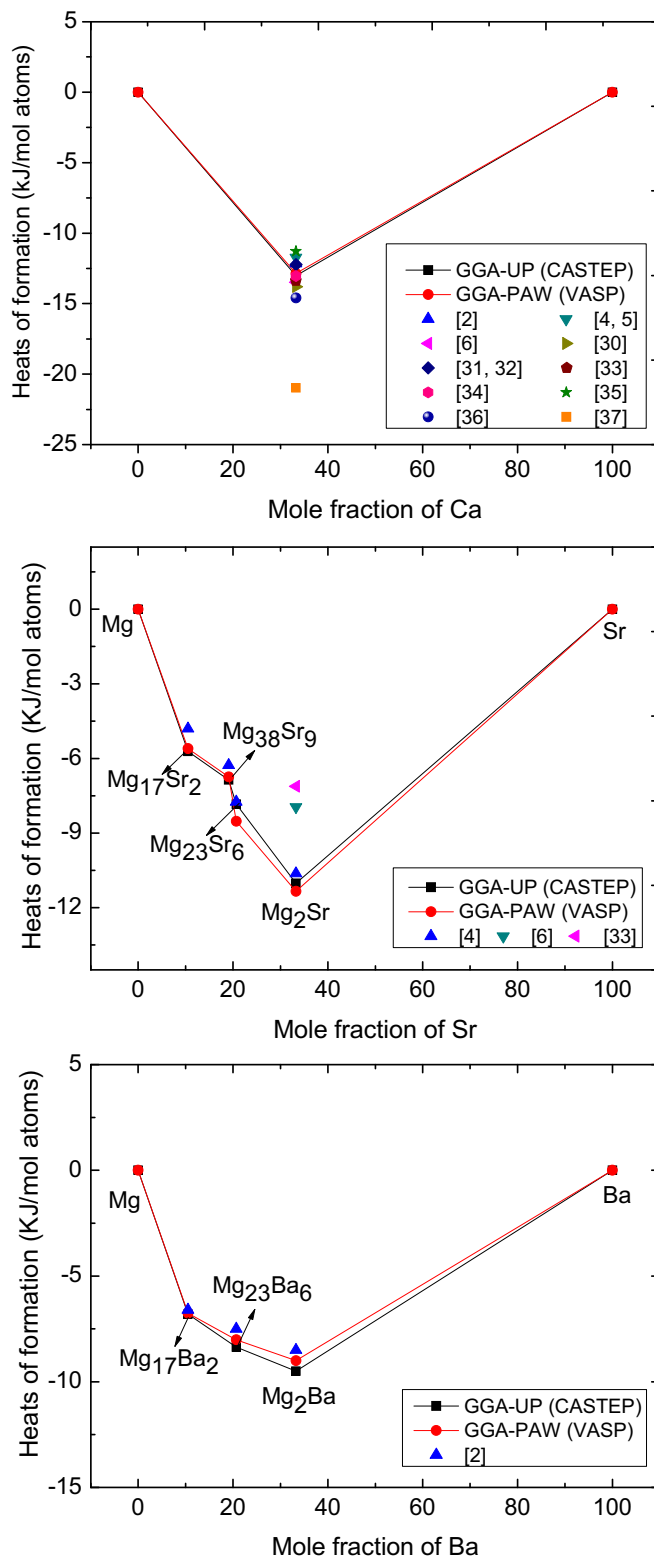
Fig. 2. Calculated heats of formation compared to experimental and theoretical values for Mg–AE system intermetallic compounds.

Table 3
Calculated elastic properties compared to experimental and theoretical values for the single crystalline Mg–AE system intermetallic compounds.

Phase	C_{11}	C_{12}	C_{13}	C_{14}	C_{22}	C_{23}	C_{33}	C_{44}	C_{55}	C_{66}	K
Mg$_2$Ca	53.7	22.9	10.1				66.8	14.6			28.9
Mg$_2$Ca [1]	59.5	17.8	12.6				66.0	17.4			30.1
Mg$_2$Ca [18]	61.2	17.6	15.0				65.5	19.2			31.4
Mg$_{17}$Sr$_2$	58.1	14.6	16.4				59.9	9.4			30.1
Mg$_{38}$Sr$_9$	51.0	12.4	12.6				57.9	19.3			26.1
Mg$_{23}$Sr$_6$	34.0	24.0						15.9			27.3
Mg$_2$Sr	43.8	19.8	10.6				57.2	12.4			25.2
Mg$_{17}$Ba$_2$	72.1	10.2	11.6	−1.7	63.6	16.7	61.3	22.7	22.3	20.9	30.4
Mg$_{23}$Ba$_6$	40.0	15.2						16.1			23.5
Mg$_{23}$Ba$_6$ [1]	41.5	15.9						17.2			24.4
Mg$_2$Ba	33.1	20.7	9.5				41.0	11.0			20.7
Mg$_2$Ba [1]	39.8	14.5	9.8				46.2	11.0			21.5

C_{ij}, elastic stiffness (in GPa); K, bulk moduli (in GPa).

Table 4
Polycrystalline bulk moduli, shear moduli, Young's moduli, Poisson's ratios for Mg–AE system intermetallic compounds deduced by Voigt, Reuss, and Hill (VRH) approximations.

Phase	K_V	K_R	K_H	G_V	G_R	G_H	E	G/K	ν
Mg$_2$Ca	28.9	28.9	28.9	17.7	16.6	17.1	44.1	0.61	0.2457
Mg$_2$Ca [1]	30.1			20.6			50.3	0.68	
Mg$_2$Ca [18]	31.4			21.3			52.3	0.68	
Mg$_{17}$Sr$_2$	30.1	30.1	30.1	16.7	14.2	15.4	42.3	0.55	0.2659
Mg$_{38}$Sr$_9$	26.1	26.0	26.1	19.7	19.7	19.7	47.2	0.75	0.1985
Mg$_{23}$Sr$_6$	27.3	27.3	27.3	11.5	8.5	10.0	30.3	0.42	0.3153
Mg$_2$Sr	25.2	25.2	25.2	14.3	13.4	13.8	36.1	0.57	0.2614
Mg$_{17}$Ba$_2$	30.4	30.4	30.4	23.8	23.2	23.5	56.6	0.78	0.1896
Mg$_{23}$Ba$_6$	23.5	23.5	23.5	14.6	14.4	14.5	36.3	0.62	0.2427
Mg$_{23}$Ba$_6$ [1]	24.4			15.4			38.2	0.63	
Mg$_2$Ba	20.7	20.7	20.7	10.1	8.8	9.5	26.1	0.49	0.2901
Mg$_2$Ba [1]	21.5			13.0			32.5	0.60	

K, bulk moduli (in GPa); G, shear moduli (in GPa); E, Young's moduli (in GPa); ν, Poisson's ratio.

mechanical stability criteria for trigonal structure can be expressed as [41]: $C_{11}-|C_{12}| > 0$, $(C_{11} + C_{12})C_{33}-2C_{13}^2 > 0$, $(C_{11}-C_{12})C_{44}-2C_{14}^2 > 0$. As can be seen from Table 3, the elastic constants of Mg$_{17}$Ba$_2$ satisfy all the above constraints, which indicate that Mg$_{17}$Ba$_2$ is mechanically stable.

Table 4 presents calculated polycrystalline bulk moduli (K), shear moduli (G), Young's moduli (E), and Poisson's ratio (ν) by using the Voigt, Reuss, and Hill (VRH) approximations [42]. The relationship between the bulk moduli and concentration of AE has also been depicted in Fig. 3. As we can see from Fig. 3, with

increasing concentration of AE (in atoms%), the bulk moduli decreases monotonously for the Mg–AE system intermetallic compounds. This can be explained by the calculated bulk moduli of 35.0, 17.3, 12.1, and 8.7 GPa for pure Mg, Ca, Sr, and Ba. With increasing atom weight of AE, the bulk moduli decrease gradually for Mg–Ca, Mg–Sr and Mg–Ba intermetallic compounds. It was considered that the increase of atom radius of AE with increasing atom weight of AE is the main reason for the decrease of the bulk moduli. Moreover, this trend is in accordance with the calculated results for Mg–Ca and Mg–Ba intermetallic compounds performed
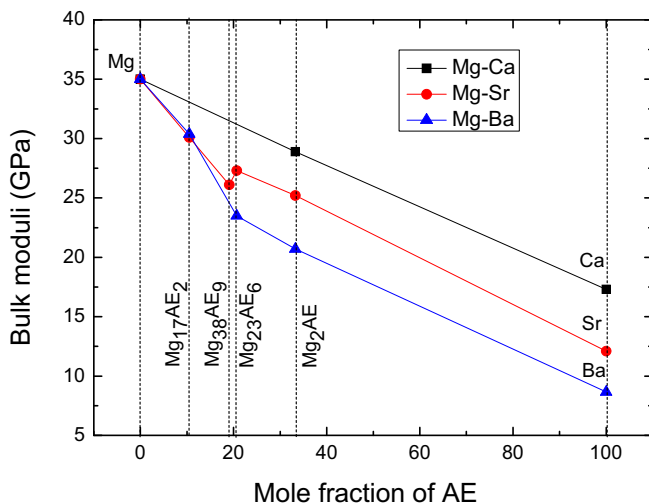
Fig. 3. Calculated bulk moduli of Mg–AE system intermetallic compounds.
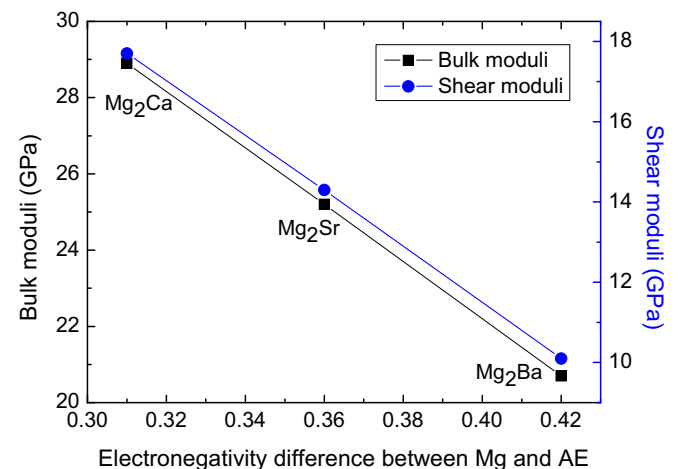
Fig. 4. The relationship between bulk moduli and shear moduli with electronegativity difference of AE versus Mg.
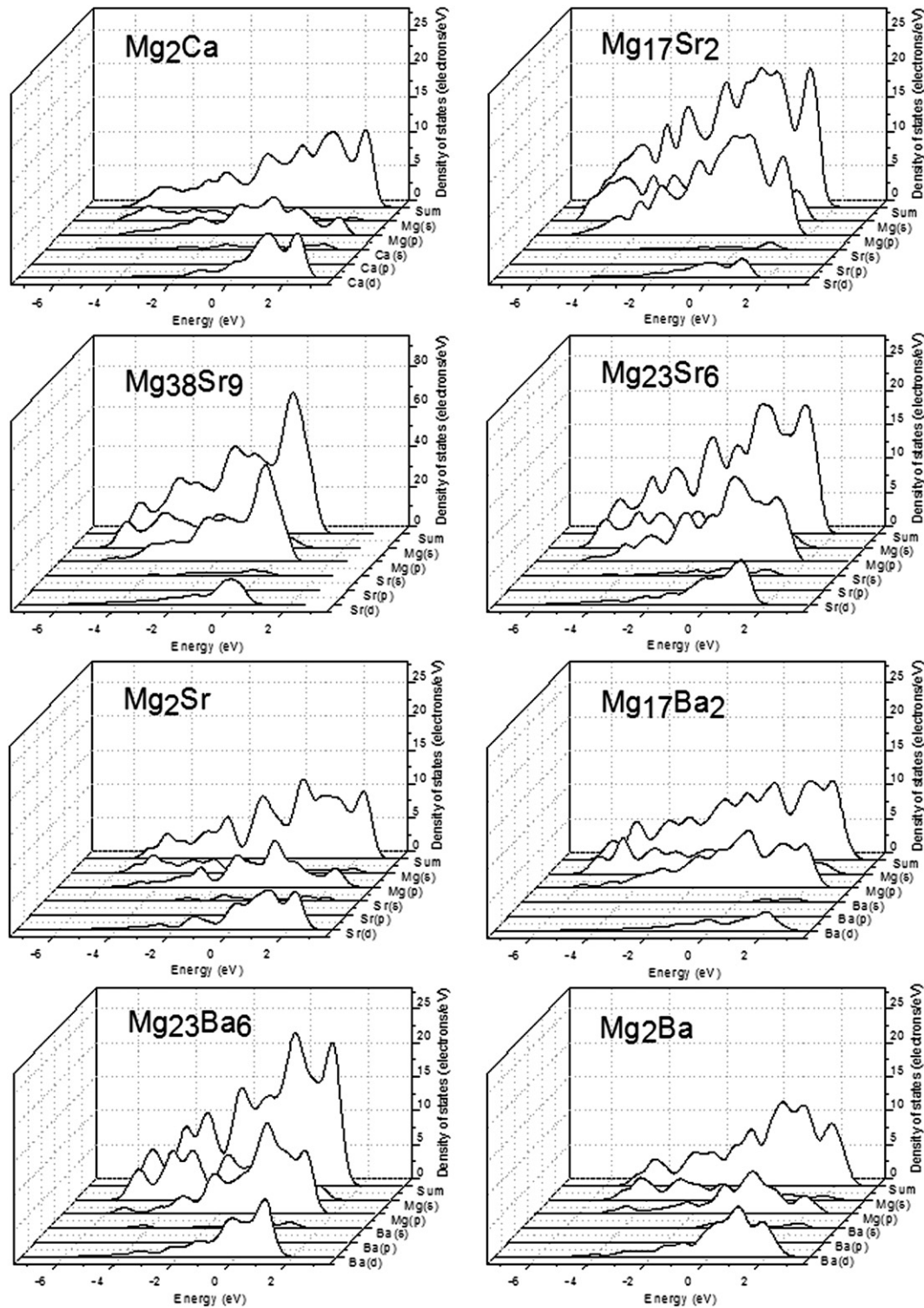
Fig. 5. PDOS plots calculated for Mg–AE system intermetallic compounds.

by Ganeshan et al. [1]. Frantsevich et al. indicated that the hardness and strength of materials are related to their elastic moduli, and the general trend is the larger the moduli, the harder the materials [43]. It was found that the hardness of Mg–Ca system intermetallic compounds is larger than that of Mg–Sr and Mg–Ba systems intermetallics due to their larger elastic moduli. Fig. 4 presents the relationship between bulk moduli and shear moduli with

electronegativity difference of AE versus Mg. Using the Pauling scale [44], the electronegativity of Mg, Ca, Sr, and Ba are 1.31, 1.00, 0.95, and 0.89, respectively. As we can see from Fig. 4, the bulk moduli and shear moduli of Mg_2Ca, Mg_2Sr, and Mg_2Ba decrease with increasing the electronegativity difference between AE and Mg. Thus, it can be concluded that the larger the electronegativity difference is, the smaller the elastic modulus would be.

Based on the values of elastic moduli, the ratio of shear moduli to bulk moduli (G/K) has been utilized to analyze their brittleness and ductility properties; calculated G/K values are presented in Table 4. Pugh [45] has proposed that if G/K ratio is larger than 0.57, metals behave in a brittle manner, otherwise the material are considered as ductile, and this criterion has been demonstrated successfully in intermetallic compounds [1,46–48]. The lower the value of G/K, the more ductile the material would be. As it can be seen from Table 4, the G/K value of Mg_2Ca is 0.61, indicating that Mg_2Ca is brittle. This result is in a good agreement with the reported results obtained by Sumer et al. [18] and Ganeshan et al. [1]. For the Mg–Sr system intermetallic compounds, the G/K ratios of $Mg_{38}Sr_9$ and Mg_2Sr are larger than 0.57, and the G/K values of $Mg_{17}Sr_2$ and $Mg_{23}Sr_6$ are smaller than 0.57. These results indicate that $Mg_{38}Sr_9$ and Mg_2Sr behave in a brittle manner, and $Mg_{17}Sr_2$ and $Mg_{23}Sr_6$ behave in a ductile manner. For the Mg–Ba system intermetallic compounds, the values of G/K ratio for $Mg_{17}Ba_2$ and $Mg_{23}Ba_6$ are larger than 0.57, implying that $Mg_{17}Ba_2$ and $Mg_{23}Ba_6$ are brittle. For the Mg_2Ba, the G/K ratio is 0.49, indicating that Mg_2Ba is ductile. It is noted that the brittle behavior of $Mg_{23}Ba_6$ is in accordance with the reported results by Ganeshan et al., while the ductile behavior of Mg_2Ba is different from the earlier reported results [1]. As for all the considered eight Mg intermetallic compounds, the $Mg_{17}Ba_2$ is the most brittle, and the $Mg_{23}Sr_6$ is the most ductile.

3.4. Electronic structures

The partial density of states (PDOS) of the eight Mg intermetallic compounds, which are obtained using GGA-UP (CASTEP) method, are shown in Fig. 5. Zero energy in the plotted figures corresponds to the Fermi energy. It can be seen that the densities of states of Mg_2Ca are dominated by Mg s, p-states and Ca d-states, which is in accordance with the calculated results performed by Jaswal et al. [19]. For Mg–Sr system compounds, at Fermi energy, the $Mg_{38}Sr_9$ has the largest value of densities of states, and the value of densities of states for Mg_2Sr is the smallest. Mg s, p-states and Sr d-states contribute to the densities of states. For the Mg–Ba system compounds, $Mg_{23}Ba_6$ has the largest value of densities of states, and the value of densities of states for Mg_2Ba is smaller than the corresponding values for $Mg_{17}Ba_2$. The densities of states are mainly dominated by Mg s, p-states and Ba d-states. Therefore, we can find that the densities of states of Mg–AE (AE = Ca, Sr, Ba) systems intermetallic compounds are all mainly having the Mg s, p-states and AE d-states as major contributors. In addition, the values of the densities of states at Fermi energy for Mg_2Ca, $Mg_{17}Sr_2$, $Mg_{38}Sr_9$, $Mg_{23}Sr_6$, Mg_2Sr, $Mg_{17}Ba_2$, $Mg_{23}Ba_6$ and Mg_2Ba are 8.9, 19.7, 58.64, 15.8, 10.7, 11.7, 18.7, and 11.4, respectively. These results indicate that the eight Mg intermetallic compounds are all conductors.

4. Conclusions

By using first principles calculations based on density functional theory, we have studied the structural, heats of formation, elastic properties, and densities of states of eight Mg–AE (AE = Ca, Sr, Ba) systems intermetallic compounds. Calculated results indicate that the bulk moduli decrease monotonously with increasing atom weight and concentration of AE, and the bulk moduli and shear moduli of Mg_2Ca, Mg_2Sr, and Mg_2Ba decrease with increasing the electronegativity difference between AE and Mg. Ductility and brittleness have been analyzed based on the Pugh's criteria. It was found that Mg_2Ca, $Mg_{38}Sr_9$, Mg_2Sr, $Mg_{17}Ba_2$ and $Mg_{23}Ba_6$ are brittle, and $Mg_{17}Sr_2$, $Mg_{23}Sr_6$ and Mg_2Ba are ductile. By investigating the calculated densities of states, heats of formation, and elastic constants of all the eight Mg compounds, it was observed that they are all conductors, thermodynamically and mechanically stable.

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