Investigating Possibility of CrSb Application in Spintronic by Theoretical Calculation of Electronic and Magnetic Properties Related to Spin of CrSb Base on Ab-Initio Calculations

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Abstract

In this article, the theoretical study about structure of spin electron bands and magnetic properties of Bulk CrSb in Zinced Blende structure have been considered according to density functional theory by using LSDA approximation for exchange-correlation energy and potential calculations using FP-LAPW method by theoretical calculation of electronic band structure, spin energy bands, total and partial states density, electronic charge density of atoms at (110) and (100) crystalline plane. In this calculation, the degree of spin polarization and the total energy of bulk state are also studied by considering magnetic coupling between Cr spins and its neighbors. The results indicate that Cr by positive local magnetic momentum cause to arising total magnetic momentum equals to 3.0000 μΒ in a unit cell, which confirm by a theoretical rule known as Rule of 8, too. This material completely shows metallic properties in up spin, energy bands of up spin have cut Fermi surface, so valence electrons with up spin can easily move from valence band to conduction band. But at down spin, valence bands were separated from conduction bands by indirect gap equals to 1.64377 eV, that indicates the clear characteristic of a nonconductor, therefore in this material only electrons with up spin participate in density of Fermi surface's states and appearance of metal property, CrSb can be considered as a half metal, in general the total density of up and down spin states also proves this result and CrSb's half metallic property and introduces its electronic properties related.

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Keywords: Spintronic; DFT; Half metal; Band structure; Density of states; LSDA; CrSb

Introduction

Spintronic technology is practical usage of free degree of electron's charge and spin in electronic system synchronized. The spin injection process in devices which are used in this industry is the controllable transition of electrons from a high polarized spin substrate such as half metallic ferromagnetic to a semiconductor, so it must be kept a relative spin forms of transmitted electrons for the development and maintenance of spin injection in this process. So most of transmitted electrons have the same spin. Since the manufacturing of spin electronic devices and the study of their physical properties have a main role for their great applications in the future of information technology, magnetic memories, giant magneto resistance, tunneling magneto resistance and nonvolatile memories, the research for finding ideal materials with these special physical properties were considered by most of researchers. The development and maintenance of spin injection process require the maintenance of relative unbalance in transmitted electron's spin states, so that most of transmitted electrons have up or down spins. An appropriate electrode for spin injection at spintronic devices should remained ferromagnetic at room temperature and should maintain its high spin polarization, and also should form a schotky barrier by semiconductor in interface, so that the structure of spin injector material would be stable on mentioned semiconductor and the interface between them would have the minimum of possible Ohmic contact. The main factors in making problems in production of such compounds are interface structural disorder and atomic intermixing that can be lead to the formation of dead layers, or to the destroying of electron's spin polarization in interface with semiconductor. Furthermore, mismatch between ferromagnetic and semiconductor (1) are another obstacle in spin injection process. Since one of the main advantages of spin injectors in ferromagnetic is their polarization, the attempt for finding more appropriate ferromagnetic resulted in half metallic property discovery by de Groot (2) in 1983. These materials are spin polarized at Fermi surface in ideal mode certainly. The half metallic properties were observed in some materials such as some Proveskite structures (3)Transition oxides like FeO₃, CrO₂, (4), some Heusler Alloys (2) like NiMnSb, PtMnSb (5,6).

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and some Diluted Magnetic Semiconductors (DMS) like Zn_{1-x}Mn_xGeP_2 (7) and Zn_{1-x}Cr_xTe (8) which a magnetic ion was doped into semiconductor in them. DMS would have a good structural compatible with semiconductors because they are from semiconductors family, but the main problem of DMS which produce by adding a magnetic ion such as V, Co, Fe, Mn or Cr into semiconductors is their low Curie temperature. The main problem of using transition metals oxides in spintronic materials refers to their difficult experimental growth as thin film oxide state, too. One of the reasons of effectiveness decrease in half metal Magnetic transition metals compounds as an injector on semiconductors is the possibility of a magnetic dead layer formation on interface due to the mismatch of crystal structure’s lattice constant (9). Furthermore, Heusler Alloys and transition metals oxides aren’t an appropriate selection for HM-FM because of the current problems in stoichiometry control and the defects that result in their spin transition destruction (10).

With above descriptions, the half metal ferromagnetics which have a high Curie temperature will have also the capability of spin flow injection in spin polarized material certainly. The half metal ferromagnetics of transition compounds with Zinc-Belende (Zb) structure (11) on III-V semiconductors groups geometrically are more appropriate for an interface formation with minimum spin dispersion degree on interface, because in addition to minimum dispersion due to the disorder on their interface there is less on atomic environment of their interface with semiconductor in comparison with Heusler compounds half metal ferromagnetics which prevent from entering interface forms into the down spin energy Gap, and maintains half metallic property. In spite of recent progresses in the fabrication of these materials, the presence of some issues such as high Curie temperature, effective spin injection and spin transition, search for ideal materials are also continuing. Since the spintronic materials place on a sublayer of semiconductor as a thin film, the compatibility with semiconductor’s lattice structure is considered as a main condition of a good injector.

In CrSb application with semiconductor sublayers for better compatibility with semiconductor sublayer which has Zb structure, it must be grown in the form of Zb thin films with semiconductor sublayer’s lattice constant. But Since CrSb structure in the nature isn’t in the form of Zb, in that case its stability must be studied. In this article, first of all the ab-initio theoretical studies on CrSb bulk structure have been considered for studying CrSb experimental growth possibility on lattice constant of semiconductors sublayer and comparison of extension and mismatching effects on half metallic properties on CrSb/InSb interface, in comparison with CrSb bulk state, as a first step in calculation Which the results will be introduced as flowing. Since CrSb has a high Curie temperature, it can be a good choice for using in spintronic, if half metallic property of CrSb can be proved when it is grown on semiconductor’s lattice constant, because it is expected that in experimental growth by MBE (Molecular Beam Epitaxy) method on several primary layers, it will accept its semiconductor sublayer’s lattice constant and will be compatible with it.

**Calculation Method**

The theoretical study about electronic bands structure of CrSb (Zb) figure (1) and its magnetic properties in
The bulk state is carried out based on the density functional theory with LSDA approximation for XC potential by FP-LAPW method. At first, by using experimental lattice constant, energy curve is drawn versus unit cell volume and from the minimum of this curve, the equilibrium lattice constant equal to $a=6.15\,\text{Å}$ is resulted, and then the degree of applied stress upon each atom is minimized by relaxation of atomic positions. The calculations are done in a fcc unit cell with Cr (0, 0, 0) and Sb (0.25,0.25,0.25) local coordinates which have the equilibrium lattice constant equals to $a= 6.15\,\text{Å}$. In FP-LAPW method, potential and charge density are considered completely without any approximation, and the base functions in MT sphere are developed according to spherical harmonics to angular momentum $L=10$ and out of MT sphere in interstitial regions developed according to plane waves. In order to control and decrease computational error and for high accuracy achievement, at first by doing calculation with $K$ points in the range of 300 to 3000 with length step of 100 and considering energy changes according to this parameter, the certain quantity of $k$ points was selected 3000 points. Also, the optimum quantity of $R_{K_{\text{max}}}= 8.5$ selected by recomputing with $R_{K_{\text{max}}}$ in the range of 6 to 9 with 0.5 length step. The separating energy $E_{\text{cutoff}}=6$ Ryd is used as a standard for separating core electrons from valence electrons. Which with core state treated completely relativistic and with semicore state treated half relativistic. Self consistent calculations up to convergence (0.00001) are carried out at charge quantity with 35 step iteration. In other word, calculations would be convergent only when
$\int |\rho - \rho_{n-1}| \, dr$ result is less than (0.00001). In which $\rho_n$ is input charge density and $\rho_{n-1}$ is output charge density. In this calculation the amount of total energy and Fermi energy is (-15053.954292 Ryd) and (0.10994 Ryd) respectively and the total magnetization in a unit cell is 3.0000 µB. Since there is no state for down spin on Fermi surface, it can be resulted that CrSb-Zb with InSb lattice constant has half metal property, but if the lattice constant of selective semiconductor be too small for CrSb, the d and p states overlap like GaP and the therefore result in expanding of down spin state hybridization in a band, so that the Fermi surface would be cut then the half metallic property would be disappeared.

**Result**

**Magnetization**

The results of theoretical computations for each atom's magnetization are shown in figure (2) through 35 iteration steps. it shows Sb's local magnetization direction antiparallel with Cr magnetization. It means that Cr atom inspires a positive local magnetic momentum in a cell, while Sb atom inspires a negative local magnetic momentum that its quantity refers to the local amount and the replacement of P wave functions around atom. In these calculations the numerical amount of Sb's local magnetization is (-0.31930 µB) and Cr's local magnetization is (3.31931 µB), then the total magnetization of CrSb in a unit cell includes one Cr atom and one Sb atom is equal to 3.0000µB, which is compatible with experimental quantity. As the numbers shows, the main part of magnetization is due to the Cr atom which inspires positive local magnetic in a unit cell. The total magnetization of half metal Zb compounds in a unit cell due to the remaining valence electrons numbers would be computed by following formula which is known as rule of 8. Since in each orbital, two electrons with opposite spins can be placed, there are 2 electrons in s orbital and they
can fill that orbital (s²), there are 6 electrons in p orbital (p⁶), so eight valence bands were filled with eight valence electrons (6+2=8) and the rest of electrons begin to fill d orbital with up spin. First the eg states which have lower energy can be filled, and then t₂g states can be filled. According to this rule, the total magnetic of half metallic systems should be an integer number, so for CrSb we will have:

\[ M = (Z_{\text{tot}}-8) \mu_B = (11-8) \mu_B = 3 \mu_B \]

which confirms the accuracy of theoretical evaluated quantities in present result.

Table 1. Comparison between \(E_{\text{gap}}\) in this and other works

<table>
<thead>
<tr>
<th>Researcher</th>
<th>Method</th>
<th>(E_{\text{gap}}) (eV)</th>
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<tbody>
<tr>
<td>Pask [12]</td>
<td>LAPW</td>
<td>1.58</td>
</tr>
<tr>
<td>Current Work</td>
<td>FP-LAPW</td>
<td>1.64377</td>
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Energy spin bands structures

The up and down spin energy bands structures in Zb-CrSb are represented in figures (3-5) along the high symmetry lines in first Brillouin zone at Kelvin zero temperature. The vertical axis of bands energy is calculated upon eV and zero energy scale indicates Fermi surface area which is shown by dash vertical line. As shown by the figures, the up spin energy band have cut Fermi surface completely, so this compound represents completely metallic property by itself, so that the valence band electrons with up spin can move easily from valence band into conductance band. But in down spin, valence band is separated from conducance band by indirect gap equals to 1.64377 eV which indicates the clear property of an inductor, while in ferromagnetic materials, both spin directions have role in Fermi’s density of states, then according to these results CrSb can be considered as a half metal.

\[ E_{\text{gap}} = \text{Min Conductance Band} - \text{Max Valance Band} = (1.60187) - (-0.04190) = 1.64377\text{eV} \]

Total density of states

The total density of spin states in CrSb is shown in figures 6-13 which indicate the number of allowed electron’s states at different distances of energy. These results confirm band structure and represent half metallic property in down spin states clearly. The horizontal axis is according to energy (eV) and the vertical axis indicates the number of states. For better comparison, in figures (7-8) partial density of states of Cr and Sb orbitals for studying their contribution in CrSb’s total density of states are shown. As shown in these figures, Sb and Cr atoms in dn spin never cut Fermi surface. The main part of CrSb-dn conductance band is made of Cr-dn orbitals, and the main part of CrSb-dn valence band is made of Sb-dn and Cr-dn bands. While the main parts of up density of states of conductance and valance bands are made of Cr-up states. In figure (7), Sb-s orbital energy is about (-7eV) and p orbital is began from (-2 eV) and they make the main part of Sb valence band in both up and down spin states. While p-dn orbitals make a great peak in Sb-dn valence band, but they have a little role in Sb-dn conduction band formation. The main role of p-up orbitals of Sb is completely visible in cutting Fermi surface at Sb-up states. For better comparison of
CrSb’s total density, the energy band structure of up and down spin states are shown in figure (8) at the same axis. In figure (9), for better comparison between contributions of each orbital from total density of states, the related figures are shown synchronized. As shown in this figure, s-dn, p-dn Cr orbital have a little role in valence and conduction bands. But d-up orbitals of Cr is very localized and are effective in cutting the Fermi surface, the main role of Cr orbital is in formation of density of state around Fermi surface.

**Electron charge density**

The electron charge density of (110) and (100) crystalline plane in CrSb on two or three dimension in real space in figures (10-11) indicates the electron charge distribution around Cr and Sb atoms according to (e/A³). The chemical bond type between crystal elements are recognizable by drawing charge density in different crystal plane and studying density of electronic cloud around each atom. Cr atom is related to 6B group of alternative table and its electron arrangement is Cr: [Ar] 3d⁵, 4s¹ while Sb is in 5A group and its electronic arrangement is Sb: [Kr] 4d¹⁰, 5s², 5p³. Then the bond between these two atoms seems covalent, but by considering their binding to the crystal lattice and their participation in bond, electron charge distribution in lattice have considerable changes in comparison to isolate atoms regarding the electronegativity percentage of each atom. Since electronegativity of Sb is more than Cr, it absorbs the common electrons between two atoms in bond to its direction and therefore it has negative charge and Cr has positive charge, as a result chemical bond between these two atoms is found ionic nature. Electronic charge density |ψ²| in overlap area due to the attraction between Cr and Sb atoms and wave function of two atoms ψ_r=ψ_Cr+ψ_Sb has maximum quantity and as a result the density of electronic cloud is very dens in this area. So the issue of electronic charge density in area between Cr and Sb indicates and confirms that the bond between these atoms in crystal is ionic.

**Conclusion**

Since the spintronic materials lie on sublayer of semiconductor in the form of thin film, the compatibility with semiconductor lattice structure which has Zb crystalline structure, in general is considered as a main condition for a good injector. Regarding the results of CrSb theoretical calculations in order to recognizing its magnetic and electronic properties for application as a thin film on a sublayer of Insb semiconductor for using in spintronic industry with Insb lattice constant would be resulted that this material represents high spin polarization if growth in the form of Zb thin film on a sublayer of Insb and behaves as a half metallic. Therefore, Insb can be a good candidate for CrSb growth on it and practical usage in spintronic industry by proving the presence of half metallic property in CrSb with lattice constant of Insb. So it is expected from the result that in experimental growth by MBE method, this material will accept Insb lattice constant in several primary layers as its sublayer and could be compatible with it.
Fig. 9. contribution of up & down Cr orbitals in total DOS of Cr
Fig. 10. spin electronic charge density of CrSb in crystalline plane (110)

Fig. 11. spin electronic charge density of CrSb in crystalline plane (100)
References