Theoretics-directed effect of copper or aluminum content on the ductility characteristics of Al-based (Al_3Ti, AlTi, AlCu, $AlTiCu_2$) intermetallic compounds*

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First-principle simulations have been applied to investigate the effect of copper (Cu) or aluminum (Al) content on the ductility of Al_3Ti, AlTi, AlCu, and $AlTiCu_2$ alloys. The mechanical stable and elastic properties of Al-based intermetallic compounds are researched by density functional theory with the generalized gradient approximation (DFT-GGA). The calculated lattice constants are in conformity with the previous experimental and theoretical data. The deduced elastic constants show that the investigated Al_3Ti, AlTi, AlCu, and $AlTiCu_2$ structures are mechanically stable. Shear modulus, Young's modulus, Poisson's ratio, and the ratio B/G have also been figured out by using reckoned elastic constants. A further analysis of Young's modulus and Poisson's ratio reveals that the third added element copper content has significant effects on the Al–Ti-based ICs ductile character.

Keywords: intermetallics, brittleness and ductility, elastic properties, *ab-initio* calculations

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1. Introduction

Since the early part of the last century, intermetallic compounds (ICs) have attracted considerable attention due to their unique physical properties and wide prospects in industries and electronics,[1–5] such as: mechanical help, welding alloys, alloy materials of sacrificial anodes, heat-resistant alloys, electricity, preferred material of mechanical heart valve and components.[6,7] As one potential industrial applied material, aluminum–titanium alloys possess elevated-temperature strength, low density, high melting points and strength.[8] They have been the desirable candidate-materials for structural applications, electricity and electronic devices.[9] Unfortunately, Al–Ti alloys are hard to be applied directly in practice industry for Al–Ti ICs brittleness and bad plastic deformation.[10–15] In order to improve the ductile properties of Al–Ti ICs, we put out a hypothesis added copper element into Al–Ti alloys that could improve Al–Ti ICs ductile and mechanical properties.

As we all know, Cu-based ICs have showcased for a new talent in biomechanical applications, aerospace and connectors with their perfect mechanical and physical ductile properties.[16–19] Especially, their brittleness is mainly due to the strong directional metallic-covalent bonds, which is based on the bonding mechanism by Osman *et al.*[20] In view of the present situation, an original plan is revised that the added element could decrease the content of Al percent, and increase the ductile character of Al–Ti alloy with the content of Cu. Of course, there are some corroborated experiments and theory evidences to support this initial hypothesis.[21] Other scientists have found that the mechanical characters can be improved due to the phase transition, especially, Al_3Ti structure.[22,23] Hence, we can add the third element copper into Al–Ti alloys to make Al–Ti ICs become an eminent and ductile material. In this way, adding the third element copper into the binary systems would be an elegant way of gaining ideal Al–Ti-based alloys. At the same time, Zhang *et al.*[21] has proved that Cu could increase the strength of the *in situ* composites substantially due to the introduction of more strengthening modes and more reinforcing particles. However, there is no related evidence that the added Cu can improve Al–Ti–*X* ductile character.

To gain more knowledge about Al–Ti–*X* ductile character, this study mainly focuses on Al_3Ti, AlTi, AlCu, and

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$AlTiCu_2$ structural and mechanical properties. In this paper, we present a detailed study of these mechanical and physical properties of $AlTiCu_2$ by using the first-principles plane-wave pseudopotential method.

2. Computational details

All calculated works were done by using the Cambridge Serial Total Energy Package Code (CASTEP) based on the density functional theory (DFT) scheme and an implementation of the ultra-soft pseudo-potential plane-wave (UPPW) methods.[17–20] Exchange and correlation theory was employed with the generalized gradient approximation or called GGA.[21,22] $3s^2 3p$ of Al, $3d^2 4s^2$ of Ti, and $3d^{10} 4s^2$ of Cu were considered as valence electrons. In this paper, the cutoff energy of plane-wave was 450 eV. The other parameters were set as a total energy convergence of 5.0×10^{-6} eV/atom, a maximum force of 0.01 eV/Å, a maximum stress of 0.02 GPa, and a maximum displacement of 5.0×10^{-4} Å. Al_3Ti, AlTi, AlCu, and $AlTiCu_2$ parameters were reckoned and probed by the popular Brodyden–Fletcher–Goldfarb–Shanno (BFGS) means.[23–26] For the different kinds of structures calculated, the Brillouin zone integrations were sampled with various (Γ point centered) k points which are generated by the scheme of Monkhorst–Pack grids (shown in Table 1).[27]

Table 1. Lattice parameters (a and c), space groups, and k-point mesh.

Phase		Space group	k-point mesh	a/Å	b/Å	c/Å	β
Al_3Ti	this work	$I4/mmm$	$6\times6\times3$	3.84900	3.84990	8.63204	90
	exp[28]	$I4/mmm$		3.85370	3.85370	8.58390	90
	error/%			−0.09861	−0.09861	0.56081	0
AlTi	this work	$P4/mmm$	$18\times18\times12$	2.82559	2.82559	4.07692	90
	exp[29]	$P4/mmm$		2.83730	2.83730	4.05910	90
	error/%			−0.41272	−0.41272	0.43901	0
AlCu	this work	$C12/m1$	$6\times6\times6$	12.0712	4.11606	6.94830	55.2512
	exp[30]	$C12/m1$		12.0660	4.10500	6.91300	55.0400
	error/%			0.04310	0.26943	0.51063	0.38372
$AlTiCu_2$	this work	Fm/mmm	$8\times8\times8$	6.03963	6.03963	6.03963	90
	exp[31]	Fm/mmm		6.02370	6.02370	6.02370	90
	error/%			0.26446	0.26446	0.26446	0

3. Results and discussion

3.1. Calculated structural

The different space groups of Al_3Ti, AlTi, AlCu, $AlTiCu_2$ are studied and shown in Fig. 1. Calculated lattice parameters are compared with experimental data and summarized in Table 1.

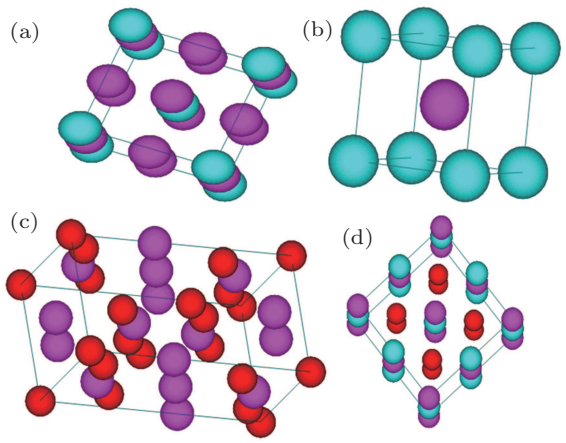


Fig. 1. (color online) Crystal structures of Al-based alloys: (a) Al_3Ti, (a) AlTi, (a) AlCu, and (a) $AlTiCu_2$.

Clearly, the calculated lattice constants are in good agreement with the previous experiments data. The deviations are less than 1%. Through these reliable calculated results, the structural data indicate that this method is a credible and applied method in this research work. Thereby, the GGA-PBE method and optimized lattice constant could be suited for subsequent calculations, including Al_3Ti, AlTi, AlCu, $AlTiCu_2$ mechanical properties, even other physical characters.

3.2. Elastic constants

Elastic constants of different Laves phases are important for the actual application of our life. Simultaneously, elastic properties of solids are very closely related to various fundamental physical properties, such as bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson's ratio (v), melting point, Debye temperature, and thermal expansion coefficient. Maybe, this is the reason why elastic constants C_{ij} play a significant role in ICs materials. The gross energy and a small strained equation is given by[32]

$$\varepsilon(V,\delta) = E(V_0,0) + V_0\left(\sum_i \tau_i\xi_i\delta_i + \frac{1}{2}\sum_{ij}\tau_{ij}\xi_i\delta_j\right). \quad (1)$$

As momentous parameters, elastic constants are also key physics quantities between structural stability and mechanical behaviors. The mechanical stability of Al_3Ti, AlTi, AlCu, and $AlTiCu_2$ is tested and verified by elastic constants C_{ij}. For

cubic crystals, mechanical stability criteria are[33]

$$C_{11} > 0, \tag{2}$$
$$C_{44} > 0, \tag{3}$$
$$C_{11} - C_{12} > 0, \tag{4}$$
$$C_{11} + 2C_{12} > 0. \tag{5}$$

The stability for tetragonal structures can be tested through[34]

$$C_{ii} > 0, \quad i = 1-6, \tag{6}$$
$$C_{11} - C_{12} > 0, \tag{7}$$
$$C_{11} + C_{22} - 2C_{12} > 0,$$
$$C_{11} + C_{33} - 2C_{13} > 0,$$
$$C_{22} + C_{33} - 2C_{23} > 0, \tag{8}$$
$$C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23}) > 0. \tag{9}$$

For the complex monoclinic structure, the following restrictions are the basic evaluation standard:[35]

$$C_{ii} > 0, \quad i = 1-6, \tag{10}$$
$$C_{33}C_{55} - C_{35}^2 > 0, \tag{11}$$
$$C_{44}C_{66} - C_{46}^2 > 0, \tag{12}$$
$$C_{22}C_{33} - C_{23}^2 > 0, \tag{13}$$
$$C_{11} + C_{22}C_{33} + (C_{12} + C_{13} + C_{23}) > 0, \tag{14}$$
$$C_{22}(C_{33}C_{55} - C_{35}^2) + 2(C_{23}C_{25}C_{35} - C_{25}^2C_{55} + C_{25}^2C_{33}) > 0, \tag{15}$$
$$2[C_{15}C_{25}(C_{33}C_{12} - C_{13}C_{23}) + C_{15}C_{35}(C_{22}C_{13} - C_{12}C_{23}) + C_{25}C_{35}(C_{11}C_{23} - C_{12}C_{13})] - C_{15}^2(C_{22}C_{33} - C_{23}^2) + C_{25}^2(C_{11}C_{33} - C_{13}^2) + C_{35}^2(C_{11}C_{22} - C_{12}^2) + C_{55} > 0, \tag{16}$$

Elastic constants are shown in Table 2. For Al_3Ti, AlTi, AlCu, $AlTiCu_2$, these stability are fulfilled with Eqs. (2)–(16). In addition, all structures are situated in a stable phase under zero pressure and temperature surrounding. Here, C_{11} or C_{33} is an elastic stiffness constant, shows the a- or c-direction resistance to linear condensation easily. From Table 2, we can see that the calculated C_{11} is lower than C_{33} for the calculated structures, except AlCu. The c axes of Al_3Ti and AlTi are not easily compressed along the a axes. Instead, AlCu is easy to be compressed along the a axis for the low C_{33}.

Table 2. Calculated elastic constants.

Phase	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{15}	C_{23}	C_{25}	C_{35}	C_{46}
Al_3Ti	202.7	202.7	226.4	96.5	96.5	133.9	76.3	38.9	–	38.9	–	–	–
AlTi	198.9	198.9	173.1	111.4	111.4	39.5	54.5	81.2	–	81.2	–	–	–
AlCu	228.1	209.8	185.2	65.8	63.2	76.5	53.0	56.5	8.2	66.5	20.9	11.6	13.2
Ref. [36]	223.0	227.4	181.1	66.3	59.5	77.7	58.4	71.3	–0.3	68.0	8.5	8.7	6.9
$AlTiCu_2$	179.8	179.8	179.8	103.6	103.6	1036	1219	1219	–	1219	–	–	–

3.3. Elastic modulus

As a systematical response to Al_3Ti, AlTi, AlCu, $AlTiCu_2$ alloy material mechanical properties, bulk modulus B, shear modulus G, Young's modulus E, and Poisson's ratio σ are also summarized in Table 3. These medial elastic properties are based on the added hypotheses such as isostress, entitled as Reuss or Voigt states.

For the cubic structure, the shear modulus G and bulk modulus B are given approximately as[33,35]

$$G_{\rm V} = (C_{11} - C_{12} + 3C_{44})/5, \tag{17}$$
$$G_{\rm R} = [5C_{44}(C_{11} - 2C_{12})]/[4C_{44} + 3(C_{11} - C_{12})], \tag{18}$$
$$B_{\rm V} = B_{\rm R} = (C_{11} + 2C_{12})/3. \tag{19}$$

For Monoclinic, bulk modulus B and shear modulus G were given by Reuss and Voigt as follows:[35,37]

$$\begin{aligned} G_{\rm V} &= [C_{11} + C_{22} + C_{33} + 3(C_{44} + C_{55} + C_{66}) \\ &\quad - (C_{12} + C_{13} + C_{23})]/15, \end{aligned} \tag{20}$$

$$\begin{aligned} G_{\rm R} &= 15\{4[(C_{33}C_{55} - C_{35}^2)(C_{11} + C_{22} + C_{12}) \\ &\quad + (C_{23}C_{55} - C_{25}C_{35})(C_{11} - C_{12} - C_{23}) \\ &\quad + (C_{13}C_{35} + C_{15}C_{33})(C_{15} + C_{25}) \\ &\quad + (C_{13}C_{55} - C_{15}C_{35})(C_{22} - C_{12} - C_{23} - C_{13}) \\ &\quad + (C_{13}C_{25} - C_{15}C_{23})(C_{15} - C_{25}) + f]/\Omega \\ &\quad + 3[g/\Omega + (C_{44} + C_{66})/(C_{44}C_{66} - C_{46}^2)]\}^{-1}, \end{aligned} \tag{21}$$

$$B_{\rm V} = [C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})]/9, \tag{22}$$

$$\begin{aligned} B_{\rm R} &= \Omega[(C_{33}C_{55} - C_{35}^2)(C_{11} + C_{22} - 2C_{12}) \\ &\quad + (C_{23}C_{55} - C_{25}C_{35})(2C_{12} - 2C_{11} - C_{23}) \\ &\quad + (C_{13}C_{35} + C_{15}C_{33})(C_{15} - 2C_{25}) \\ &\quad + (C_{13}C_{55} - C_{15}C_{35})(2C_{12} + 2C_{23} - C_{13} - 2C_{22}) \\ &\quad + 2(C_{13}C_{25} - C_{15}C_{23})(C_{25} - C_{15}) + f]^{-1}, \end{aligned} \tag{23}$$

$$\begin{aligned} f &= C_{11}(C_{22}C_{55} - C_{25}^2) - C_{12}(C_{12}C_{55} - C_{15}C_{25}) \\ &\quad + C_{15}(C_{12}C_{25} - C_{15}C_{22}) + C_{22}(C_{23}C_{35} + C_{25}C_{33}), \end{aligned} \tag{24}$$

$$\begin{aligned} g &= C_{11}C_{22}C_{33} - -C_{11}C_{23}^2 - C_{22}C_{13}^2 \\ &\quad - C_{33}C_{12}^2 + 2C_{12}C_{13}C_{23}, \end{aligned} \tag{25}$$

$$\begin{aligned} \Omega &= 2[C_{15}C_{25}(C_{33}C_{12} - C_{13}C_{23}) + C_{15}C_{35}(C_{22}C_{13} - C_{12}C_{23}) \\ &\quad + C_{25}C_{35}(C_{11}C_{23} - C_{12}C_{13})] - [C_{15}^2(C_{22}C_{33} - C_{23}^2) \\ &\quad + C_{35}^2(C_{22}C_{11} - C_{13}^2) + C_{35}^2(C_{22}C_{11} - C_{12}^2)] + gC_{55}. \end{aligned} \tag{26}$$

For tetragonal structure, the Voigt (G_V) and Reuss (G_R) shear modulus G, and the Voigt (B_V) and Reuss (B_R) bulk modulus are extrapolated by[35,38]

$$G_V = [12(C_{44}+C_{66})+C_{11}+C_{12}+2C_{33}-4C_{13}]/30, \quad (27)$$

$$G_R = [5(C_{11}+C_{12})C_{44}]/[4C_{44}+3(C_{11}-C_{12})], \quad (28)$$

$$B_V = [2(C_{11}+C_{22})+4C_{13}+C_{33}]/9, \quad (29)$$

$$B_R = [C_{33}(C_{11}+C_{12})-2C_{13}^2]/(C_{11}+C_{12}+2C_{33}-4C_{13}). \quad (30)$$

In the end, polycrystalline bulk modulus B, shearmodulus G, Young's modulus E, and Poisson's ratio σ are calculated by the Voigt–Reuss–Hillapproximation for the Al_3Ti, AlTi, AlCu, $AlTiCu_2$ ICs through[35,39,40]

$$B = (B_V + B_R)/2, \quad (31)$$

$$G = (G_V + G_R)/2, \quad (32)$$

$$E = 9B_HG_H/(3B_H + G_H), \quad (33)$$

$$\sigma = (3B_H - 2G_H)/2(3B_H + G_H). \quad (34)$$

Bulk modulus B, shear modulus G, and Young's modulus E for Al_3Ti, AlTi, AlCu, $AlTiCu_2$ are calculated according to Eqs. (17)–(34) and shown in Table 3. For the calculated result, there are a few differences between our results and other theoretical results. The small fraction is caused by the effective inward relaxations of some atomic seats under different strains. Because, the different distortion of the unit cell revolutionized could lead to the seat of different atoms within the cell changing relative to the positions given by a single shear effective. This change often engenders different energy and maybe counteracts the energetic value of the little deformation. The fractional error yields unpredictable results and cannot be avoided at present. Hence, we believe that the little fractional error could be ignored in this paper. For this reckoned bulk modulus (B), the calculated value can bear closer analysis. As shown in Table 3 and Fig. 2, $AlTiCu_2$ has the largest B, the best capacity of resistance to volume change under different pressures.

Table 3. Calculated bulk modulus B, shear modulus G, and Young's modulus E of Cu–Ti ICs.

Phase	B			G			B/G	E	σ
	B_V	B_R	B_H	G_V	G_R	G_H			
Al_3Ti	103.30	103.14	103.22	89.40	84.57	86.98	1.19	203.72	0.17
AlTi	111.65	111.65	111.65	76.08	67.35	69.72	1.60	173.12	0.24
AlCu	108.35	105.06	106.70	70.91	68.31	69.91	1.53	172.21	0.23
Cal[41]	–	–	112.1	–	–	64.9	–	163.2	0.26
Cal[42]	114.1	112.9	113.5	69.6	67.8	68.7	1.65	171.5	0.25
$AlTiCu_2$	141.23	141.23	141.23	73.76	51.00	62.38	2.26	163.12	0.31
Cal[43]	–	–	138.72	–	–	56.11	2.47	148.34	0.32
Cal[44]	–	–	134.99	–	–	54.48	2.47	–	–

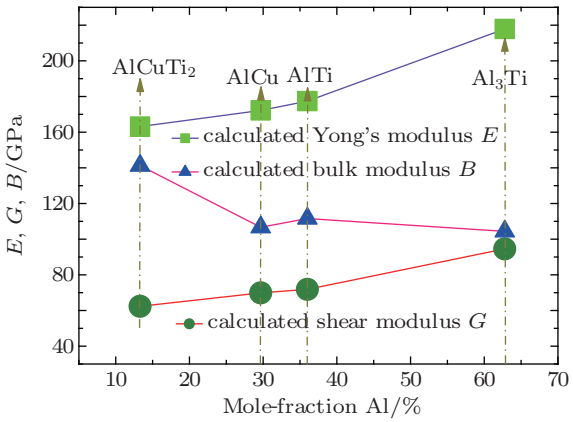


Fig. 2. (color online) Bulk, shear, and Young's moduli of Al_3Ti, AlCu, AlTi, $AlTiCu_2$.

Young's modulus is always a pretty character about the stiffness of ICs materials. The larger Young's modulus is, the harder the material is. In Fig. 2, Young's modulus decreases in the following sequence: Al_3Ti>AlCu>AlTi>$AlTiCu_2$. The Young's modulus of Al_3Ti is obviously larger than that of others, implying the worst plasticity. Young's modulus E also reflects the ratio of stress and strain and provides a measure of the stiffness of the solid. The smaller value of E responds to the ductile material. This result is the same as the ratio of bulk modulus to shear modulus (B/G), shown in Fig. 3.

In this part, plasticized properties of Al_3Ti, AlCu, AlTi, $AlTiCu_2$ are characterized by the ratio of bulk modulus to shear modulus (B/G), which can describe the plastic characteristic of materials.[40,45] A large B/G value means that the material tends to perform with a ductile property, while, a small value means it has a tendency to a brittleness property. The standardized value distinguishing ductile and brittle materials has been evaluated to be 1.75.[40] The B/G ratio is shown in Table 3 and Fig. 3. According to these, $AlTiCu_2$ is a kind of special ductile material, the brittleness of these materials ranks as follows: Al_3Ti>AlCu>AlTi>$AlTiCu_2$.

Poisson's ratio σ is distinguished by the level of different bonds in this work. For Ionic crystal, σ is usually looked at as 0.25. While, for the value of covalent materials, σ is not equal ionic crystals ($\sigma = 0.1$).[45] The calculated σ is given in Table 3. Obviously, the value of σ of $AlTiCu_2$ is larger than

0.25. It means that the ionic contribution to the inter atomic bonding for $AlTiCu_2$ is dominant.

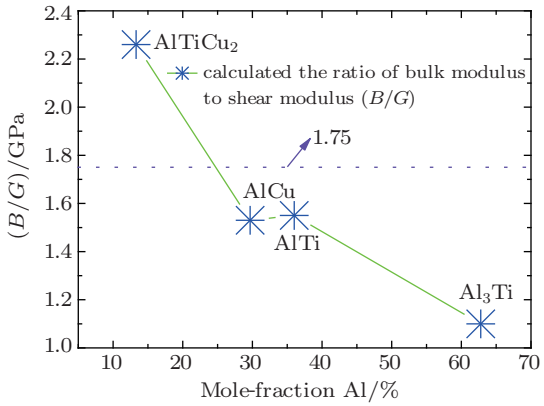


Fig. 3. (color online) Theoretically calculated the ratio of bulk modulus to shear modulus (B/G) of Al_3Ti, AlCu, AlTi, $AlTiCu_2$as a function of Al content.

4. Conclusions

In this paper, we have systemically investigated the alloying stability, the mechanical and thermodynamic properties of Al_3Ti, AlCu, AlTi, and $AlTiCu_2$ by the first-principles method. The conclusions are listed in the following points.

(I) The calculated lattice constants of Al_3Ti, AlCu, AlTi, and $AlTiCu_2$ are in good agreement with previous experimental data.

(II) The mechanical properties such as shear modulus and Young's modulus are obtained from single-crystal elastic constants. Through the data in Table 2, we believe that Al_3Ti, AlCu, AlTi, and $AlTiCu_2$ are mechanically stable and have strong alloying ability.

(III) From the simulation results, it has been proved that the third element copper has significant effects on Al–Ti-based ICs ductile character. The Poisson's ratio and B/G ratio are calculated. According to these calculated values, Al_3Ti, AlCu, AlTi are brittle materials, except $AlTiCu_2$. The ductile ranks as follows: $Al_3Ti<AlTi<AlCu<AlTiCu_2$.

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