



Ab-initio study of structural, electronic, elastic and mechanical properties of $\text{RuAl}_{1-x}\text{Ga}_x$ ($x=0, 0.25, 0.50, 0.75$ and 1)



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ARTICLE INFO

Article history:

Received 6 February 2014

Received in revised form

26 September 2014

Accepted 20 November 2014

Available online 25 November 2014

Keywords:

Intermetallic compounds

Ab initio calculations

Elastic properties

Electronic structure

Mechanical properties

ABSTRACT

We have used special quasirandom structure to study the structural, electronic, elastic and mechanical properties of $\text{RuAl}_{1-x}\text{Ga}_x$ alloys for different compositions ($x=0, 0.25, 0.50, 0.75$ and 1) using a FP-LAPW method based on Density Functional Theory. The exchange and correlation potential is treated within the generalized gradient approximation. Ground state properties such as lattice constant (a_0), bulk modulus (B), its pressure derivative (B') and elastic constants are calculated. The ductility of these alloys has been analyzed by calculating the ratio of B/G_H , Cauchy pressure ($C_{12}-C_{44}$) and Frantsevich rule. From this study RuAl and RuGa are found to be brittle, but their alloys show ductile behavior; $\text{RuAl}_{0.50}\text{Ga}_{0.50}$ is found to be most ductile. Mechanical properties such as Poisson's ratio (σ), Young's moduli (E), and the ratio of elastic anisotropy factor (A) are estimated. We have also correlated the ductility and bonding behavior of these alloys.

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1. Introduction

Intermetallic compounds have emerged as materials with vast potential for application in a wide range of technologically important areas. The enormous potential of these intermetallics stems from their many attractive properties, such as high oxidation and corrosion resistance, thermal stability and relatively low densities, combined with their ability to retain strength and stiffness at elevated temperatures [1–5]. Tens of thousands of binary intermetallic compounds are known, however only a few dozen show appreciable room temperature ductility. During the last few years considerable experimental efforts have been devoted to understand not only their deformation and fracture behavior but also their property/microstructure relationships, in order to identify both intrinsic and extrinsic factors governing their brittleness [6].

Mehl et al. have studied the structural properties of ordered high-melting temperature intermetallic alloys (SbY , CoAl , RuZr and NbIr) using first-principles total energy calculations [7]. A theoretical study of structural, electronic, elastic, thermal and mechanical properties of nonmagnetic B_2 -type intermetallics YM ($M=\text{Cu}$, Zn and Ag) has been reported by Chouhan et al. [8] using first principles density functional theory based on the full

potential linearized augmented plane wave (FP-LAPW) method. The elastic and brittle properties of B_2 -MgRE ($\text{RE}=\text{Sc}$, Y , Ce , Pr , Nd , Gd , Tb , Dy , Ho , and Er) intermetallics have been investigated by Wu et al. [9] using first-principles density functional theory. These authors have found that all MgRE compounds are brittle; MgSc is most brittle, while MgHo is least brittle. Wang et al. [10] have investigated the phonon and thermodynamic properties of rare-earth-aluminum intermetallics AlRE ($\text{RE}=\text{Y}$, Gd , Pr , and Yb) with B_2 -type structure by using density functional theory and density functional perturbation theory within the quasiharmonic approximation. The cohesive and electronic properties of NiAl and RuAl have been studied by Lin et al. [11] by using first principles local density linearized muffin-tin orbital (LMTO) and full-potential linearized augmented plane wave (FP-LAPW) methods. Nguyen et al. [6] have studied the binding energies for the $4d$ transition metal (TM) aluminides (TMAI) with respect to 12 different binary type structures, using FP-LMTO method within LDA. The elastic constants and various elastic moduli of RuAl have been reported by Mehl et al. [12] while Villars et al. [13] have calculated the lattice constant of RuAl .

RuAl is a very unusual intermetallic compound amongst the large number of B_2 structured intermetallics that has been identified and investigated in recent years. Fleischer et al. [14] have pointed out the unusual ductility and toughness of RuAl in context of other intermetallics. RuAl has recently been considered as a bond coat for ZrO_2 -based thermal barrier coatings (TBCs) [15,16]. The high temperature capability and potentially excellent mechanical behavior of RuAl has triggered extensive interest in this

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particular alloy. The mechanical properties of RuAl-based alloys are also affected by addition of different elements, such as boron, which was found to increase the ductility of the stoichiometric and Ru-rich alloys approximately two fold with only 0.5% addition [14]. However, the exact mechanism through which boron contributes to the improved ductility of RuAl is still unclear [17]. Other alloying additions that have been found to have positive effects on the mechanical properties of RuAl include Sc, which aids to increase the high temperature strength without deteriorating room temperature toughness [14]. In the present paper we investigate the structural, electronic, elastic and mechanical properties of $\text{RuAl}_{1-x}\text{Ga}_x$ with Ga concentration varying between 0.0 and 1.0 using the full potential-linearized augmented plane wave (FP-LAPW) method. The primary aim is to study how ductility of RuAl changes by addition of Ga and to determine the alloying effects on bonding, crystal ordering and symmetry, using first principle density functional theory.

2. Method of calculation

The total energy calculations are performed for $\text{RuAl}_{1-x}\text{Ga}_x$ for x varying from 0.0 to 1.0 in step of 0.25. The calculations of electronic structure and other properties of $\text{RuAl}_{1-x}\text{Ga}_x$ alloys have been performed using the full potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code [18], based on the density functional theory (DFT). The generalized gradient approximation (GGA) in the scheme of Perdew, Burke and Ernzerhof (PBE) is used for the exchange and correlation effects [19]. In this study we have adopted the special quasirandom structure (SQS) approach proposed by Zunger et al. [20]. SQS are specially designed periodic structures with only a few atoms per unit cell, which closely mimic the most relevant local pair and multisite correlation functions of the random substitutional alloys [21–24]. Due to small sizes of SQSs, essentially any DFT method can be employed, including full-potential methods capable of accurately capturing the effects of atomic relaxations.

We have considered SQSs for random pseudo-binary $\text{RuAl}_{1-x}\text{Ga}_x$ alloy, where Al and Ga atoms are randomly distributed on one B_2 sublattice while the second sublattice is completely occupied by Ru atoms. The structural properties of the $\text{RuAl}_{1-x}\text{Ga}_x$ compounds for composition $x=0.0, 0.25, 0.50, 0.75$ and 1.0 are presented generating various SQS- N structures for the random pseudobinary $\text{RuAl}_{1-x}\text{Ga}_x$ alloys (with $N=1, 2$ and 4 simple-cubic sites per unit cell, or a total of $2N$ atoms per unit cell) for compositions where $x=0.0$ –1.0 with steps of 0.25. Thus, we use SQS-1, SQS-2 and SQS-4 to represent the random $\text{RuAl}_{1-x}\text{Ga}_x$ alloy as SQS-1 for $x=0$ and $x=1$, SQS-2 for $x=0.50$ (4 atom supercell) and SQS-4 for $x=0.25$ and 0.75 (8 atom supercell).

In order to achieve convergence, we expand the basis function up to $R_{MT} \times K_{max}=7$ where R_{MT} is the smallest atomic radius in the unit cell and K_{max} gives the magnitude of the largest K vector in the plane wave expansion. The maximum value for partial waves inside the atomic sphere is $l_{max} x=10$ while the charge density is Fourier expanded up to $G_{max} x=12$. The self-consistent calculations are converged when the total energy of the system is stable within 10^{-4} Ry. A dense mesh of 1000k points and the tetrahedral method [25] has been employed for the Brillouin zone integration. The total energies are fitted to Birch [26] equation of state to obtain the ground state properties. The muffin-tin radius was chosen to be 2.50, 2.22 and 2.22 au for Ru, Al and Ga respectively.

The elastic moduli require knowledge of the derivative of the energy as a function of the lattice strain. It is well known that a cubic system has only three independent elastic constants namely, C_{11} , C_{12} and C_{44} . Hence, a set of three equations is needed to determine all the constants. The first equation involves calculation of

bulk modulus (B), related to the elastic constants as

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \quad (1)$$

The second step involves volume-conservative tetragonal strain given by the following tensor:

$$\begin{bmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \frac{1}{(1+\delta)^2} - 1 \end{bmatrix} \quad (2)$$

where $\delta=(1+e)^{-1/3}-1$ with e as strain tensor. Application of this strain has an effect on the total energy from its unstrained value as follows:

$$E(\delta) = E(0) + 3(C_{11} - C_{12}) + V_0\delta^2 + O(\delta^3) \quad (3)$$

where V_0 is the volume of the unit cell.

Finally, for the last type of deformation, we use in the volume-conserving rhombohedra strain tensor given by

$$\frac{\delta}{3} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \quad (4)$$

which transforms the total energy to

$$E(\delta) = E(0) + \frac{1}{6}(C_{11} + 2C_{12} + 4C_{44}) + V_0\delta^2 + O(\delta^3) \quad (5)$$

3. Result and discussion

3.1. Structural properties

To model the $\text{RuAl}_{1-x}\text{Ga}_x$ alloys, we employed special quasirandom structures (SQS) [20]. SQS scheme allows us to select the simplest unit cell for each analyzed composition. In order to study the structural properties of ternary $\text{RuAl}_{1-x}\text{Ga}_x$ alloys for compositions $x=0, 0.25, 0.50, 0.75$ and 1, first we calculate the structural properties of the binary compounds RuAl and RuGa in the CsCl structure. Taking CsCl standard unit cell of $2 \times 2 \times 2$, we obtained the structures of $\text{RuAl}_{1-x}\text{Ga}_x$ by replacing the Al atoms with Ga to get the alloys with 25%, 50% and 75% concentration respectively. For alloys randomness can be reproduced for the first few shells around a given site, with the help of SQS's approach [20]. For the considered structures, we performed the structural optimization by minimizing the total energy with respect to the volume using the FP-LAPW method. The plots of total energy versus volume are given in Fig. 1. The calculated total energies are fitted to the Birch equation of states [26] to determine the ground state properties, such as equilibrium lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') which are listed in Table 1. Bulk modulus of $\text{RuAl}_{1-x}\text{Ga}_x$ alloys increases as concentration of Ga increases. The calculated values of lattice parameter of RuAl is in agreement with the experimental [13,14] and other theoretical [11] results.

3.2. Electronic properties

The calculated non-spin polarized electronic band structures along high symmetry directions of RuAl as well as for Ga doped alloys are presented in Fig. 2(a)–(e) where Fermi level is considered at zero. The total and partial densities of states (DOS) for these compounds at ambient pressure are presented in Fig. 3(a)–(e). For RuAl, in Fig. 2(a) the lowest lying bands are due to Al 's' like states. It can also be seen from partial density of states in Fig. 3(a) that there are many peaks between -6.5 eV and 4.0 eV

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