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Electronic And Mechanical Properties Of Zr_2TiAl: A First Principles Study

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Abstract. First principles study of electronic and mechanical properties of ternary phase Zr_2TiAl intermetallic compound has been carried out by using full potential linear augmented plane wave (FP-LAPW) method. Our calculated lattice parameter is in good agreement with the experiment. We find the magnetic phase of the compound to be stable with a magnetic moment of 1.95 μ_B. The major contribution to the total magnetic moment arises mainly from the Ti atom with the local magnetic moment of 1.22 μ_B. From the density of states plots we find the Ti-*d* and Zr-*d* to dominate at the Fermi level (E_F) with enhanced crystal field splitting and exchange splitting found in Ti. The mechanical stability of the compound is confirmed from the calculated elastic constants, and we find the compound to be ductile in nature from the calculated Pugh's ratio and Cauchy's pressure.

Keywords: Intermetallic, First-principle study, Electronic structure, Band structure, Mechanical properties.
PACS: 71.20.Lp, 63.20.dk, 71.20.Ps, 62.10.+s.

INTRODUCTION

Isoelectric intermetallic compounds Zr_3Al and Ti_3Al have high temperature applications with different structures[1]. By replacing the Zr and Ti atoms in these two compounds, a ternary Ti_2ZrAl and Zr_2TiAl phases can be obtained. Among these two compounds a lot of attention has been paid towards Ti_2ZrAl[2], whereas there is no study available for Zr_2TiAl. In the present study we focus on the details of electronic structure, magnetic and mechanical properties of Zr_2TiAl.

METHODOLOGY

All the calculations are carried out by using the FP-LAPW method as implemented in the WIEN2k code[3]. For the exchange correlation potential we have used PBE-GGA (Perdew-Burke-Ernzerhof parameterization of the Generalized Gradient Approximation) approximation. Throughout the calculation, the R_{MT} value for each atom was fixed as 2.39 *a.u* for Zr and 2.45 *a.u* for both Ti and Al atoms. For the energy convergence, the criterion $R_{MT}*K_{max}$ = 9 was used, where K_{max} is the plane wave cut-off. The potential and charge density were Fourier expanded up to G_{max} = 9. All the calculations are performed with 44x44x44 k-mesh which gives 2168 k-points in the irreducible part of the Brillioun zone (BZ). Birch–Murnaghan (BM) equation of states was used to fit the total energies as a function of primitive unit cell volume to obtain the bulk modulus and the equilibrium lattice parameter for the present compound.

RESULTS AND DISCUSSIONS

The ground state, electronic and mechanical properties are elaborated in this section.

Ground State Properties

The calculated lattice parameter agree well with the experiment[4] and the values are reported in Table 1, along with the available experimental data. From Fig.1, we confirm the magnetic phase of Zr_2TiAl to be stable with the energy difference of 6.8 *mRy/unit cell* between the magnetic and non-magnetic phase. The total magnetic moment is found to be 1.95 μ_B with maximum contribution from Ti around 1.22 μ_B. From the calculated band structure (BS) plots as shown in Fig.1 we find the *s* orbital to inert and position separately from the other bands in the lower energy region. Apart from this we can see one band to cross the E_F in both spin-up and spin-down channel

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indicating the metallic nature of the compound. We have also plotted the Fermi surface (FS) plots as shown in Fig.2 and are mainly of the mixture of hole and electron character which again is evident from the BS plots. We have also calculated the density of states

TABLE 1. Ground state properties of Zr_2TiAl.

Parameter	Present work	Exp[4].
Lattice parameter ($\AA$)	6.840	6.842
Volume $(\AA)^3$	80.003	80.073
Bulk modulus (GPa)	96.875	---
Mag. moment (μ_B)	1.95	---

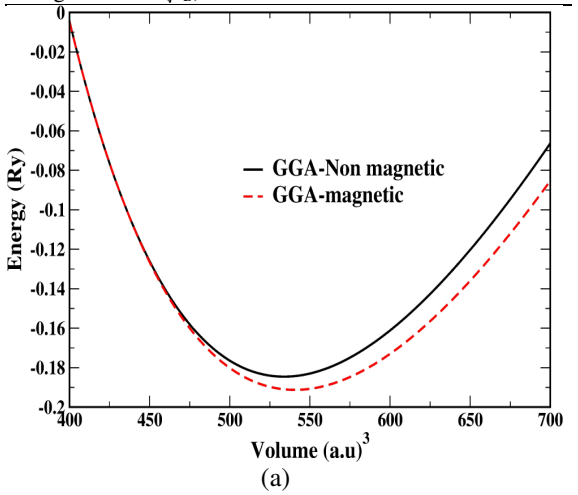

FIGURE 1. Energy optimization (a), band structure for spin-up (b) and spin-down (c).

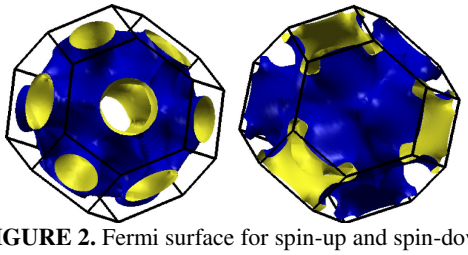

FIGURE 2. Fermi surface for spin-up and spin-down.

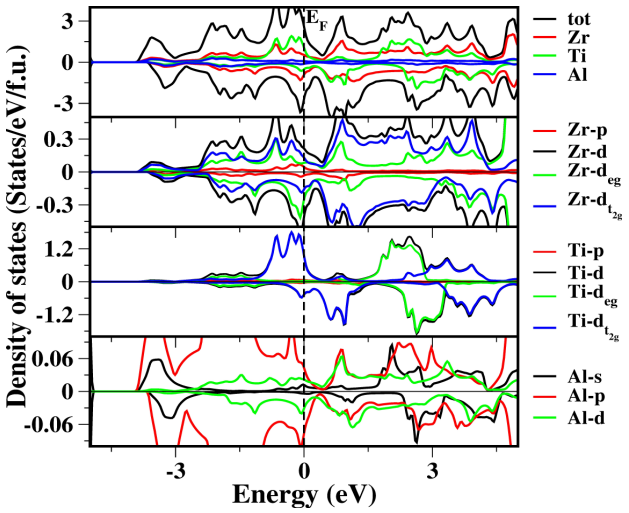

FIGURE 3. Density of states for Zr_2TiAl.

(DOS) and find Zr-*d* and Ti-*d* orbitals to dominate at E_F. From the projected DOS as shown in Fig.3, it is evident that the crystal field as well as the exchange splitting is more in Ti-*d* and well support the dominating nature of Ti atom towards the total magnetic moment. From the local magnetic moment we find the ferromagnetic interaction to exist between Zr-*d* and Ti-*d* orbital and is well evident from the partial DOS from Fig.3.

Mechanical Properties

In order to know the mechanical stability of the Zr_2TiAl we have also calculated the elastic constants (EC) and are given in Table 2. Zr_2TiAl compound crystalize in cubic structure and have three nonzero C_{11}, C_{12} and C_{44} elastic constants. These calculated EC satisfy the Born's criteria, and ultimately show the mechanical stability of Zr_2TiAl. The calculated bulk modulus from the EC is in good agreement with the value calculated from equation of states confirming the

TABLE 2. The calculated elastic constants and derived quantities for Zr_2TiAl in *GPa*

Parameter	Present work
C_{11}	109.006
C_{12}	90.782
C_{44}	58.129
B=Bulk modulus	96.875
E=Young's modulus	77.892
σ = Poisson's ratio	0.366
CP = Cauchy's Pressure	32.652
PR = Pugh ratio	0.294
A = Anisotropy factor	6.360
Θ_D = Debye temp. (K)	359.942

validity of the EC calculations. From the value of the Poisson's ratio[5], which is nearer to the upper limit of 0.5, indicate the stiffness of the compound[5]. The positive value of the Cauchy's pressure indicate the ductile nature of the present compound and again ductility is also confirmed from the Pugh ratio[5], which possess the value below the critical value 0.57 to satisfy the compound to be ductile.

CONCLUSIONS

We have investigated the electronic, magnetic and mechanical properties of the Zr_2TiAl. The obtained structural parameters are in good agreement with the experimental data. We have reported the magnetic nature of Zr_2TiAl for the first time with total magnetic moment to be around 1.95 μ_B. From the calculated elastic and the related mechanical properties we predict Zr_2TiAl to be ductile.

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