Spin-Orbit and Strain Induced Modification in Electrical Properties of Monolayer InSb

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Abstract
In this work, the electrical properties of monolayer InSb in the presence of biaxial strain using density functional theory are investigated. Here, we first explore the band structure of InSb with and without spin-orbit coupling (SOC) consideration. The electron and hole effective mass modify with SOC consideration. The electron and hole effective masses lowered two and ten times, respectively. The location of valleys in conduction and valence band for various strains are explored, and the corresponding effective masses are reported. A lower effective mass is obtained for both electron and hole with applying tensile strain, whereas, the bandgap closes for large tensile strain. A numeric fitting has applied to effective mass versus strain, and an equation for every curve is reported. Finally, the work function of this material for different strains is obtained.

Keywords: InSb, Monolayer, Effective mass, Spin-Orbit Coupling, Work function.

1. Introduction
Since the birth of graphene in 2004, it has been paid considerable attention in the scientific world toward exploring properties of new two-dimensional (2D) materials [1, 2]. The 2D materials have been getting intense research since the last decade because of their unique structure and outstanding electronic, optical, and transport properties [3, 4], which have potential for future applications. Also, 2D materials with high specific surface areas and no dangling bond on the surface give advantages to the bulk.

The III-V compound materials have been known as semiconductors with high mobility and direct bandgap. GaAs and InSb, two members of this family, have shown colossal capability in photoelectric industries. The bulk GaAs and InSb widely used in industry because of their unique optoelectronic properties, high mechanical stability, and direct bandgap [5-8]. The indium-based compounds demonstrate materials with small and direct bandgap. Due to their narrow bandgap, they proposed suitable applications for free-space communications, infrared imaging systems, and gas-phase detection systems [9, 10]. The high electronic mobility (78,000 cm²/Vs) of InSb points to it as a potential candidate in optoelectronic materials [11]. The bulk InSb with a narrow bandgap (0.18 eV at room temperature) can be used in thermal imaging, Schottky diodes, and infrared detectors. The InSb nanosheets display high electron mobility and ambipolar behavior. InSb nanowires demonstrate high electron mobility as 2.5 × 10⁴ cm²/Vs that is affected by large spin-orbit coupling [12, 13].

Furthermore, a strong interest has recently emerged in group III-V two dimensional and these monolayers have both graphene-like planners and buckled structure [14, 15, 16, 17, 18, 19, 20, 21, 22]. Based on density functional theory (DFT) calculations, [23, 24] the stability and electronic band structure of monolayer honeycomb structure of group III-V binary compound has been studied. Monolayer and multilayer boron-nitride with wide bandgap proposed as a high-quality substrate for other monolayers that demonstrates low effects on the transport in monolayer [25, 26, 27]. Some of these compounds demonstrate a topological insulator phase in mono and bilayer due to their strong spin-orbit coupling (SOC) [28, 21]. Bi and Sb atoms from group V, and In and Tl from group III posses high SOC where topological insulator in III-V compounds are based on these atoms [29, 30, 31]. InSb contains two heavy atoms (In and Sb), and one can expect SOC can highly be modify the electrical properties. Strain and functionalize with halogen atoms or methyl can drive these materials in...
the quantum spin hall effect phase \[32, 33\].

In this paper, the electronic properties of monolayer InSb are studied using density functional theory (DFT). The effective masses for electron and hole are calculated with and without SOC consideration. After that, the effective masses and location of valleys are explored for various biaxial strain. Finally, the work function is investigated in the different strains.

2. Computational details

Our results are based on density functional theory calculations as implanted in the Quantum ESPRESSO package \[34, 35\]. Projector augmented plane waves (PAW) pseudopotentials within the PerdewBurkeErnzerhof (PBE) parametrization of the generalized gradient approximation (GGA) were utilized as an exchange-correlation potential \[36\]. Electron-ion interactions were described by the norm-conserving pseudopotentials \[37\]. In order to include the spin-orbit interaction, fully relativistic approximation was adopted. The energy cutoff of 612 eV for the plane-wave basis expansion was used throughout all calculations. During calculation, a 12 \times 12 Monkhorst-Pack k-point grid was used \[38\]. We were first performed full geometry optimization until the forces on the atoms are less than 0.001 eV/Å and the total energy difference lower than $10^{-8}$ eV.

The effective masses of electron and hole are calculated by using the following equation \[39\]:

$$m^* = \frac{\hbar^2}{\partial^2 E / \partial k^2} \quad (1)$$

Here, $\h$ is the reduced Planck constant, $E$ and $k$ are the energy and wave vector of the conduction band minimum (CBM) and valence band maximum. The work function can be obtained the difference between Fermi energy ($E_F$) and vacuum energy ($E_{\text{vac}}$) as: $\phi = E_{\text{vac}} - E_F$.

3. Results and discussion

The structure of InSb with honeycomb configuration is depicted in Fig. 1. The map energy for the first valence and conduction band is plotted in the first Brillouin zone. As one can observe, $\Gamma$-valley is the conduction band minimum, and $K$- and $M$-valleys is much higher than $\Gamma$-valley. On the other hand, both $\Gamma$ and $K$-valleys contribute to the valence band maximum. The band structure is plotted around the reduced Brillouin zone in a path ($\Gamma$-$K$-$M$-$\Gamma$). The band structure of InSb with and without spin-orbit coupling is plotted in Fig. 2(a). The SOC modifies the band structure and changes electrical properties. The CBM and VBM are located in the $\Gamma$-valley and this material is a direct semiconductor. There is one band at the bottom of the conduction band, whereas, two bands are located at the top of the valence band. Therefore, one band contributes electron effective mass and two bands to hole effective mass.

The bandgap, electron, and hole effective masses are compared for with and without SOC consideration in Table 1. First, the bandgap decreases from 0.6930 to
0.4729 eV with applying SOC. Our band gap without SOC is close 0.68 eV and 0.79 eV in other works [23, 40] and lower than 1 eV reported by Ref. [41]. The effective mass of the electron is 0.0816\(m_0\), which decreases to 0.0482\(m_0\) with applying SOC. Our electron effective mass is much lower than 0.33 and 0.28\(m_0\) reported in other works [24, 40]. The bulk electron effective mass is 0.014, which is three times lighter than the 2D limit. One can find that two bands at \(\Gamma\)-point and one band at \(K\)-point contribute to VBM and affects the hole effective mass. The effective masses of these three are listed in Table 1. The effective masses at \(\Gamma\)-point as 0.5664 and 0.1087\(m_0\) can be considered as a heavy hole (HH) and light hole (LH). SOC decreases masses for HH and LH to 0.0708 and 0.1355\(m_0\), respectively. Both LH and HH in without SOC state crosses at \(\Gamma\)-point whereas, SOC splits two bands 0.5039 eV. The energy of these effective masses is inserted in the Table. Hole effective mass in the two-dimensional limit can be calculated as:

\[
m^*_h = m^*_{h,\Gamma} + m^*_{h,\Gamma 2} \exp(-\Delta E_{\Gamma 1,\Gamma 2}/K_B T) + N_K m^*_{h,k} \exp(-\Delta E_{\Gamma 1,K}/K_B T)
\]

where \(K_B\) is Boltzmann constant, and \(T\) is the temperature in Kelvin. \(N_K\) accounts number of \(K\)-valley in the first Brillouin zone that \(N_K = 2\). \(\Delta E_{\Gamma 1,K} = E_{\Gamma 1} - E_K\) accounts the energy difference between first and second band at \(\Gamma\)-point. \(\Delta E_{\Gamma 1,K} = E_{\Gamma 1} - E_K\) also defines as the energy difference between \(\Gamma\) and \(K\) valleys in the first band. The hole effective mass is obtained using the above equation as 0.0709 and 0.7978\(m_0\) for with and without SOC consideration, respectively. The hole effective mass in bulk is 0.263\(m_0\) four times larger than the 2D limit. The SOC decreases hole effective mass and makes monolayer InSb as a material with light hole and electron for application as NFET and PFET.

In the following, we apply Bi-axial strain to modify the electrical properties. The compressive and tensile strain is applied, and the resultant structure is completely relaxed, then band structure is obtained, and its electrical properties are extracted. At first, the bandgap as a function of strain is studied with and without SOC, and the results are plotted in Fig. 2. The amount of reduction is higher in the compressive regime, and this indicates SOC is more important in the compressive regime. We observed similar effects in group-III monocalchagonides [42]. The bandgap decreases with applying tensile strain, and it goes to zero at 4.5% tensile strain. For strain larger than this strain, the CBM is located at \(\Gamma\)-valley, whereas the VBM at \(M\)-valley. The bandgap is zero, but the conduction band and valence band don’t cross. InSb is a semi-metal for strain larger than 4.5% tensile strain. The bandgap first increases with applying compressive strain then decreases for larger compressive strain. The maximum band gap is obtained 0.7386 eV at strain -2.75%. As one can observe, the SOC decreases bandgap in InSb. After this, all calculations are done with consideration of SOC.

| Band gap | Eg [eV] | 0.4729 | 0.235 |
|----------|---------|--------|--------|

Table 1: The effective masses and corresponding energy of the valleys for electron and hole. The effective mass and energy are in the units of \(m_0\) and eV, respectively.

| m* | w/o SOC | w SOC | Bulk Exp [7] |
|-----|---------|-------|-------------|
| \(m^*_{\alpha,\Gamma}\) | 0.0816 | 0.0482 |
| \(E_T\) | 0.3371 | 0.2392 |
| \(m^*_{\alpha}\) | 0.0816 | 0.0482 | 0.014 |
| \(m^*_{\alpha,\Gamma 1}\) | 0.1087 | 0.0708 |
| \(m^*_{\alpha,\Gamma 2}\) | 0.5664 | 0.1355 |
| \(m^*_{h,\Gamma}\) | 0.6630 | 0.7070 |
| \(E_{\Gamma 1}\) | -0.3559 | -0.2395 |
| \(E_{\Gamma 2}\) | -0.3559 | -0.7434 |
| \(E_K\) | -0.3996 | -0.4787 |
| \(m^*_{h}\) | 0.7978 | 0.0709 | 0.263 |

Figure 3: The energy of valleys in (a) the conduction and (b) valence bands for various strain.
The location of the CBM affects electron transport. This modulates electron density and effective mass. The location of valleys in the conduction band relative to Fermi energy for three valleys (Γ, K, and M valleys) are plotted in Fig. 3. As one can observe, the CBM is placed in Γ-valley in tensile strain, and its energy decreases with increasing strain. The energy of valleys increases with applying compressive strain, whereas, K- and M-valleys decrease. At strain -2.75, CBM goes to M-valley; however the energy of K-valley is located close to M-valley. Both M- and K-valley contribute to the conduction band in strain range [-6,-2.75]. In the following, we fit a line to these curves and find the best fitting. We use two ranges of strain for fitting due to breaking in the curves. The first range is [-6,-2.75], and the other is in the interval [-2.75,6]. The relation for fitting is as: for \(-6 \leq x \leq -2.75\)

\[
E_\Gamma = -0.145x - 0.005308, \\
E_K = 0.06857x + 0.5512, \\
E_M = 0.06535x + 0.6355,
\]

and for \(-2.75 \leq x \leq 6\)

\[
E_\Gamma = -0.02838e^{1.247} + 0.2727e^{-x/7.413}, \\
E_K = -0.01056x^2 + 0.1363x + 0.8176, \\
E_M = -0.01287x^2 + 0.1122x + 0.8555.
\]

Two bands at Γ-point is separated by applying SOC. The energy of two bands at Γ point (Γ1 and Γ2) and K-valley versus strain are plotted in Fig. 3. The second band at Γ-the point is far from the first one and doesn’t contribute to transport. It is obvious that in compressive strain and tensile strain up to 3.25 tensile strain, the VBM is located at Γ point. The VBM switches to K-valley for strain larger than 3.25%. The strain is divided into two regimes, first [-6,-2.75] and second [-2.75,6]. The relation for fitted lines is as follow: for \(-6 \leq x \leq -2.75\)

\[
E_\Gamma = 0.006515x^2 - 0.024 - 0.4892
\]

for \(-2.75 \leq x \leq 6\)

\[
E_\Gamma = 0.001166x^3 - 0.002163x^2 + 0.0513x - 0.24, \\
E_K = -0.01066x^2 + 0.1365x - 0.4741.
\]
are:

\[
m_{\Gamma}^{v}(-6 \leq x \leq 1) = 0.000138e^{-x/1.084} + 0.057e^{-x/14.9} \\
+ 0.000364e^{-x/1.065} \\
m_{\Gamma}^{v}(1 \leq x \leq 6) = 0.0575e^{-x/15.625} \\
+ 0.000364e^{-x/1.065} \\
m_{\Gamma \rightarrow \Gamma}^{v} = 0.4414e^{-x/11.25} + 0.1416e^{x/6.215} \\
m_{\Gamma \rightarrow M}^{v} = 1.855e^{-x/51.18} + 0.2011e^{x/2.09} \\
m_{\Gamma \rightarrow K}^{v} = 0.5358e^{-x/54.7} + 0.1146e^{x/4.11} \\
m_{M \rightarrow K}^{v} = 0.5286e^{-x/6.77} + 0.002322e^{x/1.94}
\]

The effective mass for the valence band is shown in Fig. 5. The hole at \(\Gamma\)-valley shows a low effective mass but larger than the electron. \(m_{\Gamma}^{v}\) increases with applying compressive strain, whereas, decreases with tensile strain up to 4\%, after that increases. The lowest \(\Gamma\) effective mass 0.0534\(m_{0}\) can be obtained at tensile strain 4\%. Hole effective mass at K-valley increases with increasing strain. For strain larger than 3.25\% tensile strain, VBM is located at K-point, and InSb indicates a high effective mass for the hole. The fitted line to hole effec-

Another important parameter for studying the electrical property is work function (\(\phi\)) or electron affinity (\(\chi\)). The difference between these two parameters is half of the bandgap, \(\phi - \chi = \frac{E_{g}}{2}\). The work function is calculated by the difference between Fermi and vacuum energies. The work function for the unstrained one is 4.68 eV that is close to bulk 4.57 eV. The work function is the same for with and without SOC. The work function versus strain is plotted in Fig. 6. \(\phi\) behaves linear in interval [-6,-2.75] and parabolic in interval [-2.75,6].

\[
\phi(-6 \leq x \leq -2.75) = 0.04931x + 4.536 \\
\phi(-2.75 \leq x \leq 6) = -0.01156x^2 + 0.1043x + 4.794
\]

The work function can be tuned between 4.2 to 5 eV by applying biaxial strain.

4. Conclusions

In summary, we investigated the electronic properties of monolayer InSb. We find that the SOC highly
declines hole, and electron effective masses to 0.0482 and 0.0711 $m_0$, respectively. In the following, we study the effects of biaxial strain on the electrical properties. The maximum band gap is obtained 0.7386eV at 2.75% compressive strain, and bandgap closes at 4.5% tensile strain. The location of hole and electron’s valleys versus strain is studied and a numeric fitting has applied to every curve. The effective masses for electron and hole are calculated, and a curve is fitted to them. The lowest electron and hole effective mass occurs when CBM or VBM is located at $\Gamma$-point. At final, the work function increases when strain increases from compressive to tensile.

5. Conflict of interest

The authors declare that they have no conflict of interest.

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