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Half-Metallic Ferromagnetism in the Ti_2CoGe Heusler Compound

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Using first-principles calculations based on density functional theory, we predict the half-metallic ferromagnetism of the Ti_2CoGe Heusler compound with the $CuHg_2Ti$-type structure. The electronic band structures and density of states of the Ti_2CoGe compound show that the spin-up electrons are metallic, but the spin-down bands are semiconducting with a gap of 0.61 eV, and the spin-flip gap is 0.58 eV. The Ti_2CoGe Heusler compound is half-metallic ferromagnetic with magnetic moment of $3\mu_B$ at the equilibrium lattice constant a = 6.11 Å, which agrees with the Slater–Pauling rule.

Key words: Magnetically ordered materials, electronic band structure, Heusler compounds, half-metallic ferromagnet

INTRODUCTION

Spintronics is a nascent form of electronics which utilizes the spin degree of freedom of electrons as well as their charge.[1] Half-metallic ferromagnetic materials, in which spin-up band is metallic while spin-down band is semiconducting with an energy gap at the Fermi level, are potential prototype materials of this concept. Half-metallic materials showing a peculiar 100% spin polarization at the Fermi level have attracted great attraction from scientific researchers due to their potential spintronic device applications such as nonvolatile magnetic random-access memories (MRAM) and magnetic sensors.[2,3] The concept of half-metallic ferromagnets was first introduced by de Groot et al.,[4] on the basis of band structure calculations in NiMnSb and PtMnSb semi-Heusler phases. So far, half-metallic properties have been observed in many materials, for example, Heusler compounds,[5–10] ferromagnetic metallic oxides,[11–13] dilute magnetic semiconductors,[14,15] and zincblende transition-metal pnictides and chalcogenides.[16–20]

The Heusler compounds represent a class of ternary intermetallic compounds with general formula X_2YZ, where X and Y are transition metals and Z is a main group element.[21] The X_2YZ Heusler compounds crystallize in the cubic $AlCu_2Mn$-type structure in space group $Fm\bar{3}m$. In this structure, X, Y, and Z atoms are placed at Wyckoff positions 8*c* (1/4,1/4,1/4), 4*a* (0,0,0), and 4*b* (1/2,1/2,1/2), respectively. If the number of 3d electrons of Y atom is more than that of X atom, $CuHg_2Ti$-type structure in space group $FF\bar{4}3m$ is observed. In this structure, X atoms occupy the nonequivalent 4*a* (0,0,0) and 4*c* (1/4,1/4,1/4) positions, while Y and Z atoms are located at 4*b* (1/2, 1/2,1/2) and 4*d* (3/4,3/4,3/4) positions, respectively.[7]

Although many Heusler compounds have been theoretically predicted to be half-metallic,[5–10,22–26] electronic structure calculations of Ti_2-based Heusler compounds have not been widely studied up to now. In the present paper, the electronic structure and magnetism of the Ti_2CoGe Heusler compound with $CuHg_2Ti$-type structure are studied by means of the self-consistent full potential linearized augmented plane wave (FPLAPW) method.

COMPUTATIONAL METHOD

Electronic structure calculations were performed using the self-consistent FPLAPW method[27] implemented in WIEN2K code[28] within density functional theory (DFT). The Perdew–Burke–Ernzerhof generalized gradient approximation (GGA)[29,30] was used for the exchange correlation correction. In this method the space is divided into nonoverlapping muffin-tin (MT) spheres separated by an interstitial region. The basis functions are expanded into spherical harmonic functions inside the MT sphere and Fourier series in the interstitial region. The MT

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sphere radii were 2.25 a.u. for Ti and Co, 2.1 a.u. for Ge. The convergence of the basis set was controlled by a cutoff parameter $R_{mt}K_{max} = 7$, where R_{mt} is the smallest of the MT sphere radii and K_{max} is the largest reciprocal lattice vector used in the plane wave expansion. The magnitude of the largest vector in the charge density Fourier expansion (G_{max}) was 12. The cutoff energy, which defines the separation of valence and core states, was chosen as −6 Ry. We select the charge convergence as 0.0001e during self-consistency cycles. In these calculations, we neglected the effect of spin–orbit coupling because it has little effect on results.[31] For the Brillouin zone (BZ) integration, the tetrahedron method[28] with 72 special k points in the irreducible wedge (2000 k points in the full BZ) was used to construct the charge density in each self-consistency step.

RESULTS AND DISCUSSION

The calculated total energy as a function of unit-cell volume for both magnetic and nonmagnetic configurations is plotted in Fig. 1 for the $CuHg_2Ti$-type structure. It can be seen that the magnetic phase has lower energy than the nonmagnetic phase. The calculated minimal total energy of the magnetic state is 0.36 eV lower than that of the nonmagnetic state at the equilibrium lattice constant. The energy difference between the magnetic and nonmagnetic states increases slightly with increasing lattice constant. The calculated total energies versus volume were fitted using the empirical Murnaghan's equation of state[32] to determine the ground-state properties. For Ti_2CoGe in the magnetic state of the $CuHg_2Ti$-type structure, the computed lattice parameter, bulk modulus and its first derivative are a = 6.11 Å, B = 147.079 GPa, and B' = 4.434, respectively. Up to now, an experimental or theoretical lattice constant value has not been reported.

Figure 2 presents the spin-polarized total densities of states (DOS) and atom-projected DOS of the Ti_2CoGe compound at its equilibrium lattice constant. The calculated total magnetic moment of the Ti_2CoGe compound is $3\mu_B$, while the atomic magnetic moments are $1.31\mu_B$ for Ti(1), $0.67\mu_B$ for Ti(2), $0.40\mu_B$ for Co, and zero μ_B for Ge. The magnetization of interstitial region, which is due to itinerant electrons, is $0.62\mu_B$. The calculated integer magnetic moment of the Ti_2CoGe compound, which indicates stability of half-metallic behavior, obeys the Slater–Pauling rule. The local magnetic moments of the titanium atoms are different from each other, indicating different atomic environments. It is clear that the majority-spin band is metallic, while the

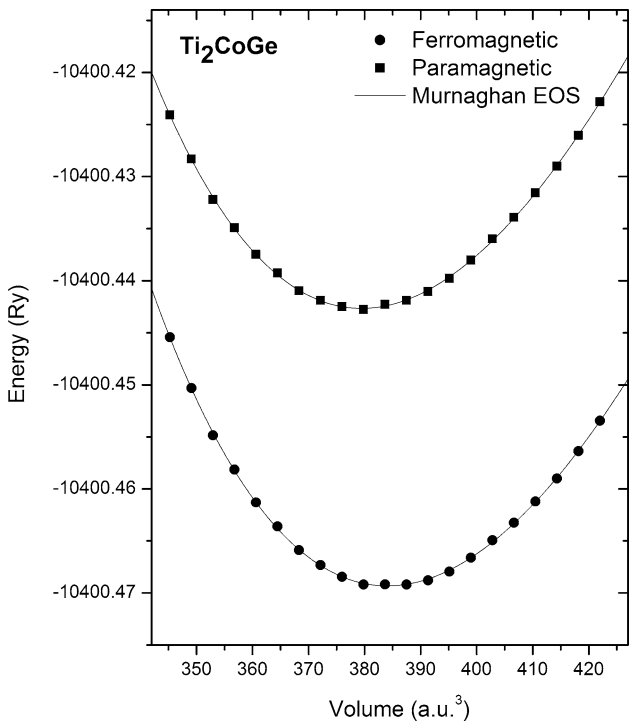

Fig. 1. Volume optimization for the Ti_2CoGe Heusler compound.

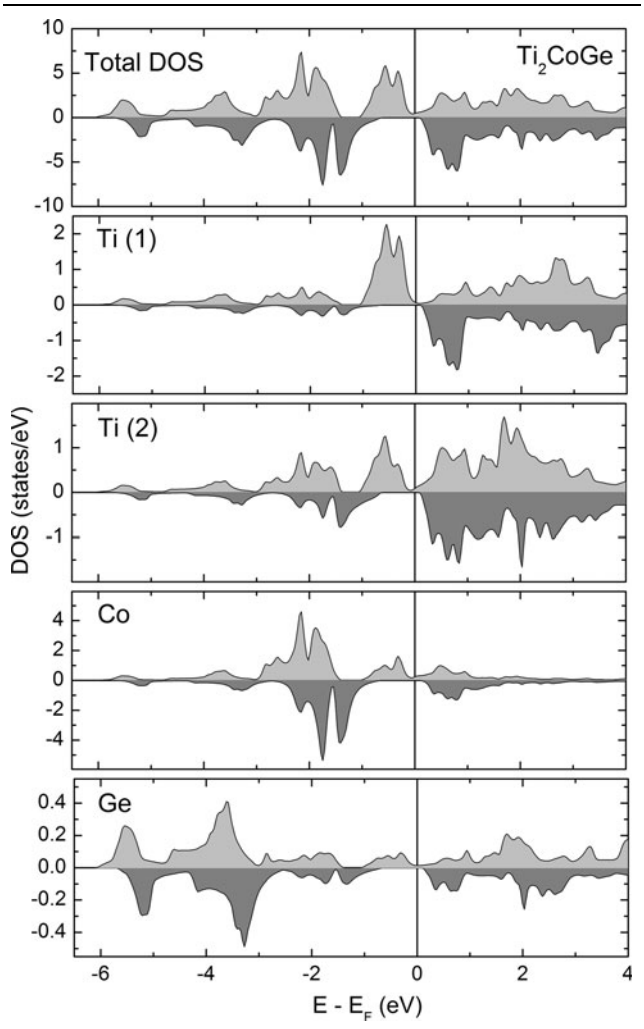

Fig. 2. The spin-polarized total DOS and atom-projected DOS.

minority-spin band shows a semiconducting gap around the Fermi level. In the minority-spin band, the valance band maximum is located at −0.58 eV and the conduction band minimum at 0.03 eV. The energy gap for spin-down electrons at around the Fermi level is 0.61 eV and close to the energy gap values for the Co_2TiAl and Co_2TiSn compounds.[33] This energy gap in the minority-spin band gap leads to 100% spin polarization at the Fermi level, resulting in the half-metallic behavior at equilibrium state. In the spin-down band, the total density of states around the Fermi level is predominantly due to Co d, Ti(1) d, and Ti(2) d electrons. The projected density of states of Co atom lies mainly below the Fermi level and makes the main contribution to the total DOS. The spin-down density of states of Ti(1) and Ti(2) atoms lies mainly above the Fermi level. The energy region between −6.0 eV and −2.5 eV consists mainly of p electrons of Ge atoms.

The band structures of the Ti_2CoGe compound for the spin-up and spin-down electrons are plotted in Fig. 3. It is obviously seen that the spin-up band structure has metallic intersections at the Fermi level, which is a sign of metallic nature. However, the spin-down band structure has an energy gap at the Fermi level. The width of the energy gap can be calculated using the energies of the highest occupied band at the Γ point and the lowest unoccupied band at the L point. The Fermi level lies 0.58 eV above the highest spin-down valance band. Therefore, the spin-flip gap, which is the minimum energy required to flip a minority-spin electron from the valance band maximum to the majority-spin Fermi level, is 0.58 eV. This nonzero spin-flip gap indicates that the Ti_2CoGe compound is a true half-metallic ferromagnet.

To investigate the dependence of the half-metallic state on the lattice constant, the calculations were performed for lattice parameters between 5.9 Å and 6.4 Å. It is clearly seen in Fig. 4 that the Ti_2CoGe Heusler compound has a band gap at the Fermi energy above lattice constant of 6.05 Å. Weak DOS values at the Fermi level observed for lattice constants smaller than 6.05 Å lead to loss of the half-metallic property. Therefore, the Ti_2CoGe Heusler compound is half-metallic for lattice parameters above 6.05 Å. The Fermi level moves to the valance band as the lattice constant expands.

Figure 5 presents the calculated total magnetic moment, the magnetic moments of the Ti(1), Ti(2), and Co atoms, and the spin polarization as a function of lattice constant. The calculated total magnetic moment is $3\mu_B$ within the whole lattice parameter

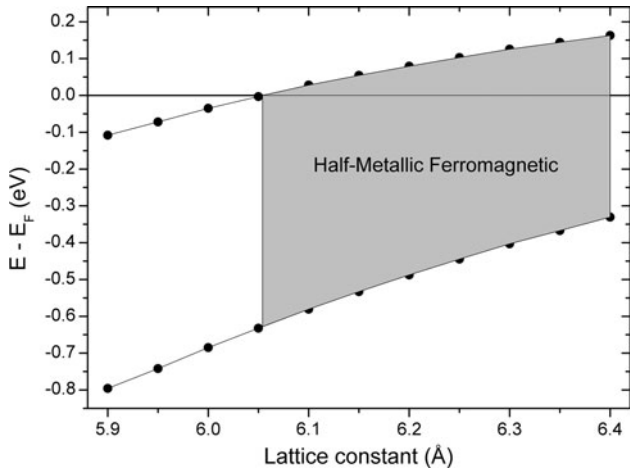

Fig. 4. Dependence of the half-metallic state on the lattice constant.

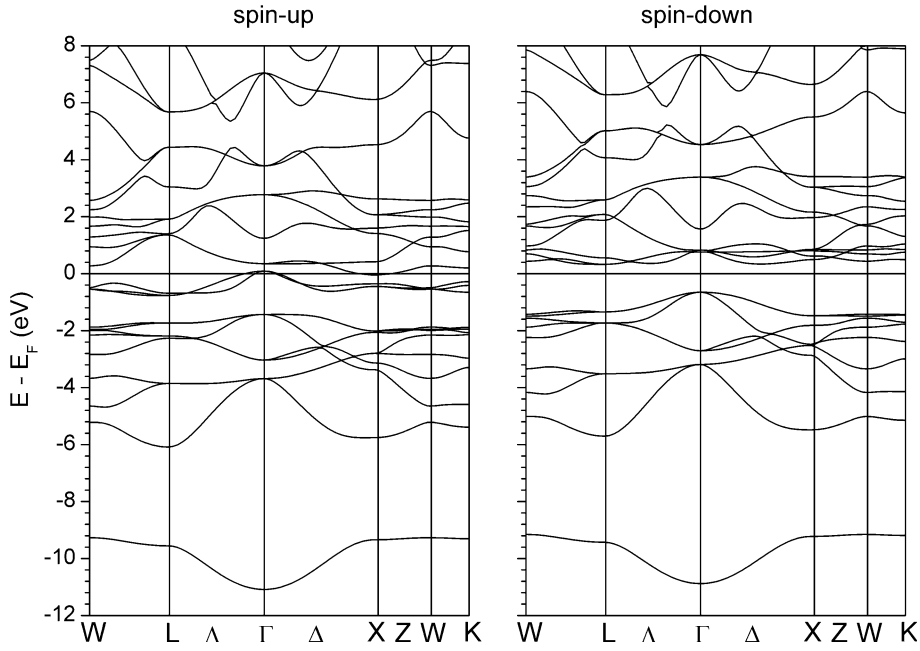

Fig. 3. Band structures of the Ti_2CoGe compound for the spin-up and spin-down electrons.

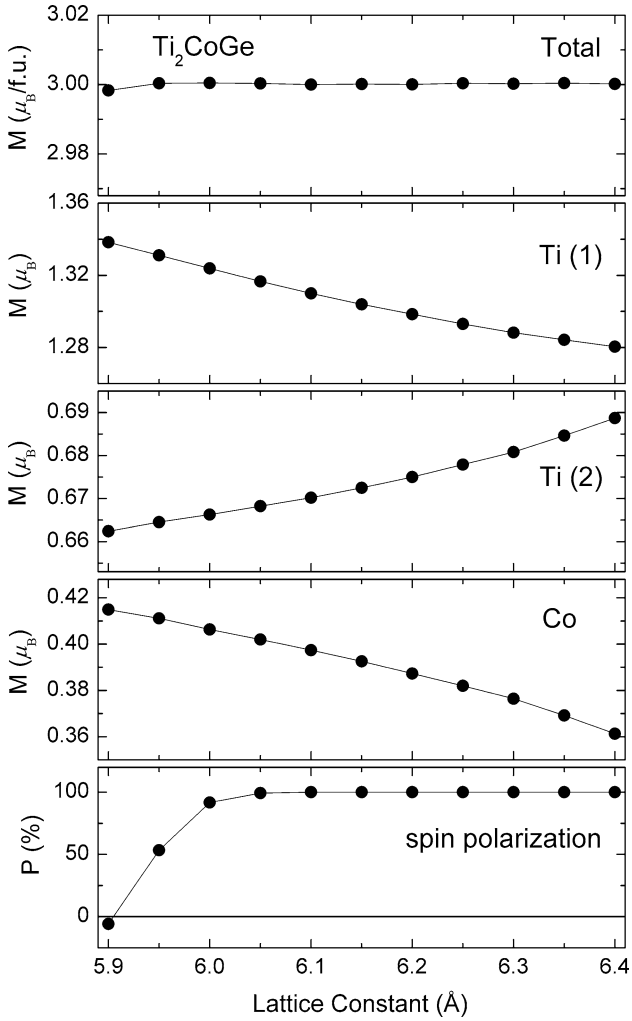

Fig. 5. The calculated total magnetic moment, the magnetic moments of the Ti(1), Ti(2), and Co atoms, and the spin polarization as a function of lattice constant.

range. The calculated magnetic moments of the Ti(1) and Co atoms decrease with increasing lattice constant, while the magnetic moment of the Ti(2) atom increases. The spin polarization ratio P is calculated as $(N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow)$, where $N_\uparrow$ and $N_\downarrow$ are the majority and minority DOS at the Fermi level, respectively. The ferromagnetic Ti_2CoGe Heusler compound maintains 100% polarization above lattice constant values of 6.05 Å. The negative spin polarization observed for a = 5.90 Å is due to the Ti 3d states which have a large density in the minority-spin channel at the Fermi energy.

CONCLUSIONS

For the Ti_2CoGe Heusler compound, the electronic structure and magnetic properties have been calculated using the first-principles FPLAPW method. The spin-polarized calculations showed that the Ti_2CoGe Heusler compound is a half-metallic ferromagnet with magnetic moment of $3\mu_B$ within the whole lattice constant range. Therefore, the Ti_2CoGe Heusler compound is a promising material for future spintronic applications.

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