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Electronic and structural properties of Sr_2YSbO_6

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Abstract

The electronic and structural properties of the cubic perovskite Sr_2YSbO_6 were predicted from *ab initio* calculations. Such properties were obtained using the density functional theory (DFT). The full-potential (linearized) augmented plane-wave ((L)APW) method was used, as it is implemented in wien2k code. We have optimized the volume of the unitary cell and the internal x parameter. The lattice constant (a) and x determine some length bonds. We have found that $a = 8.405$ Å, $x = 0.26177$, and the bond lengths Y–O and Sb–O are 2.20 and 2.00 Å, respectively. Additionally, Sr_2YSbO_6 was prepared experimentally by the solid-state reaction method using stoichiometric mixtures of high purity (99.99%). By means of X-ray and Rietveld analysis, the main structural features were determined. The experimental lattice parameter is $a = 8.249$ Å, which differs about 1.9% of the value obtained using DFT. The bulk modulus is ~133 GPa, which is not measured experimentally. DFT predicts that Sr_2YSbO_6 is an indirect semiconductor and magnetic behavior does not have to be expected because at Fermi level the dominant orbitals are p-oxygen. The gap of the material is at least 2.5 eV.

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Keywords: DFT band structure; Density of states; Rietveld analysis; Electronic and structural properties

1. Introduction

In the last few years, complex perovskite material with $A_2BB'O_6$ formula have been extensively investigated because of their interesting electric and magnetic properties, which suggest the possibility of applications in the new spintronic technology. We have reported the Sr_2YSbO_6 material as a potential compound for substrate in the deposition of $YBa_2Cu_3O_{7-\delta}$ superconductor films, due to its favorable characteristics [1,2]: chemical stability of Sr_2YSbO_6 with $YBa_2Cu_3O_{7-\delta}$; good lattice matching and no degradation of superconductor transition temperature of $YBa_2Cu_3O_{7-\delta}$ due to interaction with Sr_2YSbO_6.

In this paper we have carried out theoretical calculations in order to predict the main electronic and structural properties of Sr_2YSbO_6. We use the wien2k [3], which is a program based on density functional theory (DFT) [4,5] and that allows to perform electronic structure calculations of crystalline solids. The wien2k works with the full-potential (linearized) augmented plane-wave ((L)APW) + local orbitals (lo) method, which is the most accurate for band structure calculations. The exchange correlation potential can be treated using several approximations in the framework of local density approximation (LDA) and the generalized gradient approximation (GGA). Additionally, this program includes all-electron scheme with relativistic effects. As a consequence of our calculations, we predict that the Sr_2YSbO_6 must be an insulator.

On the other hand, structural features were studied on polycrystalline samples of Sr_2YSbO_6 synthesized by solid-state reaction method. This study was carried through Rietveld analysis on X-ray diffraction (XRD) pattern of Sr_2YSbO_6. From the experimental results, we can conclude that it crystallizes in the face-centered cubic (FCC) structure (space group #225).

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2. Calculation method

Calculations were performed using DFT, with the wien2k [3] code and exchange correlation potential was included by means of the GGA [6]. From Rietveld analysis we found that this material crystallizes in the cubic structure, space group $Fm\bar{3}m$ (#225). Fig. 1. shows the structure used for calculations. The bond between the O- and Y-atom (localized at origin) is xa, where a is the lattice constant. We observe that each atom of Y or Sb is at octahedral site formed by six oxygen, but the Sr-atom is surrounded by 12 O-atoms. The covalent and atomic radius are shown in Table 1. As we see in Fig. 1, the nearest neighbors of O-atoms are Y-atoms or Sb-atoms. From the table, we observe that the covalent radius of Sb is smaller than the one of the Ytrium. Therefore, oxygen will have to be located more nearer to the Sb and to have a bond length O–Sb smaller than the bond length O–Y.

The muffin-tin radius (RMT) used, in Å, were 1.08, 1.32, 1.14 and 0.82 for Y, Sr, Sb and O, respectively. $RMT * Kmax = 7.0$, which implies that the energy plane wave cut-off is about 277 eV or 20 Ry. We used 56 k-points over the irreducible Brillouin zone (BZ) and the maximum angular momentum inside the muffin-tin sphere is $l = 10$.

By searching the energy minimum, we optimized the unitary cell volume and x parameter. From volume the lattice parameter (a) is easily found. The procedure for volume and x optimizations was carried out in the following cyclical way: initially, we set $x = 0.25$ and the volume was optimized. After that, x was optimized with constant volume and all the processes are repeated. Energy minimum converges and the process is stopped when the difference between the energies of two successive steps is smaller or equal than 5×10^{-4} eV.

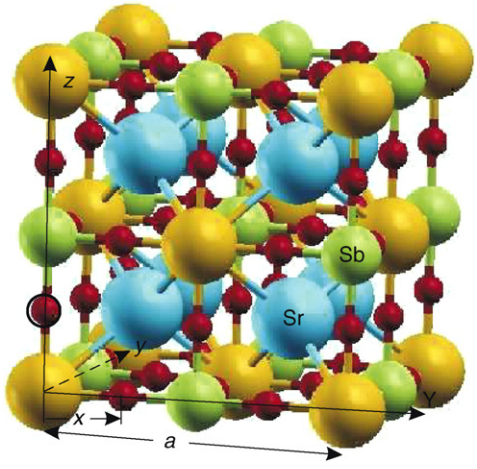

Fig. 1. Structure of Sr_2YSbO_6. In the figure the x parameter is proportional to the length bond between oxygen and Y-atoms [7–9].

Table 1
Covalent and atomic radius of the elements present in Sr_2YSbO_6

Element	Covalent radius (Å)	Atomic radius (Å)
Sr	1.91	2.45
Y	1.62	2.37
Sb	1.40	1.53
O	0.73	0.65

3. Experimental details

Sr_2YSbO_6 was prepared by the solid-state reaction method. Stoichiometric mixtures of high purity (99.99%) constituent chemicals Y_2O_3, SrO and Sb_2O_3 in adequate amounts are mixed thoroughly, pelletized and calcined at 1100 °C for 18 h. The calcined material was reground, pressed as circular discs and sintered at 1090 °C for 135 h. All the above processing was carried out in air atmosphere [1].

XRD pattern of this powder material was recorded by means of PHILLIPS PW1710 diffractometer, using the Cu-Kα radiation ($\lambda = 1.5406$ Å). We perform measurements in the 2θ interval between 15° and 85°, with a scanning step of 0.02° and 2 s exposure time. Rietveld refinement of this pattern was made by means of computer code GSAS and its graphic interface EXPGUI [10,11], using the structural parameters of the $A_2BB'O_6$ complex cubic perovskite family.

4. Results and discussion

Fig. 2 shows the energy as a function of x. Each one of the round points is an individual calculation and the dash-line corresponds to a polynomial of grade two which was obtained by the least-square fitting method [12]. The minimum of the energy is obtained for $x = 0.26177$. Also, the dependence of energy with volume by each chemical formula is shown in Fig. 2. Solid line represents the fitting to the Murnaghan's state equation [13]. Table 2 shows the structural parameters obtained from that fit. Due to the

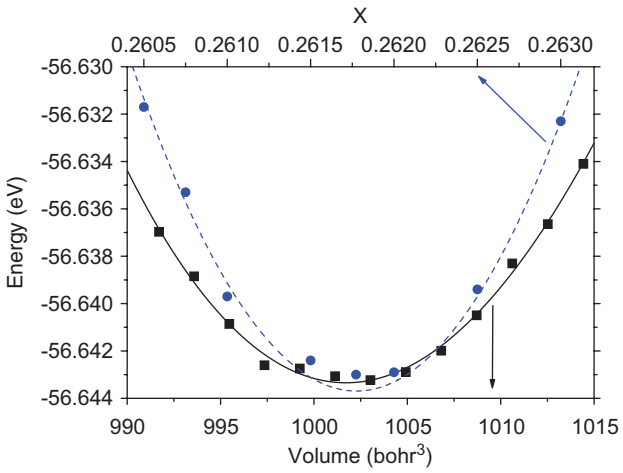

Fig. 2. Energy as a function of x (dashed line) and volume of primitive cell (continuous line) of Sr_2YSbO_6. The dashed line corresponds to a parabola of degree 2, while the solid line is the fitting to the Murnaghan's state equation. Both fittings were obtained by the least-square fitting method.