Pis'ma v ZhETF, vol. 122, iss. 6, pp. 365 – 367

Structural, electronic, magnetic, and elastic properties of quaternary ZrTM(TM = V, Cr, Mn)TiSi Heusler alloys: first-principles study

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Submitted 8 June 2025
Resubmitted 18 August 2025
Accepted 18 August 2025

First-principles calculations were used to explore the electronic,magnetic and elastic properties of ZrTM(TM = V, Cr, Mn)TiSi Heusler alloys. A detailed discussion is presented regarding the half-metallic and magnetic properties at their equilibrium lattice constants. The results showed that for all compounds ZrTM(TM = V, Cr, Mn)TiSi, the type Y1 is energetically more stable at the equilibrium volume. These compounds' band structures and density of states were examined, and the reason behind half-metallicity was explored. ZrVTiSi and ZrCrTiSi have a total magnetic moment of $1\,\mu_B$ and $0\,\mu_B$ per formula unit respectively, and it obeys the Slater–Pauling rule: $\mu_T = 18 - Z_T$ (μ_T is the total magnetic moment per unit cell and Z_T is the valence concentration). The computed elastic constants C_{11}, C_{12}, and C_{44} are all positive and follow the Born criteria, which confirmed that these Heusler compounds are mechanically stable.

DOI: 10.31857/S0370274X25090181, EDN: EEZFJI

The quest for advanced materials with tailored electronic and magnetic properties has intensified with the rapid development of spintronics – a technology that exploits not only the charge but also the spin degree of freedom of electrons [1–4]. Among the most promising candidates for spintronic applications are Heusler alloys, intermetallic compounds known for their unique half-metallic behavior, high spin polarization, and tunable magnetic properties [5, 6]. In this context, quaternary Heusler alloys (QHAs) have attracted significant attention due to their structural flexibility, compositional diversity, and potential for high Curie temperatures, making them ideal for next-generation spintronic and thermoelectric devices [7]. This study presents a comprehensive first-principles investigation into the structural, electronic, magnetic, and elastic properties of a new family of QHAs, ZrTM (TM = V, Cr, Mn) TiSi, using density functional theory (DFT) within the full-potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code [8–10].

The structural stability of ZrVTiSi, ZrCrTiSi, and ZrMnTiSi compounds was systematically evaluated by analyzing three possible atomic configurations – Y_1, Y_2, and Y_3 – based on different Wyckoff site occupancies in the cubic Y-type structure (space group # 216). The total energy versus volume curves, fitted using Murnaghan's equation of state [11], revealed that the Y_1 configuration is energetically the most favorable for all three compounds, indicating superior structural stability. The optimized lattice constants were found to be 6.38 Å, 6.32 Å, and 6.33 Å for ZrVTiSi, ZrCrTiSi, and ZrMnTiSi, respectively. A notable trend was observed: as the atomic number of the transition metal (TM) increases from V to Cr, the lattice constant decreases, which can be attributed to the decreasing atomic radius across the period. Concurrently, the bulk modulus increases, suggesting enhanced resistance to compression, with ZrCrTiSi exhibiting the highest value (149.30 GPa), reflecting its greater mechanical rigidity.

Electronic band structure calculations were performed using both the generalized gradient approximation (GGA) and the modified Becke–Johnson (mBJ) potential to accurately describe the exchange-correlation effects. The results revealed that ZrVTiSi and ZrCrTiSi exhibit half-metallic behavior at their equilibrium lattice constants. In these compounds, the majority-spin (spin-up) channel displays metallic character, while the minority-spin (spin-down) channel shows a semicon-

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ducting gap at the Fermi level, leading to 100 % spin polarization. This half-metallicity arises primarily from strong *d*-*d* hybridizations between the TM atoms (Zr, Ti, and TM), which create spin-polarized bands near the Fermi energy. In contrast, ZrMnTiSi was found to be metallic in both spin channels, lacking a band gap and thus not exhibiting half-metallic behavior. The total density of states (DOS) analysis further confirmed that the electronic states near the Fermi level are predominantly contributed by the 3*d* orbitals of the transition metals, while the Si atoms contribute mainly at lower energies, consistent with their role as a main-group element.

The magnetic properties of the compounds were analyzed in terms of total and atomic magnetic moments. ZrVTiSi was found to have a total magnetic moment of $1.00\,\mu_B$ per formula unit, while ZrCrTiSi exhibits zero net moment ($0.00\,\mu_B$). These values strictly obey the Slater–Pauling rule ($M_{\rm tot} = Z_{\rm tot} - 18$) [12, 13], where $Z_{\rm tot}$ is the total number of valence electrons (19 for ZrVTiSi and 18 for ZrCrTiSi). The magnetic moments are primarily localized on the TM atoms, with significant contributions also from Ti and Zr, whereas the Si atom and interstitial regions show negligible magnetism. The positive local moments on the TM atoms indicate ferromagnetic coupling in ZrVTiSi, while the non-integer moment of $0.76\,\mu_B$ in ZrMnTiSi confirms its non-half-metallic, likely ferrimagnetic or complex magnetic nature. The high spin polarization in ZrVTiSi and ZrCrTiSi makes them promising candidates for spin injectors and spin-filtering devices in spintronic circuits.

Mechanical stability was assessed through the calculation of elastic constants C_{11}, C_{12}, and C_{44}, which were found to be positive and satisfy the Born stability criteria for cubic crystals: $C_{11} > 0$, $C_{44} > 0$, $C_{11} - C_{12} > 0$, and $C_{11} + 2C_{12} > 0$ [14–17]. This confirms that all three compounds are mechanically stable. The elastic anisotropy factor ($A = 2C_{44}/(C_{11} - C_{12})$) deviates significantly from unity (ranging from 0.59 to 1.98), indicating pronounced elastic anisotropy, which may influence crack propagation and mechanical response under stress. Furthermore, the compounds were found to be ductile in nature, as evidenced by positive Cauchy pressure ($C_{12} - C_{44}$), Pugh's ratio (B/G) exceeding the critical value of 1.75, and Poisson's ratio (ν) greater than 0.26. These findings suggest good plasticity and resistance to brittle fracture, essential for practical device fabrication and durability [18–21].

In conclusion, this theoretical study provides the first detailed insight into the physical properties of the ZrTM (TM = V, Cr, Mn) TiSi QHAs. The Y_1 structure is identified as the most stable configuration, and ZrVTiSi and ZrCrTiSi are predicted to be half-metallic with high spin polarization, adhering to the Slater–Pauling rule. Their mechanical stability and ductile nature further enhance their suitability for spintronic applications. These results not only deepen the understanding of structure-property relationships in quaternary Heusler systems but also pave the way for future experimental synthesis and characterization of these materials. The findings serve as a valuable theoretical foundation for the design of novel spintronic materials with tailored functionalities.

Funding. We received no funding for this study.

Conflict of interest. The authors of this work declare that they have no conflicts of interest.

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