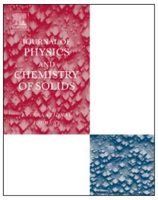
Journal of Physics and Chemistry of Solids 98 (2016) 298–308

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs



A comparative first-principles study on electronic structures and mechanical properties of ternary intermetallic compounds Al_8Cr_4Y and Al_8Cu_4Y: Pressure and tension effects

Wenchao Yang [a], Mingjun Pang [b,*], Yong Tan [c], Yongzhong Zhan [a,*]

[a] College of Materials Science and Engineering, Guangxi University, Nanning, Guangxi 530004, P.R. China
[b] SAIC-GM-Wuling Automobile Co., Ltd., Liuzhou, Guangxi 545007, PR China
[c] Shandong YuHang special alloy equipment Co., Ltd., Binzhou, Shandong 256200, P. R. China

ARTICLE INFO

Article history:
Received 14 March 2016
Received in revised form
17 June 2016
Accepted 6 July 2016
Available online 14 July 2016

Keywords:
Rare earth intermetallic compounds
First principles
Pressure
Stress–strain
Mechanical properties

ABSTRACT

An investigation into the bulk properties, elastic properties and Debye temperature under pressure, and deformation mode under tension of Al_8Cu_4Y and Al_8Cr_4Y compounds was investigated by using first principles calculations based on density functional theory. The calculated lattice constants for the ternary compounds (Al_8Cu_4Y and Al_8Cr_4Y) are in good agreement with the experimental data. It can be seen from interatomic distances that the bonding between Al1 atom and Cr, Y, and Al2 atoms in Al_8Cr_4Y are stronger than Al_8Cu_4Y. The results of cohesive energy show that Al_8Cr_4Y should be easier to be formed and much stronger chemical bonds than Al_8Cu_4Y. The bulk modulus B, shear modulus G, Young's modulus E and Poisson's ratio ν can be obtained by using the Voigt–Reuss–Hill averaging scheme. From the results of elastic properties, Al_8Cr_4Y has the stronger mechanical behavior than Al_8Cu_4Y. Our calculations also show that pressure has a greater effect on mechanical behavior for both compounds. The ideal tensile strength are obtained by stress-strain relationships under [001](001) uniaxial tensile deformation, which are 15.4 and 23.4 GPa for Al_8Cu_4Y and Al_8Cr_4Y, respectively. The total and partial density of states and electron charge density under uniaxial tensile deformations for Al_8Cu_4Y and Al_8Cr_4Y compounds are also calculated and discussed in this work.

1. Introduction

Al–T (T = transition metal) system have attracted considerable attention in recent years, which have potential applications in many fields. A great deal of experiments confirmed that rare earth (RE) element additions on Al–T system greatly improve mechanical property [1], oxidation resistance property [2], thermal stability [3] and so on. The Y element, as a common used additive, plays an important role in the behavior of Al–T alloys. For instance, it is reported that Y can promote the end-solidification temperature and decrease the quantity of eutectic in grain boundary [4], and also significantly reduce susceptibility to grain growth for Al–Cu alloy [5]. In addition, when Y additions into Al–Cr alloy, the alloys exhibit the most promising oxidation resistance [6]. It is also found that the hardness and the thermal stability can be improved after adding Y into this system [7].

However, Y added to Al–T alloys will also form various fascinating ternary intermetallic compounds, i.e. Al_8T_4Y with $ThMn_{12}$-type, AlTY with ZrNiAl-type, $Y_2(T, Al)_{17}$ with Th_2Zn_{17}-type and so on [8]. The aluminium rare earth compounds Al_8T_4Y are one of subgroup of the $ThMn_{12}$-type structure, which is always obtained with another 3d or 4d transition metal as a constituent element to stabilise the structure [9]. Especially, these compounds display favorable intrinsic properties. Gurevich et al. [10] have found Al_8Cr_4Y is superconducting compound with $T_c = 4.5$ K in 2001. It is also found that Al_8Cu_4Y has a greater electrical conductivity thereby shows a stronger metallic nature than Al_8Mn_4Y [11]. Since the existence of Al_8Cu_4Y and Al_8Cr_4Y are reported, a great deal of research is mainly concerned with their physical properties [12–15]. To the best of our knowledge, few studies are focused on electronic, elastic properties and the effect of external factors. Moreover, a complete set of information for the structure and properties of both compounds would also provide key information to practical application in the future.

In this work, the stoichiometric Al_8Cu_4Y and Al_8Cr_4Y compounds are chosen as the research objects. We present a comprehensive and systematic investigation on ground-state properties of both compounds using first principles calculations within the framework of density functional theory. In Section 2 we describe the details of the computational method used in the current

---

* Corresponding authors.
E-mail addresses: mjpang@163.com (M. Pang), zyzmatres@aliyun.com (Y. Zhan).

http://dx.doi.org/10.1016/j.jpcs.2016.07.008
0022-3697/© 2016 Elsevier Ltd. All rights reserved.

study. In Section 3.1, the equilibrium structures, phase stabilities, and electronic structures of both compounds are discussed. The elastic properties and pressure effect are presented in Section 3.2. In Section 3.3, the stress-strain relation and ideal strength for two compounds are obtained by [001](001) uniaxial tensile deformation. Finally, the conclusions are given in Section 4.

2. Computational method

The first principles calculations in the present work are based on the well-established Cambridge serial total energy package (CASTEP) code [16] within the density functional theory. The ion–electron interaction is described by the ultra-soft pseudopotential [17]. The exchange correlation potential is treated within the generalized gradient approximation (GGA) of Perdew–Burke–Ernzerh (PBE) version [18]. In the present calculations, the plane wave cutoff energy is chosen to be 400 eV. Integrations in the Brillouin–zone were performed using special *k* points generated with $6\times6\times10$ Monkhorst–Pack mesh [19]. The Pulay scheme of density mixing is applied for the evaluation of energy and stress [18]. Atomic positions and the unit cell are both relaxed by using the Brodyden–Fletcher–Goldfarb–Shanno (BFGS) minimization scheme [20]. The tolerances for the geometry optimization are selected as the difference in total energy within 5×10^{-6} eV/atom. A convergence criterion of 0.01 eV/Å was used for the maximum ionic Hellmann-Feynman force. The maximum ionic displacement is set at 5×10^{-4} Å and maximum stress within 0.02 GPa. The calculation of total energy and electronic structure are followed by cell optimization with SCF tolerance of 5.0×10^{-7} eV. For calculation of the total energies and electronic density of states (DOS), we used the linear the tetrahedron Blöchl method with corrections [21].

In the pressure calculations, we have performed a complete geometry optimization for the lattice cell in the considered range of pressure up to 50 GPa with a step of 10 GPa. The elastic constants were obtained by using the static finite strain technique [22]. As for tensile calculations, the stress-strain relations were calculated by incrementally deforming the modeled cell along the [001](001) direction of the applied strain. At each step, the lattice vectors perpendicular to the strain direction and the internal atomic coordinates were simultaneously relaxed until obtaining the equilibrium structures. To ensure that the strain path is continuous, the starting position at each strain step has been taken from the relaxed coordinates of the previous strain step.

3. Results and discussion

3.1. Bulk properties

The Al_8Cu_4Y and Al_8Cr_4Y compounds have ideal tetragonal $ThMn_{12}$ structure with space group I4/mmm (No. 139), containing 26 atoms. The Al atoms occupy the 8i and 8j Wyckoff site (0.365, 0, 0) and (0.275, 0.5, 0), respectively. The Y atoms occupy the 2a site (0, 0, 0) and the Cu or Cr atoms occupy the 8f site (0.25, 0.25, 0.25), as illustrated in Fig. 1. The experimental crystallographic data of the Al_8Cu_4Y and Al_8Cr_4Y compounds have been reported in the earlier time [23], which was considered as the original configurations in this work. The equilibrium structures of both compounds were obtained after the cell geometry and volume were fully relaxed by minimizing the total energy and forces. The calculated optimal results along with experimental values were shown in Table 1. Comparing the optimized lattice constants to the initial case, we can observe some differences between them but very small in value. In this work, the lattice constants *a* and *c* of Al_8Cu_4Y are calculated to be 8.832 and 5.169 Å, respectively. The errors between the experimental and theoretical values of lattice constants *a* and *c* are 1.28% and 0.17%, respectively. Our calculated results are also closed to the recent experimental results [24,25]. It is also found that the calculated lattice constants *a* and *c* for Al_8Cr_4Y agree well with experimental ones (the calculated values are 8.922 and 5.066 Å, respectively); the errors do not exceed 1%. Therefore, it can be demonstrated that our calculated results are well consistent with the experimental data, confirming the present calculated values of lattice parameters from our calculations are reliable. It is worth noting that the lattice constant *a* for Al_8Cr_4Y is larger than Al_8Cu_4Y while lattice constant *c* is smaller. In addition, the calculated lattice constants of Al_8Cu_4Y are both smaller than Al_8Cu_4Nb and Al_8Cu_4Sm [26], since the RE atomic radius increases in the following sequence: Y < Nb < Sm. The lattice constants of Al_8Cr_4Y are also smaller than Al_8Cr_4Nb and Al_8Cr_4Sm [26] as well as Al_8Cu_4Y.

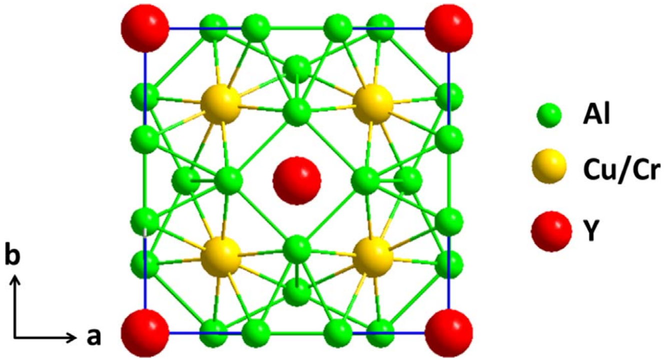


Fig. 1. Crystal structure for Al_8Cu_4Y and Al_8Cr_4Y compounds. The small green spheres are Al atoms, the middle yellow ones are Cu or Cr atoms and the large red ones are Y atoms.

Table 1
Summary of calculated structural parameters, bulk modulus B (unit in GPa) and its pressure derivative B_0' for Al_8Cu_4Y and Al_8Cr_4Y compounds at zero pressure, comparing with available previous experimental and theoretical results.

Compd.	Method	a_0 (Å)	c_0 (Å)	c_0/a_0	V_0 (Å^3)	B_0	B_0'	Ref.
Al_8Cu_4Y	Cal.	8.832	5.169	0.585	403.224	100.822	4.255	present
	Exp.	8.720	5.160	0.592	392.358	–	–	[23]
	Exp.	8.748	5.146	0.588	393.810	–	–	[24]
Al_8Cr_4Y	Cal.	8.922	5.066	0.568	403.270	123.222	3.985	present
	Exp.	8.940	5.120	0.573	409.209	–	–	[23]
	Exp.	8.920	5.130	0.575	408.100	–	–	[27]

The bulk modulus B_0 and its pressure derivative B_0' for both compounds have been evaluated in this work. In order to obtain these values, a complete geometry optimization for the unit cell in the considered range of pressure up to 50 GPa with a step of 10 GPa have been performed. The pressures were performed along *a*, *b* and *c* axis simultaneously, as shown in Fig. 2. The result obtained using the above methodology is pressure–volume data, which are fitted to a third-order Birch–Murnaghan equation of state (EOS) expressed as follows [28]

$$P=\frac{3}{2}B_0\left[\left(\frac{V}{V_0}\right)^{-7/3}-\left(\frac{V}{V_0}\right)^{-5/3}\right]\{1+\frac{3}{4}(B_0'-4)[\left(\frac{V}{V_0}\right)^{-2/3}-1]\} \tag{1}$$

where P is hydrostatic pressure; V_0 is the equilibrium volume at zero pressure; the cell volume V is constructed by carrying out geometry optimization under applied external pressure. It is shown in Fig. 2 that the relative changes of unit cell volume V/V_0 as a function of external pressure P for Al_8Cu_4Y and Al_8Cr_4Y