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Theoretical Investigations on the Mechanical, Magneto-Electronic Properties and Half-Metallic Characteristics of ZrRhTiZ (Z = Al, Ga) Quaternary Heusler Compounds

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Abstract: The electronic, magnetic, and mechanical properties were investigated for ZrRhTiZ (Z = Al, Ga) quaternary Heusler compounds by employing first-principles calculations framed fundamentally within density functional theory (DFT). The obtained electronic structures revealed that both compounds have half-metallic characteristics by showing 100% spin polarization near the Fermi level. The half-metallicity is robust to the tetragonal distortion and uniform strain of the lattice. The total magnetic moment is 2 μ_B per formula unit and obeys the Slater-Pauling rule, $M_t = Z_t - 18$ (M_t and Z_t represent for the total magnetic moment and the number of total valence electrons in per unit cell, respectively). The elastic constants, formation energy, and cohesive energy were also theoretically calculated to help understand the possibility of experimental synthesis and the mechanical properties of these two compounds.

Keywords: half-metallic materials; first-principles calculations; quaternary Heusler compound

1. Introduction

Half-metallic materials (HMMs) [1] can provide completely spin-polarized conducting electrons due to their unique electronic band structure which shows metallic characteristics in one spin channel and semiconducting/insulating properties in the other spin channel. Hence, HMMs are very much appreciated as key materials for providing high spin polarized carriers for spintronics devices.

As one of the important HMM families, Heusler compounds have a special importance due to their high Curie temperature, tunable electronic structure, and wide change of lattice constant [2,3]. Moreover, from the previous reports concerning pseudo-quaternary or ternary Heusler compounds with half-metallicity, it was found that the materials containing 4d or 5d transition metal elements generally demonstrate a wide band gap implying a robust half-metallicity in a quite uniform strain or tetragonal distortion, which is quite suitable for practical applications. Therefore, in recent years, the investigations on the Heusler compounds containing 4d or 5d transition metal elements have become the research focus [4–9]. Although many ternary Heusler compounds containing 4d or 5d transition metal elements have become the research focus [4–9]. Although many ternary Heusler compounds containing 4d or 5d transition metal elements have become the research focus [4–9]. Although many ternary Heusler compounds containing 4d or 5d transition metal elements have become the research focus [4–9]. Although many ternary Heusler compounds containing 4d or 5d transition metal elements have become the research focus [4–9]. Although many ternary Heusler compounds containing 4d or 5d transition metal elements have become the research focus [4–9]. Although many ternary Heusler compounds containing 4d or 5d transition metal elements have become the research focus [4–9].



with half-metallicity have been rarely reported. Hence, it is important to further investigate and search for new half-metallic SQH materials containing 4d or 5d transition metal elements.

In this work, we investigate two new SQH compounds, ZrRhTiAl and ZrRhTiGa, for the first time. Our prime aim in this work is to investigate the electronic and magnetic properties of both compounds and their half-metallic (HM) stability under uniform strain and tetragonal distortion. The elastic constants, formation energy, and cohesive energy were also presented to help understand the possibility of experimental synthesis and the mechanical properties of these two compounds.

2. Method of Calculations

In this work, the calculations were performed by employing CASTEP computational code [10] framed fundamentally within DFT [11]. In all the calculations, the ultra-soft pseudo-potential approach with plane wave basis set was used, and the generalized-gradient-approximation (GGA) was adopted for the exchange–correction energy functional part of the total energy [12,13]. For the expansion of electronic wave functions, the plane wave basis set expansion approach was used. To truncate the plane wave basis set expansion to attain the required convergence criterion, an energy cut-off of 450 eV and a mesh of $12 \times 12 \times 12$ k-points for the Brillouin zone sampling was used. Within our above said applied parameters, calculations ensured a high-level total energy convergence with less than a tolerance of 1×10^{-6} eV per atom for both ZrRhTiZ (Z = Al, Ga) compounds.

3. Results and Discussions

The quaternary Heusler compounds have a LiMgPdSb-type structure, which belongs to the F43m (No.216) space group. There are four crystallographic sites in Heusler compounds. For quaternary Heusler compounds, there are three possible atomic arrangements depending on each crystallographic site occupation. In this present study, the atomic arrangement properties of ZrRhTiZ (Z = Al, Ga) compounds were investigated by calculating the total energy in ferromagnetic (FM) and non-ferromagnetic (NM) states. The calculated results show that for the ZrRhTiZ (Z = Al, Ga) compound, the most stable case is that Zr and Ti atoms with less valence electrons enter into the Wyckoff sites 4a(0, 0, 0) and 4c(0.25, 0.25, 0.25), Rh atoms with more valence electrons occupy the 4b(0.5, 0.5, 0.5) site, and the main group of atoms, Z atoms, tend to locate at the 4d(0.75, 0.75, 0.75) site. The corresponding simulated crystal structure is shown in Figure 1. The stable arrangement of ZrRhTiZ (Z = Al, Ga) Heusler compounds is like the combination of inverse Zr₂RhZ [14] and Ti₂RhZ (Z = Al, Ga) [15] Heusler compounds and found to be similar to the other Zr-based SQH compounds [16,17].

Figure 2 shows the dependence of the total energy on the lattice parameters in FM and NM states for ZrRhTiZ (Z = Al, Ga) compounds. One can see that both compounds are more stable in FM than NM states according to the viewpoint of the total energy minimization. The equilibrium lattice constants corresponding to the ground state energy are 6.47 Å and 6.45 Å for ZrRhTiAl and ZrRhTiGa, respectively.



Figure 1. Crystal structure of ZrRhTiZ (Z = Al, Ga) quaternary Heusler compounds.



Figure 2. Total energy as a function of the lattice constant in the non-ferromagnetic (NM) and ferromagnetic (FM) states for ZrRhTiAl (**a**) and ZrRhTiGa (**b**) compounds. The lowest energy in the FM state is set as zero point.

The spin-projected band structures in the reduced Brillouin zone along the high symmetry directions were calculated under the equilibrium lattice constant and plotted in Figure 3 for ZrRhTiAl

and ZrRhTiGa compounds. From Figure 3, an indirect band gap can be clearly observed in the spin-down channel, and the Fermi level is located within the band gap. In the spin-up channel, the valence and conduction bands are overlapping, and the Fermi level is intersecting them for ZrRhTiZ (Z = Al, Ga) compounds, which indicates that both compounds are half-metallic materials. The band gap (E_{bg}) and HM band gap (E_{HM}) in the spin-down channel are listed in Table 1. The HM band gap is the minimum energy required to flip a minority of spin electrons from the valence band maximum (VBM) to the majority spin Fermi level. The E_{bg} is 0.432 eV for ZrRhTiAl and 0.541 eV for ZrRhTiGa. Usually, the large E_{bg} can be considered as evidence of the robustness of half-metallicity to lattice distortion. The Mulliken atomic populations quantify the charge transfer from one atom to another one and are listed in Table 2 for ZrRhTiZ (Z = Al, Ga) compounds. It is clear that the charge transfer from Ti to Rh is 0.69e and Zr to Al is 0.08e in ZrRhTiAl, and the charge transfer from Ti to Zr is 0.27e and Ga to Rh is 0.93e in ZrRhTiGa.



Figure 3. The calculated band structures for ZrRhTiAl (**a**) and ZrRhTiGa (**b**). (The black lines represent the spin-up channel, and the red lines the spin-down channel.).

Table 1. The equilibrium lattice constants (Å), total magnetic moments (μ_B), atomic magnetic moments (μ_B), valence band maximum (eV), conduction band minimum (eV), band gap (eV), half-metallic (HM) band gap (eV), and the number of valence electrons for ZrRhTiZ (Z = Al, Ga) compounds.

Compound	Total	Zr	Rh	Ti	Ζ	a (Å)	СВМ	VBM	E_{bg}	E_{HM}	Z_t	S-P rule	P (%)
ZrRhTiAl	- 2.00	1.26	-0.32	1.18	-0.14	6.47	0.350	-0.082	0.432	0.082	20	$M_t = Z_t - 18$	100
ZrRhTiGa		1.22	-0.32	1.32	-0.22	6.45	0.360	-0.181	0.541	0.181			

Species	Species Atom		р	d	Total	Charge(e)	
	Zr	2.54	6.37	3.02	11.93	0.07	
7 01 7 41	Rh	0.89	0.60	8.20	9.69	-0.69	
ZrKhIiAl	Ti	2.53	6.12	2.65	11.30	0.70	
	Al	1.05	2.03	0.00	3.08	-0.08	
	Zr	2.64	6.67	2.96	12.27	-0.27	
	Rh	0.97	0.76	8.20	9.93	-0.93	
ZrKhliGa	Ti	2.70	6.37	2.65	11.73	0.27	
	Ga	-0.17	2.26	9.99	12.08	0.92	

Table 2. Mulliken population analysis of ZrRhTiAl and ZrRhTiGa.

Figure 4 shows the total density of state (TDOS) and partial density of state (PDOS) patterns. It is clear that the main contributions to the TDOS near the Fermi level are the strong d-d hybridization among the Zr-4d state, Ti-3d state, and Rh-4d state. The spin polarization (P) at Fermi energy is

100% for ZrRhTiZ (Z = Al, Ga), for the Fermi level lies in a band gap in the spin-down channel. For Heusler compounds with half-metallicity, the origin of the half-metallic band gap is usually owed to the hybridization of the d electrons between the transition metal atoms. Through the classical molecular orbital approach, Zr-4d and Rh-4d hybridization within tetrahedral symmetry has been considered, as presented in Figure 5. In ZrRhTiZ (Z = AI, Ga) Heusler compounds, the 4d orbitals hybridization of Rh and Zr atoms generated five bonding bands $(3t_{2g} \text{ and } 2e_g)$ and five non-bonding bands ($2e_u$ and $3t_{1u}$). Then, the 3d orbitals of Ti atom hybridize with the five bonding 4d hybridized orbitals $(3t_{2g} \text{ and } 2e_g)$ of Rh and Zr atom, while the five non-bonding hybridized 4d orbitals ($2e_u$ and $3t_{1u}$) still hold with no hybridization. Finally, the distribution of the 15 d orbitals in the spin-down channel can be determined, i.e., $3 \times t_{2g}$, $2 \times e_g$, $2 \times e_u$, $3 \times t_{1u}$, $3 \times t_{2g}$, and $2 \times e_g$ are arranged from high energy to low energy. The main-group of Z atoms generate $1 \times s$ orbital and $3 \times p$ orbitals which are distributed below the 15 hybridized d orbitals and totally occupied in ZrRhTiZ (Z = AI, Ga) compounds. The triple-degeneracy t_{1u} states are not occupied in the spin-down direction, and a band gap is formed between t_{1u} (non-bonding) and t_{2g} (bonding) orbitals in the spin-down channel of ZrRhTiZ (Z = Al, Ga) compounds. Similarly, from Table 1, it can be seen that the number of valence electrons is 20 per ZrRhTiZ (Z = Al, Ga) unit cell, and the calculated total magnetic moment is 2 μ_B , which follows the Slater-Pauling rule $M_t = Z_t - 18$ and is also consistent with the reported Zr-based SQH materials [4–7,16–18].



Figure 4. Calculated total density of states and partial density of states of ZrRhTiAl (a) and ZrRhTiGa (b).



Figure 5. Schematic diagram of possible d-d hybridization between the transition-metal elements Zr-4d, Rh-4d, and Ti-3d in the ZrRhTiZ (Z = Al, Ga) compounds. The main group of elements Z (Z = Al, Ga) are not taken into account because the sp-bands are located at deep energy levels and barely contribute to the gap formation.

Figure 6 displays total magnetic moment and atomic magnetic moments as a function of lattice constant for ZrRhTiAl and ZrRhTiGa compounds. It can be noted that the total magnetic moment is constant at $2\mu_B$ over the range of the lattice constant, from 6.09 (6.10) to 6.61 (6.75) Å for ZrRhTiAl (ZrRhTiGa) compounds. The atomic magnetic moment is appreciably increasing with the lattice constant values for the Rh and Ti atoms, whereas the atomic magnetic moment of Zr as well as Al/Ga was not found to change appreciably over the wide range of lattice constants. The constant total magnetic moment can be attributed to the antiparallel arrangement of the magnetic moments of Rh and Ti atoms. The main contributors to the magnetic moment are Zr and Ti atoms. The Rh and Z atoms only carry small magnetic moments antiparallelly aligned to those of the Zr and Ti atoms.

The half-metallicity is very much sensitive to the change of lattice constant. Therefore, it is very useful to acquire knowledge about the sensitivity of the half-metallicity to the uniform strain (US) for the ZrRhTiZ (Z = Al, Ga) compounds. Here, the CBM (conduction band minimum) and VBM in the spin-down channel at different lattice constants have been recorded to show the effects of the US on half-metallic behavior, as plotted in Figure 7. Obviously, the half-metallicity can be maintained in the lattice constant range of 6.09–6.61 Å for ZrRhTiAl and 6.10–6.75 Å for ZrRhTiGa. In addition, the effects of the US on the E_{bg} and E_{HM} are also shown in Figures 8 and 9 for the ZrRhTiZ (Z = Al, Ga) compounds, respectively. The obtained results revealed both E_{HM} and E_{bg} first increase and then decrease with the increasing lattice constant.



Figure 6. Cont.



Figure 6. Plots for total spin magnetic moment and atomic spin magnetic moment as a function of lattice constant for ZrRhTiAl (**a**) and ZrRhTiGa (**b**) compounds.



Figure 7. Conduction band minimum (CBM) and valence band maximum (VBM) in the spin-down channel as a function of lattice constant (US) for ZrRhTiAl (**a**) and ZrRhTiGa (**b**).



Figure 8. Band gaps as a function of the lattice constant (US) for ZrRhTiAl and ZrRhTiGa.



Figure 9. The half-metallic band-gap as a function of the lattice constant (US) for ZrRhTiAl and ZrRhTiGa.

The half-metallicity of most Heusler compounds will be influenced and even be broken by the tetragonal distortion (TD) of the lattice. To analyze the effect of TD on half-metallicity and magnetic moments, the unit-cell volume was fixed at the equilibrium bulk volume and then the c/a ratio changed. In Figures 10 and 11, the TD effects on the half-metallicity properties and magnetic moments are described by the magnetic moment and the CBM and VBM dependence on c/a ratio. It is clear that the total and atomic magnetic moments of ZrRhTiZ (Z = Al, Ga) are nearly unchanged, and the half-metallicity can be kept in the c/a ratio range of 0.96–1.06 for ZrRhTiAl and 0.92–1.12 for ZrRhTiGa, respectively. We further plotted the curves of E_{bg} and E_{HM} have a similar variation tendency and showed a rise-fall characteristic with increasing c/a ratio. The largest E_{bg} and E_{HM} occur in the cubic structure (c/a = 1) instead of tetragonal phase.



Figure 10. Total spin magnetic moment and atomic spin magnetic moment as a function of c/a ratio (TD) for ZrRhTiAl (**a**) and ZrRhTiGa (**b**).



Figure 11. CBM and VBM in the minority channel as a function of c/a ratio (TD) for ZrRhTiAl (**a**) and ZrRhTiGa (**b**).



Figure 12. Band gaps as functions of the c/a ratio (TD) for ZrRhTiAl and ZrRhTiGa.



Figure 13. The half-metallic band-gaps as functions of the c/a ratio (TD) for ZrRhTiAl and ZrRhTiGa.

Next, the elastic properties were investigated for ZrRhTiZ (Z = Al, Ga) compounds by calculating the single crystal elastic constants C_{ij} . Heusler compounds belong to a cubic structure which needs only three independent elastic constants (C_{11} , C_{12} , and C_{44}) for the complete description of their elastic properties.

The following expressions are used to depict the elastic behavior of a material given in Reference [19]:

$$B = \frac{C_{11} + 2C_{12}}{3} \tag{1}$$

$$G = \frac{G_R + G_V}{2} \tag{2}$$

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5} \tag{3}$$

$$G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})}$$
(4)

$$E = \frac{9GB}{3B+G} \tag{5}$$

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \tag{6}$$

where B, G, E, and A stands for bulk modulus, shear modulus, Young's modulus, and anisotropy factor, respectively. The estimated elastic constants and the mechanical properties for ZrRhTiAl and ZrRhTiGa are given in Table 3.

For cubic structures, the following criteria for the mechanical stability must be satisfied [20]:

$$C_{44} > 0$$
 (7)

$$\frac{(C_{11} - C_{12})}{2} > 0 \tag{8}$$

$$B > 0 \tag{9}$$

$$C_{12} < B < C_{11} \tag{10}$$

Therefore, from Table 3, one can easily see that ZrRhTiZ (Z = Al, Ga) compounds are mechanically stable. The calculated results of Young's modulus (E = 57.9 and 47.8 for ZrRhTiAl and ZrRhTiGa, respectively) indicate that ZrRhTiAl is stiffer than ZrRhTiGa. The Pugh's index (B/G) and Cauchy pressure ($C_{12} - C_{44}$) are usually used to characterize the brittleness or ductility of a compound [21–23]. For our materials, the Pugh's index (B/G) is 2.92 and 4.01, and the Cauchy pressures (C12 – C44) are 41.91 and 37.91 for the ZrRhTiAl and ZrRhTiGa compounds, respectively. Elastic anisotropy (A) is also a very important parameter for engineering applications. An A value of 1.0 shows the isotropic nature of the crystal, whereas values other than 1.0 indicate anisotropy. As shown in Table 3, for the ZrRhTiAl and ZrRhTiGa compounds, the value of A \neq 1, demonstrating that they are elastically anisotropic under ambient conditions.

Finally, we have computed the formation and cohesive energies for ZrRhTiZ (Z = Al, Ga) based on the following expressions [24–28]:

$$E_f = E_{ZrRhTiZ}^{total} - (E_{Zr}^{bulk} + E_{Rh}^{bulk} + E_{Ti}^{bulk} + E_Z^{bulk})$$
(11)

$$E_c = (E_{Zr}^{iso} + E_{Rh}^{iso} + E_{Ti}^{iso} + E_Z^{iso}) - E_{ZrRhTiZ}^{total}$$
(12)

The calculated E_c and E_f for ZrRhTiZ (Z = Al, Ga) compounds have been listed in Table 3. The E_c is larger than 20 eV, which indicates that ZrRhTiZ (Z = Al, Ga) compounds are stable due to energetic chemical bonding. The E_f is smaller than 0 eV, showing the compounds are stable against separation into the four pure elements.

Table 3. Calculated elastic constants C_{ij} , bulk modulus *B*, shear modulus *G*, Young's modulus *E* (GPa), Pugh's ratio *B*/*G*, anisotropy factor *A*, and formation and cohesive energies (eV) for the stoichiometric quaternary Heusler (SQH) compounds ZrRhTiAl and ZrRhTiGa.

SQH Compound	<i>C</i> ₁₁	<i>C</i> ₁₂	C ₄₄	В	G	Ε	B/G	Formation Energy	Cohesive Energy	Anisotropy Factor
ZrRhTiAl	157.060	116.435	74.521	129.977	44.441	57.920	2.925	-2.632	22.279	3.669
ZrRhTiGa	150.857	117.550	79.645	128.652	32.073	47.895	4.011	-2.738	21.384	2.981

4. Summary

In this paper, the electronic structures, magnetic structures and moments, elastic constants, formation energies, and cohesive energies are calculated for ZrRhTiZ (Z = Al, Ga) quaternary Heusler compounds. Based on the obtained results, we predicted that ZrRhTiZ (Z = Al, Ga) quaternary Heusler compounds are half-metallic materials. These two compounds are among the rare SQH compounds with half-metallicity that contain 4d transition metal elements. The investigations on the effects of US and TD show that the half-metallicity is robust to US and TD. The half-metallicity can be sustained over

a wide lattice constant range of 6.09 Å–6.61 Å for ZrRhTiAl and 6.03 Å–6.75 Å for ZrRhTiGa. Under TD, the range of c/a ratio maintaining the half-metallicity is 0.96–1.06 for ZrRhTiAl and 0.92–1.12 for ZrRhTiGa, respectively. The calculated elastic parameters are listed in this paper for ZrRhTiZ (Z = Al, Ga) compounds to help understand their mechanical properties.

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Conflicts of Interest: The authors declare no conflict of interest.

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