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Three dimensional topological insulators of LuPdBi$_x$Sb$_{1-x}$ alloys

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ABSTRACT

The topological band structures of LuPdBi$_x$Sb$_{1-x}$ (for $x = 0$, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875, 1) alloys have been investigated using density functional theory by Wien2k package. The generalized gradient approximation (GGA) and Engel–Vosko generalized gradient approximation (GGA_EV) have been used to obtain accurate the band inversion strength and band order. The calculated results show that LuPdBi$_x$Sb$_{1-x}$ alloys for $x \geqslant 0.25$ in GGA and $x \geqslant 0.375$ in GGA_EV are candidates for three dimensional topological insulator or topological metal. Furthermore the effect of hydrostatic pressure on band inversion strength and band order of these alloys has been investigated.

1. Introduction

The phases of the general compositions XYZ, where X and Y stands for d- or f-electron transition metals and Z denotes a p-electron element, attract much attention due to their magnetic and electrical transport properties and their application [1–5]. The XYZ can be regarded as a hybrid compound of XZ with rouksalt structure, XY and YZ with the zinc blende structure [6]. These materials are best known for their thermoelectric properties and have been a regained interest in the study of half Heusler alloys. Especially, LuPdBi and LuPdSb have received a lot of interest because of their application. These compounds have MgAgAs structure type (by space group $F\bar{4}3m$) at normal conditions. Feng et al. [7] and Al-Sawai et al. [8] studied the band order of LuPdBi and LuPdSb using density functional theory within local density approximation (LDA) and modified Becke Johson exchange potential with generalized gradient approximation (MBJGGA) at zero pressure. They concluded that the LuPdBi is topological insulator candidate and LuPdSb is ordinary insulator.

The search for topological insulators in the fields of condensed matter physics and materials science has intensified due to their scientific importance as representing a novel quantum state and their applications in spintronics and quantum computing. Topological insulators are materials exhibiting a novel quantum state of matter involving conducting states on edges or surfaces. There are several ways to determine the band topology of an insulator. One can count the number of band inversions within the entire Brillouin zone. An odd number of band inversions within the Brillouin zone indicate that the material may be three-dimensional topological insulators. This method depends on an accurate interpretation of the band structure calculations and is better suited for crystals with a high symmetry lattice.

In this paper the band inversion strength and band order of LuPdBi$_x$Sb$_{1-x}$ alloys for different values of x ($x = 0$, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875 and 1) are studied. The first goal of this paper is compare and investigate the band order of LuPdBi$_x$Sb$_{1-x}$ alloys within the GGA using the scheme of Perdew–Burke–Ernzerhof [9] and Engel Vosko generalize gradient approximation [10] (GGA_EV). Since the band order of LuPdBi ($x = 1$) and LuPdSb ($x = 0$) compounds at zero pressure have already been reported [7,8], then the calculated results (for $x = 0$, 1) are compared with previous calculation. This study focuses on band order of those alloys (with $x = 0.125$, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875) that has not been touched by others. The x values are varied from 0 to 1 to finding the topological phase transition. The second goal of this paper is to investigate the effect of pressure on the band inversion strength and band order of LuPdBi$_x$Sb$_{1-x}$ alloys within GGA and GGA_EV approaches.

The paper is organized as follows: Briefly summarized calculation method is presented in Section 2, following the results and discussion in Section 3. Conclusions are drawn in the last section.

2. Calculation method

The density functional theory (DFT) is one of the theoretical methods to study the physical properties of solids. The calculated results in this paper were obtained using the DFT with full potential linearized augmented plane wave plus local orbital method as implemented in the Wien2k code [11]. The exchange correlation poten-

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tial was treated using GGA and GGA_EV approaches. The GGA_EV approach is based on potential optimized that has been developed for calculation of the energy band structure but not for computations of structural parameters. In augmented plane wave method, the charge density, the electronic wave function and the crystal potential are expanded in spherical harmonics inside the non-overlapping spheres centered at each nuclear position (so-called the muffin-tin spheres), and in plane waves in the rest of the space (the interstitial region). The parameters used in these calculations were chosen as follows:

The radii of the muffin-tin spheres were chosen as $R_{\mathrm{Lu}} = 2.4$ a.u. and $R_{\mathrm{Pd,Bi,Sb}} = 2.3$ a.u. These are the optimized values producing stability in the total energy calculation. A set of 160 k-point in the irreducible wedge of the Brillouin zone was used for reliable Brillouin zone integration. A cutoff for expanding the Kohn–Sham wave functions in terms of lattice harmonics inside the muffin-tin sphere was confined to $l_{\max} = 11$. The maximum size of reciprocal lattice vectors as a cut off for expanding the wave functions in the interstitial region in terms of plane waves were confined to $K_{\max} = \frac{8}{R_{MT}}\,(\mathrm{a.u.})^{-1}$ where R_{MT} represents the smallest muffin-tin radius in the unit cell. The charge density and potential were Fourier expanded up to $G_{\max} = 13\,(\mathrm{Ry})^{1/2}$. The number of k-points, $G_{\max}$, $R_{\mathrm{MT}}K_{\max}$, and $l_{\max}$ were obtained through converged the total energy calculation.

The calculated results for the valence electrons were treated in both scalar and fully relativistic fashions, while the core electrons were performed fully relativistically. Spin–orbit coupling for the valence electrons was included by a second-variational treatment [12].

3. Results and discussions

3.1. The band order of LuPdBi$_x$Sb$_{1-x}$ alloys at zero pressure

The LuPdBi$_x$Sb$_{1-x}$ alloys are modeled at some selected compositions of $x = 0$, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875 and 1 with order structures are described in terms of periodically repeated supercell ($2 \times 2 \times 2$) constructed. The structures of LuPdBi$_x$Sb$_{1-x}$ alloys are obtained with replacing the Bi atoms with Sb to get the alloy with 12.5%, 25%, 37.5%, 50%, 62.5%, 75%, 87.5% and 100% concentration. The atomic positions of LuPdBi$_x$Sb$_{1-x}$ alloys are relaxed. The force on each atom after relaxation decreased to less than 1.0 m Ry/a.u. The formation energy per formula unit of these alloys is defined as

$$E_{formation} = E(\mathrm{LuPdBi}_x\mathrm{Sb}_{1-x}) - xE(\mathrm{LuPdBi}) - (1-x)E(\mathrm{LuPdSb}),$$

where $E(\mathrm{LuPdBi}_x\mathrm{Sb}_{1-x})$, $E(\mathrm{LuPdBi})$ and $E(\mathrm{LuPdSb})$ are energy per formula unit of LuPdBi$_x$Sb$_{1-x}$, LuPdBi and LuPdSb compounds, respectively. Using above definition, the formation energy of LuPdBi$_x$Sb$_{1-x}$ (for $x = 0$, 0.125, 0.25. 0.375, 0.5, 0.625, 0.75, 0.875, 1) alloys is calculated. The calculated results show that the formation energy of these alloys is negative for all concentrations. This means that these alloys are thermodynamically stable.

To investigate the band order of LuPdBi$_x$Sb$_{1-x}$ for different value of x, the band structures of LuPdBi$_x$Sb$_{1-x}$ alloys within GGA and GGA_EV approaches in the presence of spin orbit coupling are calculated. In these band structure calculations, the lattice constants are obtained by total energy minimization within GGA approach. The calculated band structure within GGA and GGA_EV are given in Figs. 1 and 2, respectively. The results show that the band splitting within GGA is smaller than the corresponding value in GGA_EV and decreases going from 0 to 1. The general features of the band structures of these alloys are similar, with small differences in detail such as band order. The energy bands of these alloys at the Γ point near the Fermi energy split into s-like level Γ_6 with twofold degenerate, p-like level Γ_7 with twofold degenerate $j = \frac{1}{2}$ and p-like level Γ_8 with fourfold degenerate $j = \frac{3}{2}$ states due to the spin–orbit interaction. The band order of LuPdBi ($x = 1$) and LuPdSb ($x = 0$) are from high to low energy Γ_8 Γ_6, Γ_7 and Γ_6 Γ_8, Γ_7 respectively. From the viewpoint of band topology, the main difference between these two compounds is that LuPdSb possesses a normal band order, i.e., the *s*-like Γ_6 state sits above the *p*-like Γ_8 state, while LuPdBi possesses an inverted band order in which the Γ_6 state is occupied and located below the Γ_8 state. This trend in band order of LuPdBi and LuPdSb compounds is in agreement with previous study [7,8].

The topological of electronic band structures can be characterized by band inversion between Γ_6 and Γ_8 energy levels at the Γ symmetry point in the Brillouin zone. During this process a band crossing between conduction and valence bands should occur. In compound with cubic symmetry, one can define the band inversion strength, Δ, as the energy difference between the Γ_6 and Γ_8 states, i.e.,

$$\Delta = E_{\Gamma_6} - E_{\Gamma_8}$$

A negative Δ typically indicates that the materials are in a topological nontrivial semimetal, insulators or metals phases, while those with a positive Δ are in a topologically trivial phase.

The band inversion strength of LuPdBi$_x$Sb$_{1-x}$ alloys within GGA and GGA_EV approaches for different value of x is calculated. The results show that the topological phase of LuPdBi$_x$Sb$_{1-x}$ is sensitive to x. The calculated results are plotted as a function of x in Fig. 3. The calculated band inversion strength is fitted to second order polynomials:

$$\Delta^{\mathrm{GGA}} = 0.28 - 1.61x + 0.26x^2$$

$$\Delta^{\mathrm{GGA\_EV}} = 0.57 - 1.71x + 0.27x^2$$

The physical origins of this non linear behavior of band inversion strength can be treated as three different contributions: The first contribution represents the band structure response to the hydrostatic pressure, which arises from the change of their individual equilibrium volume to the alloy volume. The second reflects a charge transfer effect, which is due to the different bonding behavior of alloy. The final contribution arises in passing from the unrelaxed to the relaxed alloy.

The calculated band inversion strength of these alloys shows that:

(i) The calculated band inversion strength within both GGA and GGA_EV decreases going from $x = 0$ to $x = 1$. The GGA results yield a smaller value of the band inversion strength Δ when compared with the GGA_EV results. In particular, if GGA calculation predicts a small negative Δ such as LuPdBi$_{0.25}$Sb$_{0.75}$, it may become positive when using GGA_EV potential. This suggests that when predicting topological phases, one need to have a good band structure calculation and must be careful with the type of exchange correlation potentials.

(ii) From the view point of band topology of these alloys for different value of x, the main difference between these alloys is that these alloys with $x \geqslant 0.25$ in GGA_EV and $x \geqslant 0.125$ in GGA possess a normal band order, while these alloys with $x \geqslant 0.375$ in GGA_EV and $x \geqslant 0.25$ in GGA possess an inverted band order in which the Γ_6 state is occupied and located below the Γ_8 state. These are candidates for topological insulators or topological metal. The band structures of these alloys for $0.75 \geqslant x \geqslant 0.375$ within GGA_EV and $0.5 \geqslant x \geqslant 0.25$ within GGA are insulator with zero band gap. These alloys are candidates for topological insulators. The band structure of these alloys for $x \geqslant 0.825$ within GGA_EV and $x \geqslant 0.625$ within GGA possesses the nontrivial metallic band structures. So, these alloys are candidates for topological metal. To the best of my knowledge, there are no experimental or theoretical results for band order of these alloys (with $x = 0.125$, 0.25. 0.375, 0.5, 0.625, 0.75, 0.875) to compare with. These results may be use as a references for future investigation.