Computational Materials Science 124 (2016) 311–315

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Topological phase transition in half-Heusler compounds HfIrX (X = As, Sb, Bi)

Guangtao Wang *, JunHong Wei

College of Physics and Information Engineering, Henan Normal University, Xinxiang, Henan 453007, People's Republic of China

ARTICLE INFO

Article history:
Received 22 May 2016
Received in revised form 27 July 2016
Accepted 7 August 2016
Available online 19 August 2016

Keywords:
Topological insulator
Weyl semi-metal
Half-Heusler

ABSTRACT

We studied the lattice constant and atoms substitution tunable topological phase transition in the half-Heusler compounds HfIrX (X = As, Sb, Bi). At the equilibrium cubic crystal structure and excluding SOC, HfIrAs and HfIrBi are topological nontrivial semimetal, while HfIrSb is a trivial topological insulator. This is because that the "internal pressure" lifts the s-type Γ_1 band above p-type Γ_5 bands in HfIrSb. When SOC is included, HfIrAs and HfIrSb become topological insulator, and normal band insulator, respectively, while HfIrBi is still a topological semimetal. When we induce compressive stress in the ab-plane of HfIrBi, it becomes a Weyl semimetal, with eight Weyl-Points (WPS) at ($\pm K_x$, 0, $\pm K_z$), (0, $\pm K_y$, $\pm K_z$), $K_x = K_y = 0.023$ Å^{-1}, $K_z = 0.108$ Å^{-1}.

According to the electronic structure, all bulk materials are divided into two classes: (1) metals, which have a finite electron density at the Fermi energy; (2) insulators, which show a finite band gap. Recently, two new classes of the so-called topological insulator and Weyl-semimetal have emerged in solid state physics. Topological insulator (TI) is a new class of materials, which have a full insulating gap in the bulk but contain topologically protected conducting states on edges or surfaces [1–6]. The surface states are chiral and inherently robust to external perturbations, which could be useful for future technological applications in spintronics and even quantum computing [8]. Since the first two-dimensional (2D) TI with quantum spin-Hall effect was predicted and realized in HgTe [3,9,10], many three-dimensional (3D) TIs have been proposed theoretically [11] and observed in experiments [12,13]. On the way to searching new TI materials, researchers find that many ternary half Hustler compounds are close to the border between the trivial and nontrivial topological insulators and will be the platform for topologically related materials [2–5,7]. Such material can be easily transformed from a trivial insulator to a nontrivial topological insulator and vice versa by a small variation of the lattice constant [5].

After the discovery of TI, a new type of topologically related materials are proposed in solid physics: Weyl semimetals [14–28], which are three-dimensional crystalline systems where pairs of bands touch at points in momentum space, termed Weyl points, characterized by a definite topological charge: the chirality. Weyl fermions were originally considered in massless quantum electrodynamics, but have not been observed until two groups [14–17,24] independently and simultaneously found the Fermi arcs on the (001) surface of TaAs single crystal [14,16]. Weyl semimetal has a band structure with double degenerated crossing bands at the Fermi level. Such crossing points are the Weyl points, where exists a linear dispersion relation in all three momentum space directions moving away from the Weyl point. The negative magnetoresistance in TaAS [16], anomalous Hall effect [25], and non-local transport properties have been attributed to the existence of Weyl points [26]. Fermi arc states on the surface are predicted to show novel quantum oscillations [27] in magneto-transport [21,28]. Because of the fundamental and practical interest in Weyl semimetals, it is crucial that robust candidate materials should be hunted and identified.

It is theoretically known that Weyl fermions only exist in the crystal where time-reversal symmetry or inversion symmetry is broken. The first way to break the time-reversal symmetry is to induce magnetism into the compounds. But the best way to generate Weyl fermions is by breaking the spatial inversion symmetry, because of two reasons: (1) Nonmagnetic Welt semimetals are more easily studied by angle-resolved photoemission spectroscopy, since alignment of magnetic domains is no longer needed. (2) Magnetic related bands structure change can be ignored when measure the Berry curvature caused unusual transport properties. Because of these reasons, half-Heusler compounds may be the good platform to seek for new classes Weyl semimetals [29–33]. The crystal lattice of ternary half-Heusler compounds is described by the space group $F\bar{4}3m$, where Hf atom and Ir are

* Corresponding author.
E-mail address: wangtao@henannu.edu.cn (G. Wang).

http://dx.doi.org/10.1016/j.commatsci.2016.08.005
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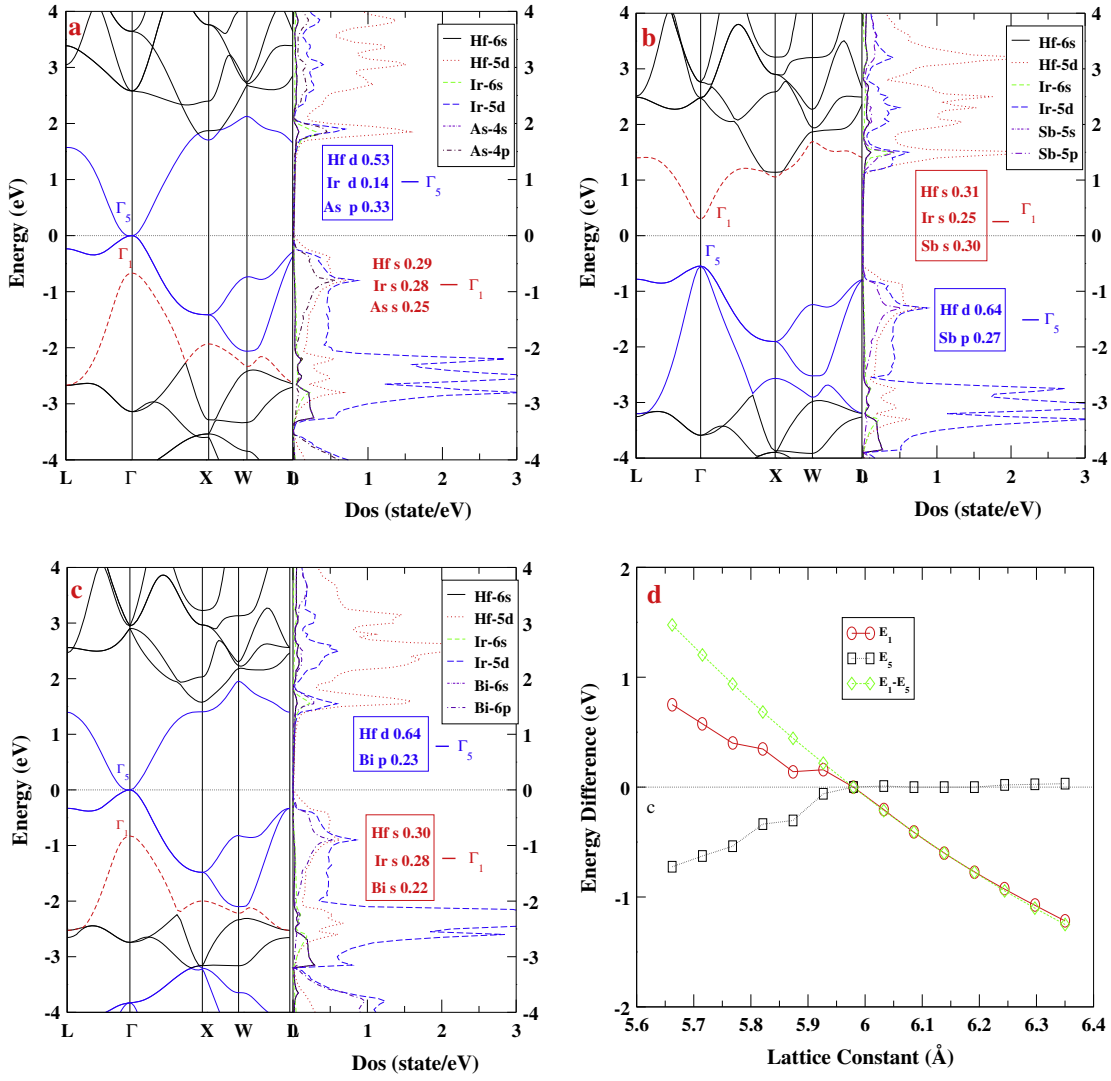

Fig. 1. Without spin-orbital coupling, the band structure and projected density of state of (a) HfIrAs, (b) HfIrSb, and (c) HfIrBi. (d) The band gap between Γ_1 and of Γ_5 changes with lattice constant of HfIrAs.

mutually tetrahedrally coordinated nearest neighbours. The Ir (4b) and As (4a) atoms form a zinc-blende-type sublattice, with Hf atoms filling in the remaining face-centered-cubic sites (4c). The number of valence electrons in the half-Heusler compounds HfIrX (X = As, Sb, Bi) is 18, with close shells as $s^2p^6d^{10}$, leading to a semiconducting or semimetal state.

Previous studies show that the alteration of the topological order by band inversion is a key ingredient of nontrivially topological material. Both spin-orbit coupling and lattice distortions are found to be essential for such band inversion [35,36]. So we studied the nontrivially topological properties of HfIrX (X = As, Sb, Bi), varying with lattice distortions and atoms substitution.

The calculations were done with the STATE [37] code, in the ultra-soft pseudopotential plane wave method. The spin-orbit coupling (SOC) effect is self-consistently included. All the equilibrium lattice constant and the atomic positions were relaxed by with generalized gradient approximation [38] calculation, with the force tolerance of 10^{-5} Ry/Bohr. The equilibrium lattice constants of HfIrAs, HfIrSb, HfIrBi are 6.16, 6.34, and 6.49 Å, respectively, in agreement with the results of Gautier's [42]. After carefully checking the convergence of calculated results with respect to the cutoff energy and the number of k-points, we adopted a cutoff energy of 500 eV and Monkhorst-Pack k-points generated with $16 \times 16 \times 16$.

In order to study how the topological phase changes with substituting Sb atoms by As atoms, we used the virtual-crystal approximation (VCA) established by Bellaiche and Vanderbilt [39]. The berry curvatures were calculated by the maximally localized Wannier functions [34,40].

We first present the band structure and projected density of state of HfIrAs, HfIrSb, and HfIrBi without spin-orbit coupling in Fig. 1(a–c). Without SOC, the bands around the Fermi level consist of the s-type singlet Γ_1 band and p-type triplet Γ_5 bands at Γ-point. For both HfIrAs and HfIrBi, the Γ_1 band is below Γ_5, but it is reverse for HfIrSb. It was called "band inversion" [32,34], If s-typed Γ_1 band is below p-typed Γ_5 bands. This means that, even without SOC, band inversion takes place in the HfIrAs and HfIrBi compounds. In Fig. 1a–c, the bands of Γ_5 are mainly derived from p-d hybridized states, while the Γ_1 band is mainly derived from the s states of Hf, Ir, and As (Sb, Bi) atoms. From HfIrAs to HfIrSb the atomic radius (at 4a) increase about 13% (from 1.21 Å of As to 1.41 Å of Sb), but the lattice constants only increase 3% (from 6.16 Å of HfIrAs to 6.34 Å of HfIrSb). So HfIrSb can be regarded as "compressed" HfIrAs, because their valance electrons are equal as $s^2p^6d^{10}$. When HfIrAs is compressed by the external pressure, both energies of Γ_1 and Γ_5 bands will increased. But the energy of Γ_1 band will increase fast than that of Γ_5, because that the orbital