

ARTICLE

First Principles Study of Al-Li Intermetallic Compounds

Hai-li Yu, Xiao-hui Duan*, Yong-jun Ma, Min Zeng

State Key Laboratory Cultivation Base for Nonmetal Composites and Functional Materials, Southwest University of Science and Technology, Mianyang 621010, China

(Dated: Received on August 22, 2012; Accepted on October 8, 2012)

The structural properties, heats of formation, elastic properties, and electronic structures of four compositions of binary Al-Li intermetallics, Al_3Li , AlLi , Al_2Li_3 , and Al_4Li_9 , are analyzed in detail by using density functional theory. The calculated formation heats indicate a strong chemical interaction between Al and Li for all the Al-Li intermetallics. In particular, in the Li-rich Al-Li compounds, the thermodynamic stability of intermetallics linearly decreases with increasing concentration of Li. According to the computational single crystal elastic constants, all the four Al-Li intermetallic compounds considered here are mechanically stable. The polycrystalline elastic modulus and Poisson's ratio have been deduced by using Voigt, Reuss, and Hill approximations, and the calculated ratios of bulk modulus to shear modulus indicate that the four compositions of binary Al-Li intermetallics are brittle materials. With the increase of Li concentration, the bulk modulus of Al-Li intermetallics decreases in a linear manner.

Key words: First principles, Al-Li intermetallic compound, Mechanical property, Formation heat, Elastic properties

I. INTRODUCTION

Intermetallic compounds have long been considered as potential candidate materials for advanced structural applications because of their high melting temperature, high modulus, low density, and excellent resistance to oxidation and corrosion as well as their unique anomalous strengthening behavior [1–6]. Among these intermetallic compounds, Al-X (X=Ni, Cu, Ru, *etc.*) system compounds have been studied systematically [2, 7–9]. As for the Al-Li intermetallic compounds, the studies have mainly focused on their electronic properties [10] or properties of Al_3Li intermetallic compound [11–13]. However, systematical studies on the properties of Al-Li intermetallic compounds are still lacking.

During the past decades, the binary alloy systems of Al-Li have received a great deal of attention from both the materials-science and physics communities due to their unique structure and potential application in aerospace industry [14]. They have been studied experimentally and theoretically. The first Al-Li phase diagram was published in 1958 [15]. Afterwards, such phase diagram was revised [16–21]. Based on these Al-Li phase diagrams, it is known now that four intermetallic compounds can exist in the Al-Li system compounds, namely Al_3Li , AlLi , Al_2Li_3 , and Al_4Li_9 . From

the results in Refs.[28–31], the Al_3Li compound is a cubic crystal, the Pearson symbol is cP4. The crystal cell has 3 Al atoms and 1 Li atom. The AlLi compound is tetragonal crystal, the Pearson symbol is tI8. The crystal cell has 4 Al atoms and 4 Li atoms. For Al_2Li_3 compound, it is a trigonal crystal and the Pearson symbol is hR5. The crystal cell has 6 Al atoms and 9 Li atoms. For Al_4Li_9 compound, it is a monoclinic crystal and the primitive cell has 4 Al atoms and 9 Li atoms.

Now the interest in low-weight and high-capacity anode materials for secondary batteries has initiated a detailed investigation of the binary Al-Li system again. To the best of our knowledge, the addition of small amounts of lithium will greatly increase the strength of the aluminum alloys with little change in the ductility. In order to systematically study the effects of the Li concentration on some properties of the Al-Li intermetallic compounds. The structural properties, heats of formation, elastic properties, and electronic structures of four compositions of Al-Li intermetallic compounds will be investigated using first principles methods.

II. COMPUTATIONAL METHOD

In the present work, four Al-Li binary systems intermetallics (Al_3Li , AlLi , Al_2Li_3 , and Al_4Li_9) are investigated computationally using density functional theory (DFT) and plane-wave pseudopotential technique implemented in the Cambridge Serial Total Energy Package (CASTEP) [22]. In this code, the Kohn-Sham equations are solved within the framework of DFT [23, 24]

*Author to whom correspondence should be addressed. E-mail: duanxiaohui@swust.edu.cn, Tel.: +86-186-2485116, FAX: +86-186-2419201.

TABLE I Experimental and optimized crystallographic data and mass density of Li-Al intermetallics of different phases*.

Phase	Space group	Lattice parameters						Mass density (kg/m ³)
		<i>a</i> /nm	<i>b</i> /nm	<i>c</i> /nm	α /(°)	β /(°)	γ /(°)	
Al	Fm-3m	4.049	4.049	4.049	90	90	90	2.699 [32]
		4.045	4.045	4.045	90	90	90	2.708
Al ₃ Li	Pm-3m	4.010	4.010	4.010	90	90	90	2.260 [28]
		4.030	4.030	4.030	90	90	90	2.221
AlLi	I41/amd	4.478	4.478	6.234	90	90	90	1.770 [29]
		4.494	4.494	6.404	90	90	90	1.740
Al ₂ Li ₃	R-3m	4.508	4.508	14.26	90	90	120	1.480 [30]
		4.459	4.459	14.17	90	90	120	1.527
Al ₄ Li ₉	B2/m	19.16	5.429	4.499	90	90	107.7	1.269 [31]
		18.97	5.379	4.480	90	90	107.7	1.300
Li	Im-3m	3.510	3.510	3.510	90	90	90	0.533 [33]
		3.452	3.452	3.452	90	90	90	0.560

by expanding the wave function of valence electrons in a basis set of plane waves with kinetic energy smaller than the specified cut-off energy. The presence of tightly-bound core electrons is represented by non-local ultrasoft pseudo-potentials of the Vanderbilt-type [25]. The states $Al3s^23p^1$ and $Li1s^22s^1$ are treated as valence states. The ion-electron interaction is modeled by ultrasoft pseudopotentials [26]. Generalized gradient approximation (GGA) with the PBE exchange-correlation functional is used [27]. The kinetic cutoff energy for plane waves is set as 400 eV. The *k* point separation in Brillouin zone of the reciprocal space is 0.05 nm^{-1} , that is, $8 \times 8 \times 8$ *k* points grid for Al₃Li, AlLi, Al₂Li₃, and Al₄Li₉. For the calculation of the elastic properties, which usually requires a dense mesh of uniformly distributed *k* points, the Brillouin zone integration is performed using a $24 \times 24 \times 24$ *k* points grid for Al₃Li, $16 \times 16 \times 16$ *k* points grid for AlLi. And for Al₂Li₃, the *k* points grid are $12 \times 12 \times 12$.

Their structural parameters are determined using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimization technique, with the following thresholds for converged structures: energy change per atom is less than 10^{-5} eV, residual force is less than 0.03 eV/\AA , and the displacement of atoms during the geometry optimization is less than 0.001 \AA . In our calculations, the crystal cell is used for Al₃Li, AlLi, and Al₂Li₃, whereas the primitive cell is adopted for Al₄Li₉.

III. RESULTS AND DISCUSSION

A. Lattice structure

Using the experimental crystallographic data of the Al-Li intermetallics phases from Refs.[28–33] as the initial configurations, the lattice parameters and internal coordinates of the Al-Li intermetallics compounds are optimized via first-principles calculations.

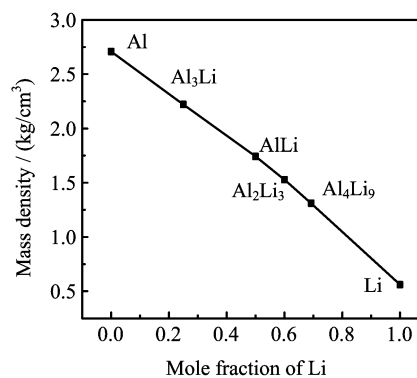


FIG. 1 Theoretical mass density as a function of Li concentration for the Al-Li intermetallic compounds.

The optimized lattice parameters and mass densities are shown in Table I in comparison with available experimental results and their corresponding crystal structures. Obviously, all the calculated lattice parameters are very close to the previous experimental results, which demonstrate that the computational methodology utilized in the present work is suitable and reliable.

The mass densities for Al-Li intermetallics of different phases from the present theoretical calculations are shown in Fig.1. It can be seen that when increasing Li concentration *C*, the mass density ρ of Al-Li intermetallics decreases approximately by a linear relationship:

$$\rho = 2.75616 - 2.12611C \quad (1)$$

B. Heats of formation

According to the optimizing 3D crystal structure of the Al-Li intermetallic compounds and the pure Li and Al, some results, including equilibrium crystal structures and ground state total energies of different Al-Li

TABLE II The calculated heats of formation for Al-Li intermetallic compounds.

	Heats of formation/(kJ/mol atom)			
	Al ₃ Li	AlLi	Al ₂ Li ₃	Al ₄ Li ₉
This work	-7.826	-18.06	-16.69	-13.20
Ref.[17]			-15.49	-16.90
Ref.[20]			-15.90	-12.60
Ref.[36]	-8.30	-16.739		
Ref.[37]	-10.89	-18.927		

intermetallic compounds, can be obtained. Taking advantage of the obtained data above, the heats of formation for Al-Li intermetallic compounds are computed by virtue of the following expression [34, 35]:

$$E_{\text{form}}^{\text{Al}_m\text{Li}_n} = \frac{1}{m+n} (E_{\text{total}}^{\text{Al}_m\text{Li}_n} - mE_{\text{solid}}^{\text{Al}} - nE_{\text{solid}}^{\text{Li}}) \quad (2)$$

where $E_{\text{form}}^{\text{Al}_m\text{Li}_n}$ is the atomic heat of formation for an Al_mLi_n alloy, $E_{\text{total}}^{\text{Al}_m\text{Li}_n}$ refers to the total energy of crystal or primitive cell used in the present calculation, m and n refer to the numbers of Al and Li atoms, respectively. $E_{\text{solid}}^{\text{Al}}$ and $E_{\text{solid}}^{\text{Li}}$ are the energies of per fcc-Al and bcc-Li atoms in the solid states, respectively.

Using Eq.(2), the heats of formation for the four compounds have been calculated via the total energies from our DFT calculations. The calculated heats of formation of the Al-Li intermetallic compounds are displayed in Table II, as well as the available experimental and theoretical results [17, 20, 36, 37]. From Table II, we can see that the heats of formation for Al_2Li_3 , AlLi, and Al_4Li_9 are in good agreement with the data from the LMTO-ASA method by Sluiter and Watanabe [20]. For Al_2Li_3 , the heat of formation is -16.69 kJ/mol atoms and it is also in good agreement with phase diagram assessment of experimental datum [17]. Such agreement further indicates that the computational methodology used in this work is reliable.

In Fig.2, we plotted the heats of formation for the Al-Li intermetallic compounds. We can see that AlLi has the smallest value of formation heat, so it is the most stable compound in the Al-Li intermetallic compounds. What is more, all the four intermetallic compounds have negative formation heat, confirming that a strong chemical interaction exists between Al and Li, and all the compounds are thermodynamically stable. Especially, with increasing the concentration of Li, the stability decreases approximately along a line in the Li-rich Al-Li compounds.

C. Electronic structures

We have calculated the total and partial density of states (DOS) of the Al-Li intermetallic compounds. The results are displayed in Fig.3 for the energy range from

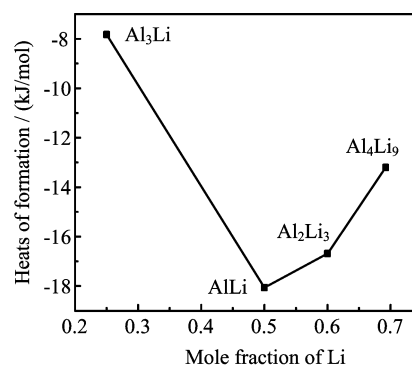


FIG. 2 Heats of formation of Al-Li system intermetallic compounds.

-10 eV to 10 eV. In Fig.3(a), it is found that the main bonding states for the Al_3Li between -10 and 0 eV are predominantly derived from Al s and p states, while the main bonding states from 0 eV to 10 eV originate from Al s, Al p, and Li s states. For AlLi in Fig.3(b), the main bonding states between -9 and -4 eV are predominantly derived from Al s and Al p states, while the main bonding states from -4 eV to 8 eV originate from Al s, Al p, and Li s states. For the Al_2Li_3 and Al_4Li_9 , their total and partial density of states have some similarities. The main bonding states between -8 and -4 eV are predominantly derived from Al s and Al p states, while the main bonding states from -4 eV to 6 eV originate from Al s, Al p and Li s states.

From Fig.3, it can be seen that the Al p and Li s peaks show evidence for the strong hybridization from 0 eV to 6 eV, while the Li's contribution is small below the Fermi level. Generally, the smaller $N(E_F)$ ($N(E_F)$ is the DOS value corresponding to the Fermi level) is, the more stable the compound is. Al_4Li_9 has the largest $N(E_F)$ (4.00 states/(eV atom)), while AlLi has the smallest $N(E_F)$ (1.55 states/(eV atom)). The $N(E_F)$ values of Al_2Li_3 and Al_3Li are equal to 3.10 and 1.92 states/(eV atom), respectively. Thus the most stable phase is AlLi, followed by Al_3Li , Al_2Li_3 , and Al_4Li_9 .

D. Elastic properties and mechanical stability

We have also investigated the elastic properties of Al-Li intermetallic compounds of different phases using DFT calculations. The results are summarized in Table III, along with the previous experimental and theoretical values [10, 38, 39].

The mechanical stability of Al-Li intermetallic compounds are studied by the calculated elastic constants of Al-Li intermetallic compounds. For a cubic crystal, the elastic constants for the mechanical stability need to satisfy the following restrictions [40]:

$$C_{11} > 0, C_{44} > 0, C_{11} > |C_{12}|, (C_{11} + 2C_{12}) > 0 \quad (3)$$

As can be seen from Table III, all the elastic constants

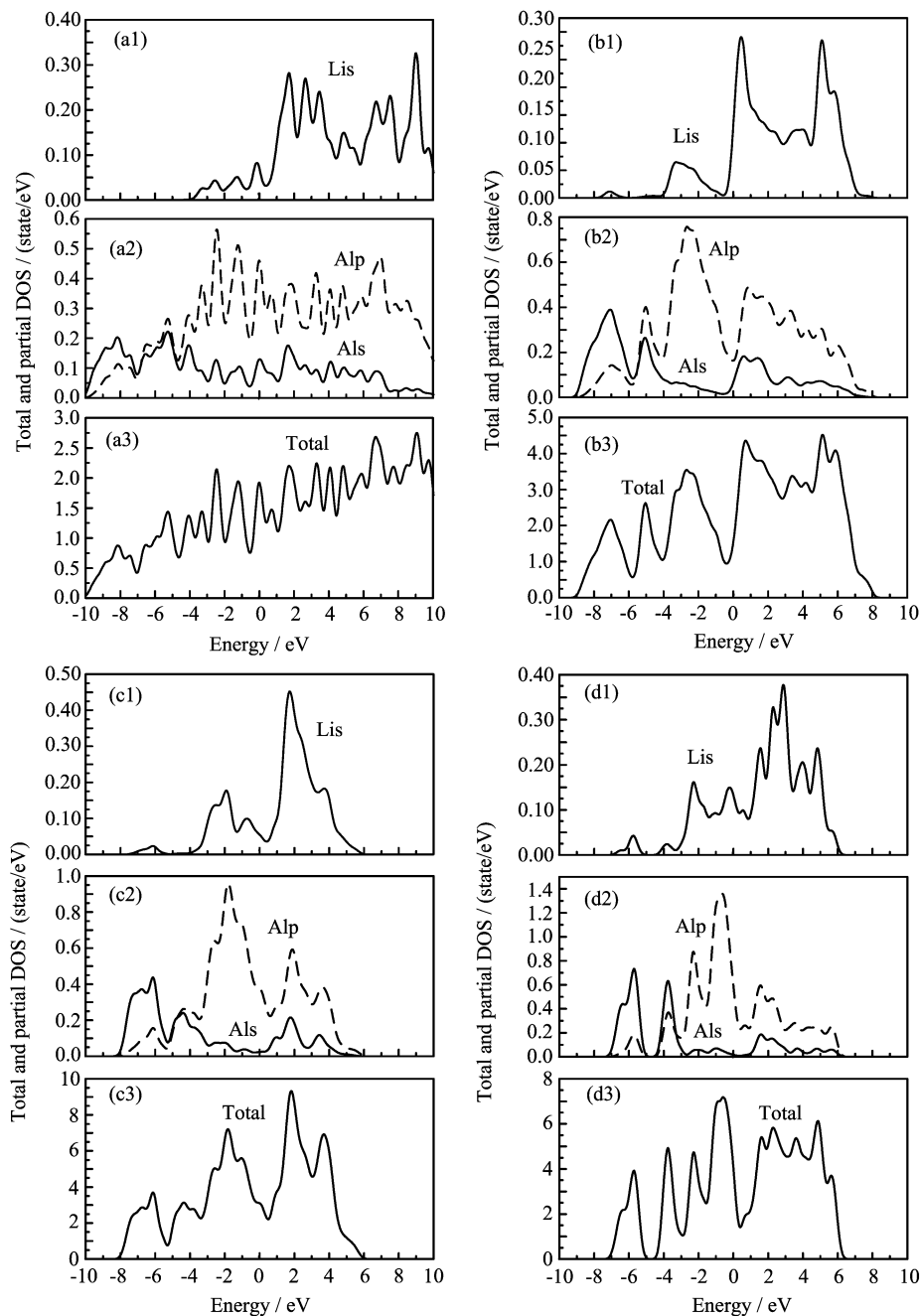


FIG. 3 The calculated total and partial density of states of Al-Li compound. (a) Al_3Li , (b) AlLi , (c) Al_2Li_3 , and (d) Al_4Li_9 .

of cubic Al_3Li satisfy the above restrictions in Eq.(3), demonstrating that Al_3Li is mechanically stable. The result is in good agreement with other works [38, 39].

For trigonal crystals, the mechanical stability criteria can be expressed as follows [3]:

$$\begin{aligned} C_{11} - |C_{12}| &> 0, \\ (C_{11} + C_{12})C_{33} - 2C_{13}^2 &> 0, \\ (C_{11} - C_{12})C_{44} - 2C_{14}^2 &> 0 \end{aligned} \quad (4)$$

Al_2Li_3 is a trigonal structure. From the Table III, we

can see that all the elastic constants of Al_2Li_3 satisfy the above restrictions in Eq.(4), and this indicates that Al_2Li_3 is also mechanically stable.

For tetragonal structures, the mechanical stability criteria can be expressed as follows [40]:

$$\begin{aligned} C_{11} > 0, C_{33} > 0, C_{44} > 0, C_{66} > 0, \\ C_{11} - C_{12} > 0, C_{11} + C_{33} - 2C_{13} > 0, \\ 2C_{11} + C_{33} + 2C_{12} + 4C_{13} > 0 \end{aligned} \quad (5)$$

In Table III, all the elastic constants of AlLi are con-

TABLE III Calculated elastic properties compared to other theoretical values for the single crystalline Al-Li system intermetallic compounds.

Phase	Elastic constant/GPa	B/GPa	
		This work	Reference
Al ₃ Li	$C_{11}=128, C_{44}=39, C_{12}=30$	63	
	$C_{11}=158, C_{44}=57.7, C_{12}=29.4$ [38]		72.3 [38]
	$C_{11}=123.6, C_{44}=42.8, C_{12}=37.2$ [39]		66 [39]
AlLi	$C_{11}=105, C_{33}=65, C_{44}=48, C_{66}=13, C_{12}=1.3, C_{13}=38, C_{16}=0$	48	
Al ₂ Li ₃	$C_{11}=114, C_{33}=88, C_{44}=28, C_{12}=13, C_{13}=2, C_{14}=-19$	38	44 [10]
Al ₄ Li ₉	$C_{11}=78, C_{22}=62, C_{33}=91, C_{44}=41, C_{55}=16, C_{66}=12, C_{12}=11, C_{13}=-8, C_{15}=-7,$	32	34 [10]
	$C_{23}=23, C_{25}=-0.5668, C_{35}=-0.5767, C_{46}=-1.8829$		

TABLE IV Polycrystalline bulk modulus B , shear modulus G , Young's modulus E , and Poisson's ratio ν for Al-Li system intermetallic compounds deduced by Voigt, Reuss, and Hill (VRH) approximations*.

Compound	B_V /GPa	B_R /GPa	B_H /GPa	G_V /GPa	G_R /GPa	G_H /GPa	E /GPa	B/G	ν
Al ₃ Li	63.3	63.3	63.3	43.1	42.6	42.8	116.8	1.479	0.1923
AlLi	47.81	47.77	47.79	35.18	23.68	29.43	78.02	1.624	0.2446
Al ₂ Li ₃	39.09	38.08	38.59	41.06	29.13	35.10	80.80	1.099	0.1510
Al ₄ Li ₉	31.35	30.33	30.84	27.53	20.58	24.05	71.26	1.282	0.1502

* The subscript V, R, H represent Voigt, Reuss, and Hill, respectively.

sistent with the above restrictions in Eq.(5) and these results demonstrate that it is mechanically stable.

There are following restrictions for the mechanical stability of monoclinic crystals [40]:

$$\begin{aligned}
 &C_{11} > 0, C_{22} > 0, C_{33} > 0, C_{44} > 0, C_{55} > 0, C_{66} > 0, \\
 &C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23}) > 0, \\
 &C_{33}C_{55} - C_{35}^2 > 0, C_{44}C_{66} - C_{46}^2 > 0, \\
 &C_{22} + C_{33} - 2C_{23} > 0, \\
 &C_{22}(C_{33}C_{55} - C_{35}^2) + 2C_{23}C_{25}C_{35} - C_{23}^2C_{55} - \\
 &C_{25}^2C_{33} > 0, \\
 &2[C_{15}C_{25}(C_{33}C_{12} - C_{13}C_{23}) + C_{15}C_{35}(C_{22}C_{13} - \\
 &C_{12}C_{23}) + C_{25}C_{35}(C_{11}C_{23} - C_{12}C_{13})] - [C_{15}^2(C_{22}C_{33} - \\
 &C_{23}^2) + C_{25}^2(C_{11}C_{33} - C_{13}^2) + C_{35}^2(C_{11}C_{22} - C_{12}^2)] + \\
 &C_{55}(C_{11}C_{22}C_{33} - C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2 + \\
 &2C_{12}C_{13}C_{23}) > 0
 \end{aligned} \quad (6)$$

In Table III, Al₄Li₉ obeys the restrictions of Eq.(6), thus it is mechanically stable.

In order to better understand the mechanical properties of Al-Li intermetallic compounds, Young's modulus E , shear modulus G , bulk modulus B , and Poisson's modulus ν for a polycrystalline material are deduced from single-crystal elastic stiffness constants by using VRH approximations [41], and the results are shown in Table IV. Figure 4(a) shows the relationship between shear modulus and concentration of Li. It is clearly shown that Al₃Li has the largest shear modulus. In addition, the relationship between bulk modulus and the concentration of Li are plotted in Fig.4(b). With in-

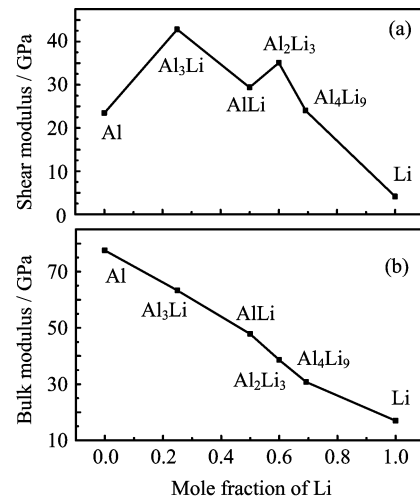


FIG. 4 Calculated (a) shear modulus and (b) bulk modulus of Al-Li system intermetallic compounds.

creasing concentration of Li C , the bulk modulus for Al-Li system compounds decrease approximately by a linear equation:

$$B = 77.66 - 62.77C \quad (7)$$

This result can be understood by the larger bulk modulus for Al ($B=72.2$ GPa [42]) compared with $B=13.5$ GPa for Li [43].

G represents the resistance to plastic deformation, while B represents the resistance to fracture [44]. To investigate the brittleness and ductility properties of Al-

Li system intermetallic compounds, the ratio of bulk modulus to shear modulus, B/G , has also been calculated. The value of B/G can classify materials as ductile or brittle by Pugh's empirical relationship [45]. If $B/G > 1.75$, the material behaves in a ductile manner; otherwise the material behaves in a brittle manner. For our computational scheme, the values of B/G are displayed in Table IV. According to the B/G values, the four compounds are brittle materials, and the brittleness of these compounds ranks as follows: $\text{Al}_2\text{Li}_3 > \text{Al}_4\text{Li}_9 > \text{Al}_3\text{Li} > \text{AlLi}$. In terms of Frantsevich *et al.*'s result [46], Poisson's ratio can be employed to discriminate between brittleness and ductility in metal or intermetallic materials. Generally, if Poisson's ratio around $1/3$, metals are ductile, otherwise metals are inferred as being brittle. The brittleness and ductility properties of the Al-Li system compounds determined by Poisson's ratio (ν) criterion based on the basis of the Poisson's ratio (Table IV), which are in good agreement with the results estimated by the B/G ratio.

IV. CONCLUSION

The structural properties, heats of formation, elastic properties, and electronic structures of four compositions of Al-Li binary system intermetallics (Al_3Li , AlLi , Al_2Li_3 , and Al_4Li_9) are systematically studied by first-principle calculations for the first time. The calculated lattice parameters for Al-Li intermetallic compounds are in good agreement with available experimental and previous theoretical values. When increasing Li concentration, the mass density of Al-Li intermetallic compounds decreases in a linear manner. The heats of formation for the Al-Li intermetallic compounds are also calculated. The values of heats of formation for Al_3Li , AlLi , Al_2Li_3 , and Al_4Li_9 are -7.826 , -18.06 , -16.69 , and -13.20 kJ/mol atoms, indicating that all of the compounds are thermodynamically stable. The computational single crystal elastic constants demonstrate that Al_3Li , AlLi , Al_2Li_3 , and Al_4Li_9 are mechanically stable. The polycrystalline elastic modulus and Poisson's ratio have been deduced by using Voigt, Reuss, and Hill (VRH) approximations, and the calculated ratios of bulk modulus to shear modulus indicate that Al_3Li , AlLi , Al_2Li_3 , and Al_4Li_9 compounds are brittle materials. With the increase of Li concentration, the bulk modulus of Al-Li intermetallic compounds decrease linearly.

V. ACKNOWLEDGEMENTS

This work was supported by the Postgraduate Innovation Fund of the Southwest University of Science and Technology (No.12ycjj03) and the 863 program of China (No.2009AA035002).

- [1] S. Ganeshan, S. L. Shang, H. Zhang, Y. Wang, M. Mantina, and Z. K. Liu, *Intermetallics* **17**, 313 (2009).
- [2] B. Wen, J. J. Zhao, F. D. Bai, and T. J. Li, *Intermetallics* **16**, 333 (2008).
- [3] D. M. Shi, B. Wen, R. Melnik, S. Yao, and T. J. Li, *J. Solid State Chem.* **182**, 2664 (2009).
- [4] F. Eshelman and J. Smith, *J. Appl. Phys.* **49**, 3284 (1978).
- [5] C. Wolverton and V. Ozolins, *Phys. Rev. Lett.* **86**, 5518 (2001).
- [6] T. Wei and A. Daud, *J. Electronic Packaging* **125**, 617 (2003).
- [7] W. Zhou, L. J. Liu, B. L. Li, Q. G. Song, and P. Wu, *J. Electron. Mater.* **38**, 356 (2009).
- [8] C. D. Yang, W. Li, and W. Zhi, *Solid State Commun.* **151**, 1270 (2011).
- [9] Z. W. Yang, D. M. Shi, B. Wen, R. Melnik, S. Yao, and T. J. Li, *J. Solid State Chem.* **183**, 136 (2010).
- [10] X. Q. Guo, R. Podlucky, and A. J. Freeman, *Phys. Rev. B* **42**, 10912 (1990).
- [11] Z. Q. Li and J. S. Tse, *Phys. Rev. B* **21**, 14531 (2000).
- [12] V. Vaithyanathan and L. Q. Chen, *Scripta Mater.* **42**, 967 (2000).
- [13] M. D. Rossell, R. Erni, M. Asta, V. Radmilovic, and U. Dahmen, *Phys. Rev. B* **80**, 024110 (2009).
- [14] T. H. Jr. Sanders and E. A. Jr. Starke, *Aluminum-Lithium. Alloys II*, New York: The Metallurgical Society of AIME (1984).
- [15] M. Hansen and K. Anoko, *Constitution of Binary Alloys*, 2nd Edn., New York: McGraw-Hill, (1958).
- [16] R. P. Elliott and F. A. Shunk, *Bull. Alloy Phase Diagrams* **2**, 353 (1981).
- [17] A. J. McAlister, *Bull. Alloy Phase Diagrams* **3**, 177 (1982).
- [18] C. Sigli and J. M. Sanchez, *Acta Metall.* **34**, 1021 (1986).
- [19] A. G. Khachatryan, T. F. Lindsey, and J. W. Morris, *Metall. Mater. Trans. A* **19**, 249 (1988).
- [20] M. H. F. Sluiter and Y. Watanabe, *Phys. Rev. B* **53**, 6137 (1996).
- [21] K. Puhakainen, M. Boström, T. L. Groy, and U. Häussermann, *J. Solid State Chem.* **183**, 2528 (2010).
- [22] M. D. Segall, P. J. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark, and M. L. Payne, *J. Phys.: Condens. Matter.* **14**, 2717 (2002).
- [23] P. Hohenberg and W. Kohn, *Phys. Rev. B* **136**, 864 (1964).
- [24] W. Kohn and L. J. Sham, *Phys. Rev. A* **140**, 1133 (1965).
- [25] D. Vanderbilt, *Phys. Rev. B* **41**, 7892 (1990).
- [26] D. R. Hamann, M. Schluter, and C. Chiang, *Phys. Rev. Lett.* **43**, 1494 (1979).
- [27] J. Dai, Z. Y. Li, and J. L. Yang, *Chin. J. Chem. Phys.* **22**, 139 (2009).
- [28] T. Yoshiyama, K. Hasebe, and M. H. Mannami, *J. Phys. Soc. Jpn.* **25**, 908 (1968).
- [29] H. Ehrenberg, H. Pauly, M. Knapp, J. Groebner, and D. Mirkovic, *J. Solid State Chem.* **177**, 227 (2004).
- [30] K. F. Tebbe, H. G. von Schnering, B. Rueter, and G. Rabeneck, *Z. Naturforsch. B* **28**, 600 (1973).
- [31] D. A. Hansen and J. F. Smith, *Acta Cryst. B* **24**, 913

- (1968).
- [32] J. Donohue, *The Structures of The Elements*, New York: John Wiley, (1974).
- [33] A. A. Nayeb-Hashemi, J. B. Clark, and A. D. Pelton, *Bull. Alloy Phase Diagrams* **5**, 365 (1984).
- [34] M. I. Medvedeva, Y. N. Gornostyrev, D. L. Novikov, O. N. Mryasov, and A. J. Freeman, *Acta Mater.* **46**, 3433 (1998).
- [35] B. R. Sahu, *Mater. Sci. Eng. B* **49**, 74 (1997).
- [36] M. Sluiter, D. de Fontaine, X. Q. Guo, R. Podlucky, and A. J. Freeman, *Phys. Rev. B* **42**, 10460 (1990).
- [37] G. P. Das, A. Aryab, and S. Banerjee, *Intermetallics* **4**, 625 (1996).
- [38] X. Q. Guo, R. Podlucky, and A. J. Freeman, *J. Mater. Res.* **6**, 324 (1991).
- [39] H. J. Axon and W. Hume-Rothery, *Proc. R. Soc. London A* **193**, 1 (1948).
- [40] Z. J. Wu, E. J. Zhao, H. P. Xiang, X. F. Hao, X. J. Liu, and J. Meng, *Phys. Rev. B* **76**, 054115 (2007).
- [41] O. L. Anderson, *J. Phys. Chem. Solids* **24**, 909 (1963).
- [42] C. Kittel, *Introduction to Solid State Physics*, 6th Ed., New York: John Wiley, (1986).
- [43] C. P. Liang and H. R. Gong, *J. Alloys Compd.* **489**, 130 (2010).
- [44] G. Vaitheeswaran, V. Kanchana, R. S. Kumar, A. L. Cornelius, M. F. Nicol, A. Savane, A. Delin, and B. Johansson, *Phys. Rev. B* **76**, 014107 (2007).
- [45] S. F. Pugh, *Philosoph. Magaz.* **45**, 823 (1954).
- [46] I. N. Frantsevich, F. F. Voronov, and S. A. Bokuta, Frantsevich Ed., *Elastic Constants and Elastic Moduli of Metals and Insulators Handbook*, Kiev: Naukova Dumka, (1983).