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An examination of the structural, electronic, elastic, vibrational and thermodynamic properties of Ru_2YGa (Y = Sc, Ti and V) Heusler alloys

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ABSTRACT

The structural, electronic, elastic, vibrational and thermodynamic properties of the Ru_2YGa (Y = Sc, Ti and V) Heusler alloys in $L2_1$ type cubic structure have been analyzed systematically using first principles density functional theory (DFT) together with the Generalized Gradient Approximation (GGA) method. The values of calculated lattice constant (a_0), elastic constants (Cij), Bulk modulus (B), Shear modulus (G), ratios of B/G, Young's modulus (E) and Poisson ratio (ν) are in good agreement with the available theoretical and experimental results. The electronic band structures, corresponding total and partial density of states have also been obtained. The calculated band structures demonstrate that Ru2YGa (Y = Sc, Ti and V) alloys are metallic. The phonon dispersion curves, total and partial density of states of these alloys have been computed for the first time by adopting the direct method. It is considered that all alloys are dynamically stable in $L2_1$ structure.

1. Introduction

Heusler alloys were first synthesized by German chemist Friedrich Heusler in 1903 by adding 3rd group elements to CuMn alloys [1]. First studied Heusler alloy was Cu_2MnSn. In this first Heusler alloy, instead of Sn atom, III-V group elements such as Al, As, Sb, Bi and B were used and similarly instead of Cu atom different transition metals were used. One of the main characteristics of Heusler alloys is that although elements forming Heusler alloy are not ferromagnetic, some Heusler alloys show ferromagnetic behavior. Heusler alloys can be divided into two main categories such as full Heusler alloys and semi-Heusler alloys. Full-Heusler alloys are in X_2YZ stoichiometric composition and have $L2_1$ body-centered cubic structure whereas Semi-Hesuler alloys are in XYZ stoichiometric composition and have $C1_b$ cubic-centered structure.

In Full Heusler alloys X is usually a transition metal, such as Cu, Fe, Ni, Co, Ru; Y is usually Mn, Cr or V and Z can be Al, Ga, Ge, Si, Sn in $L2_1$ structure. Full Heusler alloys are triple intermetallic compounds and have cubic structure [2–5]. Intermetallic alloys, crystal structured compounds or solid solutions formed in the frame of basic proportions by two pure metals which take place between metals and ceramics usually have no resemblance to each other chemically. Intermetallic alloys which are a metal attached material class at critical temperature range (T_c < 700 °C) forming regular crystal structures at long distance show metallic character. Most of the Heusler type alloys are ferromagnetic and show interesting ferromagnetic characteristics [6,7]. These alloys have the ability to

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show a violant magnetization in the exististence of a weak magnetic field. In case of removal or ceasing of the magnetic field, these alloys still show magnetism which is called remanence. Magnetic remanence value determines the permanent magnetism state. Heusler type alloys, constructed gathering of the elements has changeable magnetism which is a unique characteristics of these alloys [8]. Another important characteristics of Heusler alloys is that they can have magnetic shaped memory [9,10]. Shaped memory alloys have the ability to return to their original size or form in proper thermal and mechanical processes after their geometry is disrupted due to external factors. Because of their interesting half-metallic properties, Heusler alloys are used in many technological areas such as spintronics and magnetoelectronics [11,12]. The main characteristic of half-metallic ferromagnets is their different behavior in the two spin bands: while the majority spin band shows a typical metallic behavior, the minority spin band is semiconducting. Thus, the spin polarization at the Fermi level is 100%, that maximizes the efficiency of spintronic devices [13]. Recently, these alloys have attracted considerable interest because of their interesting magnetic properties [14–19]. Magnetic susceptibility and permeability, magnetostriction, Curie temperature and hysteresis curves studies of the Heusler alloys are fundamental topics [20,21]. Ru_2YGa (Y = Sc, Ti, and V) have been subject of various theoretical and experimental studies [22–26]. Theoretically, using the full-potential linearized augmented plane-wave (FP-LAPW) method based on the density functional theory (DFT), Abbassa et al. [22] reported the structural, electronic, elastic and thermal properties for $Ru_2VGa_{1-x}Al_x$ (x = 0, 0.25, 0.5, 0.75, 1). Gilleßen in his dissertation studied the lattice constants and magnetic moments of full Heusler alloys Ru_2YGa (Y = Sc, Ti, and V) using density functional theory [26]. On the experimental side, Ru_2VGa alloy has been synthesized for the first time by Mondal et al. [23]. The lattice constant and electrical resistivity of the Ru_2VGa alloy has been calculated using powder X-ray powder diffraction (XRD) by Mondal et al. [24]. They state that the Ru_2VGa alloy shows high resistances compared to standard metals and have low residual resistivity ratio.

In the present paper we have carried out first principles density functional theory calculations at PBE level of theory to obtain physical parameters such as lattice constant (a_0), elastic constants (C_{ij}), Bulk modulus (B), Shear modulus (G), ratio of B/G, Young's modulus (E) and Poisson ratio (ν) of Ru_2YGa (Y = Sc, Ti, and V) Heusler alloys. We have also calculated electronic band structures, corresponding total and partial density of states (PDOS), phonon dispersion relations and thermodynamic properties such as specific heat (C_v) and entropy (S) of these Heusler alloys.

Organization of this paper is as follows: We describe the theoretical method in Section 2. Results and discussions are given in Section 3. Finally, results are recapitulated in Section 4.

2. Theoretical method

All the calculations have been performed using the plane-wave pseudo-potential DFT method implemented in the MedeA-VASP package [27,28]. Projector Augmented Wave (PAW) pseudo-potentials were used to present the ionic potentials. The Perdew–Burke–Ernzerhof (PBE) [29] exchange-correlation functional was treated at the Generalized Gradient Approximation (GGA). An energy cut-off 329 eV was found to be adequate for the calculation of the structural, electronic, elastic, vibrational and thermodynamic properties of Ru_2VGa. Similarly, an energy cut-off of 313 eV was found to be adequate for Ru_2ScGa and Ru_2TiGa. The Brillouin zone integration was performed on a Monkhorst-Pack [30] 6 × 6 × 6 k-point mesh with a Methfessel–Paxton [31] smearing of 0.225 eV for Ru_2VGa and Ru_2ScGa. For Ru_2TiGa 5 × 5 × 5 k-point mesh with a smearing of 0.225 eV was used. The elastic constants were predicted using the stress-finite strain technique [32]. The phonon dispersion curves, total and PDOS of these alloys were calculated using the direct method [33].

3. Results and discussion

3.1. Structural and electronic properties

Heusler type alloys having X 2 YZ stoichiometric composition belongs to Fm-3 m (space group No. 225). This structure may conveniently be considered as four interpenetrating fcc sublattices with atoms of X, Y and Z at locations (0, 0, 0) and (1/2, 1/2, 1/2); (1/4, 1/4, 1/4); and (3/4, 3/4, 3/4), respectively [5,17]. The crystal structure of Ru_2YGa (Y = Sc, Ti, and V) Heusler alloys is given in Fig. 1. Additionally, the calculated lattice constants (a_0) are listed in Table 1. The optimized lattice constants of Ru_2ScGa, Ru_2TiGa, and Ru_2VGa are 6.229, 6.098, and 6.013 Å, respectively. It is known that ionic radius of Sc, Ti and V atoms decrease from Sc to V. Lattice constants of Ru_2YGa (Y = Sc, Ti, and V) Heusler alloys increase while ionic radius of the Y atom increases as shown in Table 1. The obtained results for Ru_2YGa (Y = Sc, Ti, and V) alloys agree well with the available experimental and theoretical results in the literature [22–26]. Therefore, there is a good agreement between our results and previously reported results.

The calculated electronic band structure, relevant total and partial DOS of Ru_2ScGa, Ru_2TiGa and Ru_2VGa along the high symmetry directions in the Brillouin zone are given in Figs. 2 and 3. It is seen that there is no band gap at the Fermi level, as a result, Ru_2ScGa, Ru_2TiGa and Ru_2VGa alloys exhibit a metallic behavior. Our calculated electronic band structure for Ru_2VGa is in good agreement with previous reported work [22].

From total and partial density of states relations of Ru_2ScGa alloy as shown in Fig. 3, the most contribution to conductivity comes from Ru-4d and Ga-4 s orbitals between −6.4 eV and −8.5 eV and similarly from Ru-4d and Ga-4 s orbitals between −4.5 eV and 0 eV (Fermi level). It is clearly seen that sharp peaks over Fermi level having energies of 2.2 eV and 3.7 eV are provided by the electrons in Ru-4d and Sc-3d.

From total and partial density of states relations of Ru_2TiGa alloy as shown in Fig. 3, the most contribution to conductivity comes from the electrons in Ru-4d and Ga-4 s orbitals between −6.5 eV and −8.7 eV and from the electrons in Ru-4d and Ti-3d orbitals between −5.0 eV and Fermi level. It is clearly seen that sharp peaks over Fermi level having energies of 2.2 eV are provided by the