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First-principles study of the half-metallic and magnetic properties for new yttrium-based full-Heusler alloys Y_2CrZ (Z = Al, Ga, In)

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ABSTRACT

First-principles calculations have been performed on the structural, electronic and magnetic properties of new yttrium-based full-Heusler alloys Y_2CrZ (Z = Al, Ga, In) in Hg_2CuTi structure. For three Y_2CrZ (Z = Al, Ga, In) alloys, the ferromagnetic states are the most favorable states among the possible magnetic configurations. At equilibrium lattice constants of 7.079, 6.979 and 7.212 Å, the Y_2CrZ (Z = Al, Ga, In) alloys are half-metallic ferromagnets with spin-up band gaps of 0.622, 0.652 and 0.489 eV, respectively. The formation energies and the cohesion energies indicate the stability of the Y_2CrZ (Z = Al, Ga, In) alloys. The much higher Curie temperatures T_C of 772.947, 842.512 and 966.184 K than room temperature show the Y_2CrZ (Z = Al, Ga, In) alloys are suitable for spintronics and magnetoelectronics applications. The origins of the spin-up band gaps are attributed to the d-d hybridization (especially) and covalent hybridization. The total magnetic moments of 3 μ_B/f.u. for these alloys satisfy the Slater-Pauling rule $M_t = 18-Z_t$. In addition, the HM characters are kept in the lattice constants range from 6.757 to 7.501 Å, 6.716 to 7.422 Å and 6.743 to 7.585 Å for Y_2CrZ (Z = Al, Ga, In) alloys, respectively.

1. Introduction

Potential candidates for spintronics applications, half-metallic (HM) magnetic compounds were intensively studied to understand their physical properties. Proposed by de Groot et al., in 1983 [1], the HM ferromagnets have been used nowadays for spintronics devices [2] which behave like semiconductor for one spin channel and like metal for the other spin channel, leading to a 100% spin polarization of electrons, at the Fermi level. Therefore, more and more HM ferromagnets with various structures have been predicted theoretically or confirmed experimentally in the past decades [3–7]. HM ferromagnets have been widely found in perovskite compounds, e.g., $BaCrO_3$ [8] and Sc_2FeMoO_6 [9], Heusler alloys, e.g., Sc_2CrZ (Z = C, Si, Ge, Sn) [10] and Cr_2MnZ (Z = P, As, Sb and Bi) [11], metallic oxides, e.g., CrO_2 [12] and Fe_3O_4 [13], dilute magnetic semiconductors (DMSs), e.g., Mn-doped GaN [13] and Cr-doped CdTe [2] and zincblende (ZB) transition-metal (TM) pnictides and chalcogenides [14–18]. Among these materials, HM Heusler alloys with high spin polarization, high Curie temperature T_C [19–21] and simultaneously a low saturation magnetization are very suitable for ultrahigh density magnetic memory storage devices [22]. So the HM Heusler alloys play a crucial role in practical applications.

The Heusler alloys can be divided into two main groups, that is, the ternary Heusler alloys and quaternary Heusler alloys. The ternary Heusler alloys have two families, half-Heusler alloys XYZ and full-Heusler alloys X_2YZ (X and Y are TM elements and Z is main group element) [23]. The full-Heusler alloys have two types of structures that are Cu_2MnAl structure (space group No. 225, $Fm\bar{3}m$) and Hg_2CuTi structure (space group No. 216, $F\bar{4}3m$). In the Cu_2MnAl structure, the X atoms occupy the Wyckoff positions A (0, 0, 0) and C (1/2, 1/2, 1/2), Y and Z atoms occupy the Wyckoff positions B (1/4, 1/4, 1/4) and D (3/4, 3/4, 3/4), respectively. While in the Hg_2CuTi structure, the X atoms occupy the A (0, 0, 0) and B (1/4, 1/4, 1/4) positions, Y and Z atoms occupy the C (1/2, 1/2, 1/2) and D (3/4, 3/4, 3/4) positions, respectively [10]. If the valence electron numbers of the Y element are more than those of the X element, the Hg_2CuTi structure will be formed, on the contrary, the Cu_2MnAl structure will be formed. From the valence electron configurations of the Y $4d^15s^2$ and Cr $3d^54s^1$, we know the Hg_2CuTi structure is preferred for the new yttrium-based full-Heusler alloys Y_2CrZ (Z = Al, Ga, In). The quaternary Heusler alloys have general formula XX′YZ which is formed by different TM elements X and X′.

In the last decades, many full-Heusler alloys have been widely investigated to be HM materials [24–35], however the Y_2-based full-Heusler alloys have not been investigated either experimentally or theoretically. Thus in this paper, the structural, electronic and magnetic properties of new Y_2-based full-Heusler alloys Y_2CrZ (Z = Al, Ga,

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In) in Hg_2CuTi structure have been investigated by first-principles calculations. Since the full-Heusler alloys Y_2CrZ (Z = Al, Ga, In) are never experimentally synthesized, this study may be helpful in preparing new full-Heusler systems usually by the arc furnace melting method. It should be pointed out that the melting point of Ga is about 29 °C and thus it is a liquid. Therefore, use of Ga in preparing full-Heusler alloy Y_2CrGa, we should control the contents of Ga to satisfy the stoichiometry. Up to now, many full-Heusler systems that are similar to our studied system have been predicted, for examples, Co_2MnZ (Z = Si, Ge, Al, Ga) [36] and Mn_2FeZ (Z = Al, Ga, Si, Ge, Sb) [37]. The paper is organized as follows. In Section 2, the calculation methods are described in detail. In Section 3, the calculation results and discussions are given. In Section 4, the calculation conclusions are summarized.

2. Calculation method

The calculations of the structural, electronic and magnetic properties of the full-Heusler alloys Y_2CrZ (Z = Al, Ga, In) in Hg_2CuTi structure are performed by using the Vienna ab-initio simulation package (VASP) [38] with the projector augmented-wave (PAW) potentials [39] based on the density functional theory (DFT). Considering the electronic correlations of the d electrons, we adopt the GGA + U method (U = 0 eV for Y atoms due to only one d electron, U = 1.8 eV for Cr atoms [40]) in the scheme of the Perdew-Burke-Ernzerhof (PBE) to represent the exchange-correlation interaction and generate the proper ground state structure of the alloys. The electronic self-consistency cycle calculations continue until the allowed error in total energy is less than 1×10^{-4} eV. The atoms relaxation will stop if Hellmann–Feynman forces are smaller than 0.02 eV/Å. The cutoff energy is chosen to be 400 eV. The Y $4d^15s^2$, Cr $3d^54s^1$, Al $3s^23p^1$, Ga $4s^24p^1$ and In $5s^25p^1$ electrons are treated as valence electrons. A $7 \times 7 \times 7$ Monkhorst-Pack grid for k-point sampling is adopted for Brillouin zone integration, together with a tetrahedron method with Blöchl corrections of 0.1 eV smearing broadening.

3. Results and discussions

3.1. Structural properties

According to the statements above, the Hg_2CuTi structure is preferred for the Y_2-based full-Heusler alloys Y_2CrZ (Z = Al, Ga, In). As shown in Fig. 1, two Y atoms occupy the Wyckoff positions A (0, 0, 0) and B (1/4, 1/4, 1/4), denoted as Y1 and Y2 in following, the Cr and Z (Z = Al, Ga, In) atoms occupy the Wyckoff positions C (1/2, 1/2, 1/2) and D (3/4, 3/4, 3/4), respectively.

In order to find the actual magnetic ground state and estimate the Curie temperatures T_C, as is shown in Fig. 2, the possible magnetic configurations of the ferromagnetic (FM), anti-ferromagnetic (AFM_1, AFM_2, AFM_3) and nonmagnetic (NM) have been considered for three magnetic sites Y1, Y2 and Cr in full-Heusler alloys Y_2CrZ (Z = Al, Ga, In) with Hg_2CuTi structure. The calculated total energy per formula unit as a function of the lattice constant is shown in Fig. 3 for the FM, AFM_1, AFM_2, AFM_3 and NM configurations. The determined equilibrium lattice constants a and total energies per formula unit E_{tot} are listed in Table 1. We can see that, for all three alloys, the total energies per formula unit E_{tot} of the FM states are the lowest as compared with the AFM_1, AFM_2, AFM_3 and NM states, showing the FM states are the stable magnetic ground states. The equilibrium lattice constants of the 7.079, 6.979 and 7.212 Å for the FM states of Y_2CrAl, Y_2CrGa and Y_2CrIn, respectively, are related to the atomic radii of Al (1.82 Å), Ga (1.81 Å) and In (2.00 Å). So following, we mainly discuss the electronic and magnetic properties of the Y_2CrZ (Z = Al, Ga, In) alloys in the FM states. To further study the formation and cohesion characters of the Y_2CrZ (Z = Al, Ga, In) alloys, the formation energy E_f is calculated according to the formula [41]

$$E_f = E_{tot} - (2E_Y^{bulk} + E_{Cr}^{bulk} + E_Z^{bulk}) \quad (1)$$

where E_{tot} is the total energy per formula unit, E_Y^{bulk}, E_{Cr}^{bulk} and E_Z^{bulk} are the energies per atom in bulks Y, Cr and Z (bulk Y with hexagonal closest packed structure, bulk Cr with body-centered cubic structure, bulk Al with face-centered cubic structure, bulk Ga with diamond cubic structure and bulk In with body-centered tetragonal structure), respectively. As listed in Table 1, the negative formation energies of −0.561, −0.453 and −0.436 eV for the Y_2CrZ (Z = Al, Ga, In), respectively, imply all three Y_2CrZ (Z = Al, Ga, In) alloys are thermodynamically stable and may be synthesized in experiment.

The cohesion energy E_{coh}, which can illustrate the strength of chemical bonds in compounds, is also calculated by the formula [42]

$$E_{coh} = 2E_Y^{atom} + E_{Cr}^{atom} + E_Z^{atom} - E_{tot} \quad (2)$$

where E_Y^{atom}, E_{Cr}^{atom} and E_Z^{atom} are the energies of the isolated Y, Cr and Z atoms, respectively. The large cohesion energies of 20.147, 19.428 and 19.112 eV for the Y_2CrZ (Z = Al, Ga, In), respectively, as listed in Table 1 as well, indicate all three Y_2CrZ (Z = Al, Ga, In) alloys are stable due to the strong chemical bonds. In summary, both the formation energy and the cohesive energy reflect the Y_2CrZ (Z = Al, Ga, In) alloys are easily formed and energetically stable.

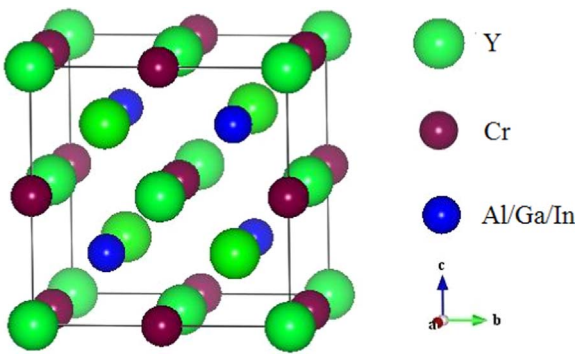

Fig. 1. The crystal structure of the full-Heusler alloys Y_2CrZ (Z = Al, Ga, In) in Hg_2CuTi structure. The Wyckoff positions are A (0, 0, 0), B (1/4, 1/4, 1/4), C (1/2, 1/2, 1/2) and D (3/4, 3/4, 3/4).

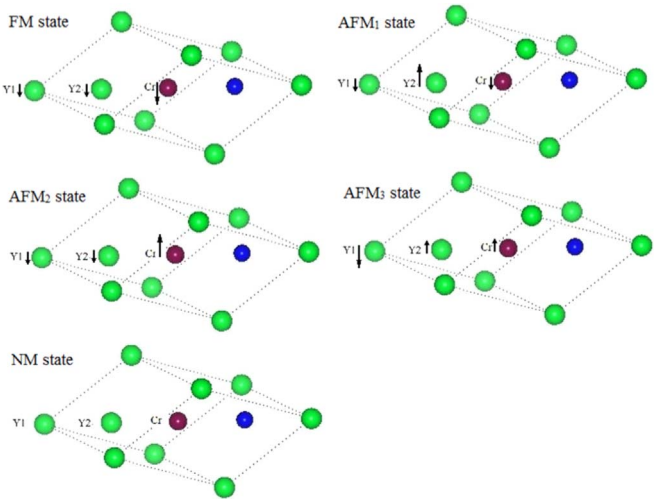

Fig. 2. The possible magnetic configurations: ferromagnetic (FM), anti-ferromagnetic (AFM_1, AFM_2, AFM_3) and nonmagnetic (NM) for three magnetic sites Y1, Y2 and Cr in full-Heusler alloys Y_2CrZ (Z = Al, Ga, In) with Hg_2CuTi structure. Arrows represent the direction of the spins.

3.2. Computation of Curie temperatures

Heusler alloys with high Curie temperatures T_C can be widely