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Electronic Modeling and Optical Properties of $CuIn_{0.5}Ga_{0.5}Se_2$ Thin Film Solar Cell

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ABSTRACT

In this work, the band structure and optical-related properties of $CuIn_{0.5}Ga_{0.5}Se_2$ thin film are presented. The calculation is performed by the full-potential linearized augmented plane wave (FPLAPW) method. The spin-orbit coupling is considered. The result for the dielectric function is in good agreement with earlier experimental measurements and simulations. Based on the complex dielectric function, the dielectric constant, the absorption coefficient, the complex refractive index and the reflectivity at normal incidence are explored. We found that they are comparable with the earlier results.

KEYWORDS

Thin Film; $CuIn_{0.5}Ga_{0.5}Se_2$; Band Structure; Dielectric Function; Dielectric Constant; Absorption Coefficient; Complex Refractive Index; Reflectivity; Spin-Orbit Coupling

1. Introduction

The chalcopyrite $CuIn_{1-x}Ga_xSe_2$ (CIGS) alloy is one of the most promising thin film absorber materials in thin film photovoltaic technology [1,2]. Currently, the best efficiency of solar cells based on CIGS contains around 30% Ga. However, optimum Ga content is theoretically 50% ~ 60%. Therefore, in this work, we will study band structure and optical-related properties of $CuIn_{0.5}Ga_{0.5}Se_2$ (50% Ga).

In this work, the band structure is calculated without and with the spin-orbit coupling (NonSOC and SOC), respectively. The SOC is important for the calculation of band structure. It affects the curvature of energy band strongly, especially for the valence bands (VBs) near the Γ point. The complex dielectric function is obtained based on the calculation of band structure. Therefore, the other optical properties are possible to be investigated using the complex dielectric function, such as the dielectric constant, the absorption coefficient and many others. The result based on our calculation method is reported few, although it is investigated by some experimental measurements and simulations [3-7].

2. Theoretical Details

2.1. Compuational Details

The program package Wien2k [8] is utilized to perform all the calculations. It based on the full-potential linearized augmented plane wave (FPLAPW) plus local orbitals method. The relativistic effects and SOC are considered in our calculation. The generalized gradient approximation (GGA) plus an onsite Coulomb interaction U of the Cu d states is treated as exchange correlation potential, which will improve the energy gap. The k mesh is 8 × 8 × 8 to sample the Brillouin zone (BZ). The $CuIn_{0.5}Ga_{0.5}Se_2$ has chalcopyrite structure with tetrahedral bonding character. Eight atoms are contained in primitive cell.

2.2. Optical Properties

The calculation of optical properties does not go beyond the Kohn-Sham eigenstates in Wien2k. The complex

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dielectric function can be written:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega), \tag{1}$$

where $\varepsilon_1(\omega)$ is the real part and $\varepsilon_2(\omega)$ is the imaginary part. Both of them are tensor. The imaginary part in atomic units is calculated as follows [9]:

$$\mathrm{Im}(\varepsilon_{ij}) = \frac{1}{\pi\omega^2}\sum_{n,n'}\int_{\mathbf{k}} p_{i;n,n',\mathbf{k}} p_{j;n,n',} (f_0(\varepsilon_{n,\mathbf{k}}) - f_0(\varepsilon_{n',\mathbf{k}}))\delta(\varepsilon_{n',\mathbf{k}} - \varepsilon_{n,\mathbf{k}} - \omega), \tag{2}$$

where $p_{i;n,n',k}$ is the ith momentum matrix element for the band index n and n' with crystal momentum $\mathbf{k}$. The real part of dielectric function is derived by the imaginary part tensor:

$$\mathrm{Re}(\varepsilon_{ij}) = \delta_{ij} + \frac{2}{\pi}\mathbf{P}\int_0^\infty \omega' \frac{\mathrm{Im}(\varepsilon_{ij}(\omega'))}{(\omega'^2 - \omega^2)} d\omega', \tag{3}$$

where $\mathbf{P}$ is the principal value. $n_{ii}(\omega)$ (refractive index) and $k_{ii}(\omega)$ (extinction coefficient) are the real and imaginary part of refractive index, respectively. They can be expressed by the complex dielectric function:

$$n_{ii}(\omega) = \sqrt{\{|\varepsilon_{ii}| + \mathrm{Re}(\varepsilon_{ii})\}/2},$$
$$k_{ii}(\omega) = \sqrt{\{|\varepsilon_{ii}| - \mathrm{Re}(\varepsilon_{ii})\}/2}. \tag{4}$$

The absorption coefficient is obtained by:

$$A_{ii} = 2\omega k(\omega)/\mathrm{c}. \tag{5}$$

The reflectivity at normal incidence can be calculated by this complex refractive index.

$$R_{ii}(\omega) = \{(n_{ii} - 1)^2 + k_{ii}^2\}/\{(n_{ii} + 1)^2 + k_{ii}^2\}. \tag{6}$$

The loss function can be calculated by:

$$L_{ij}(\omega) = -\mathrm{Im}(1/\varepsilon(\omega))_{ij}, \tag{7}$$

and the real part of the optical conductivity is:

$$\mathrm{Re}(\sigma_{ij}(\omega)) = \omega/(4\pi)\,\mathrm{Im}(\varepsilon_{ij}(\omega). \tag{8}$$

3. Results and Discussion

3.1. Band Structure

The electronic band structure of $CuIn_{0.5}Ga_{0.5}Se_2$ is presented without and with spin-orbit coupling in **Figure 1**. It is plotted in the energy range from −3 eV to −4 eV (upper panel), which is the visible sunlight spectrum. It demonstrates that it has direct band gap and the band gap for NonSOC case is 0.81 eV, and it is around 0.75 eV for the SOC case. However, the plot has been corrected the band gap to 1.33 eV.

Figure 1 demonstrates that the energy band dispersion is strongly affected by SOC, especially for the valence bands (VBs) near the Γ point (lower panel), where the SOC split is ~0.2 eV. However, the conduction bands are only affected slightly by the SOC. Therefore, it is important to consider the SOC when calculating energy band dispersion for semiconductor, because it will directly impact on the calculation of effective mass and carrier concentration. It is consistent with earlier results [10,11].

3.2. Optical Properties

The average of complex dielectric function is presented in **Figure 2**. The band gap is corrected to 1.33 eV for the calculations of optical properties. The main shape of this complex dielectric function is similar for both of NonSOC and SOC cases. However, the main peak position is slightly different. It is around 2.81 eV and 2.85 eV for NonSOC and SOC cases, respectively. The average high frequency dielectric constant is $\mathrm{Re}(\varepsilon(\omega = 0)) = 5.74$ for the NonSOC case, and it is around 5.70 for the SOC case. It has good agreement with earlier experimental measurements and simulations results [12-15].

In **Figure 3**, the tensor of this complex dielectric function is demonstrated. There is a difference in the main

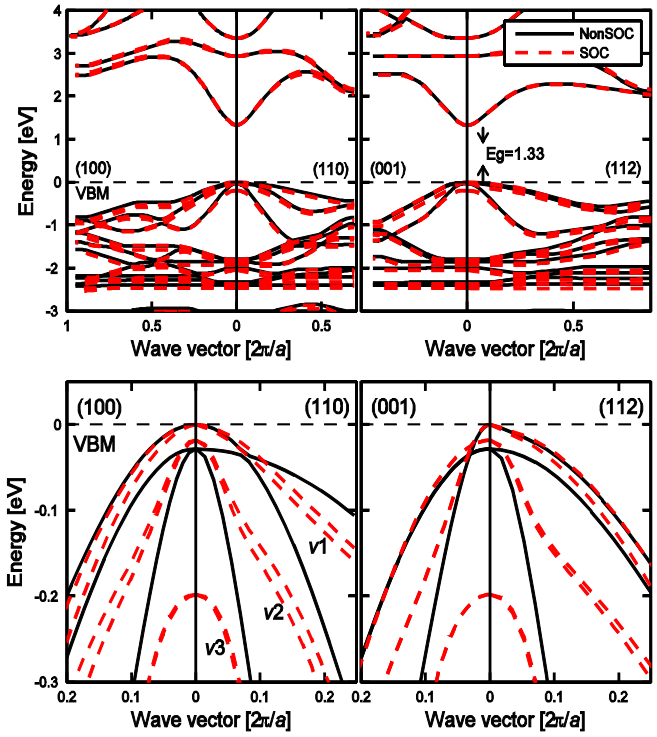

Figure 1. The electronic energy band structure of $CuIn_{0.5}Ga_{0.5}Se_2$ along the four symmetry directions (100), (100), (100) and (100) without and with spin-orbit coupling. The notation *v*1, *v*2, *v*3 and c1 refer to a spin-independent band index. The energies are referred to the VBM. The lower panel is the close-up near the Γ point VBM.

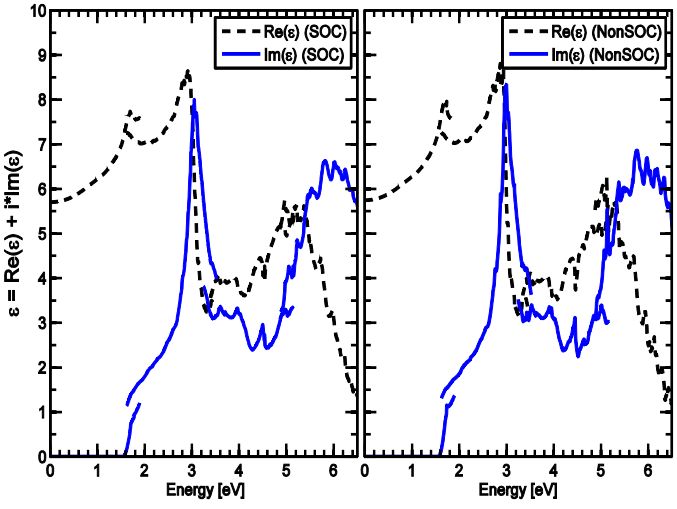

Figure 2. The average of complex of dielectric function is presented (left and right panel). Re(*ε*) is the real part of the dielectric function, and Im(*ε*) is the imaginary part of dielectric function.

and overall shape between the SOC and NonSOC calculations. However, in the lower panel of Figure 3, one can observe that there are more peaks for the SOC case than for the NonSOC case around the main peak, it comes from SOC split from band-to-band transitions ($v3 \rightarrow c1$, $v2 \rightarrow c1$ and $v1 \rightarrow c1$) at the Γ point [12] in Figure 1. Therefore, it is important to consider SOC in the more accurate calculation of the optical respond.

The absorption is shown in Figure 4. One can see that $CuIn_{0.5}G_{0.5}Se_2$ has a broader range of absorption. The main visible sunlight spectrum could be possible to be absorbed. This result is similar with the earlier measurements [13]. The difference between NonSOC and SOC calculations is subtle. However, the SOC shifts the first peak around 50 meV. This shift is due to the SOC at the Γ point (see Figure 1). It shows that the absorption in-

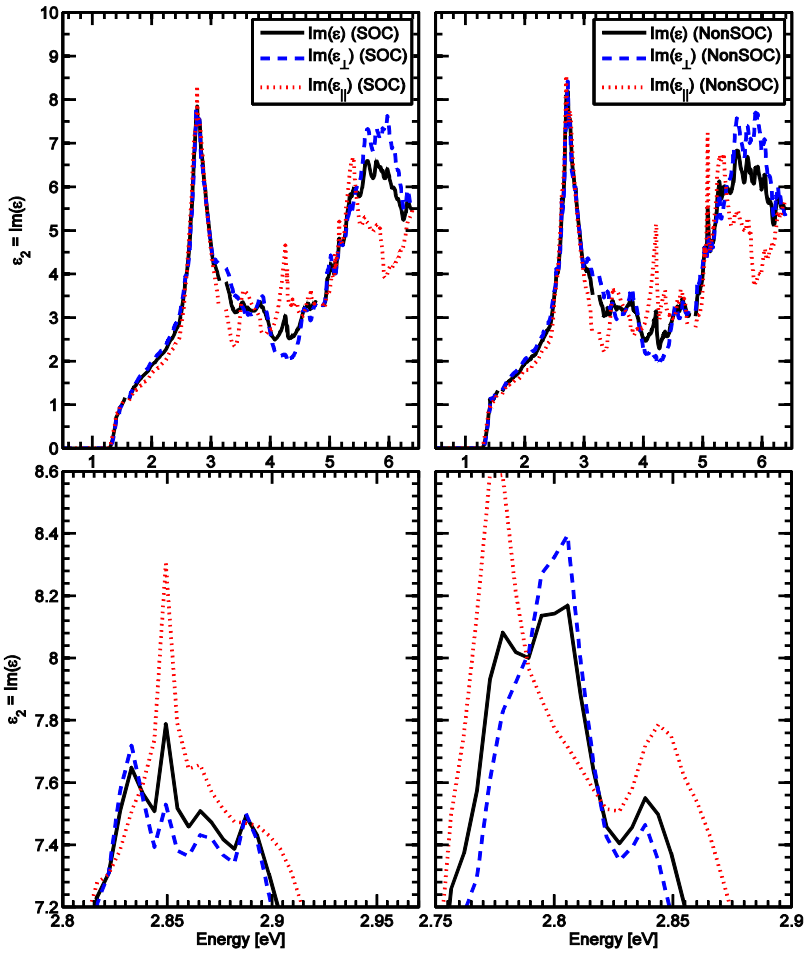

Figure 3. **The tensor of complex of the dielectric function is presented (left and right panel). The average of the polarization along the x and y directions is $\varepsilon_{\perp}$ and parallel with the z direction is $\varepsilon_{\parallel}$. The main peak is presented in the lower panel.**

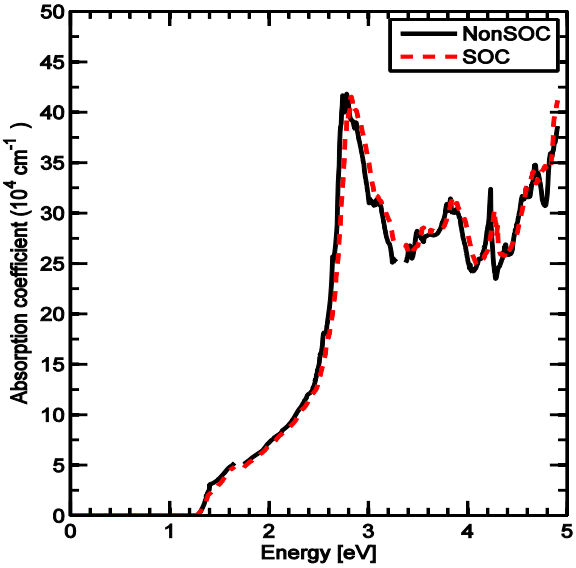

Figure 4. **The average absorption coefficient is presented (solid and dashed line), the result is presented in the range of visible sunlight spectrum.**

creases rapidly from the energy range 1.33 eV to 2.80 eV, and it is stable up to 4.60 eV, then it increases rapidly again.

Figure 5 demonstrates that the average of real (left panel $n(\omega) = (2n_{\perp}(w) + n_{\parallel}(w))/3$) and imaginary (right panel $k(\omega) = (2k_{\perp}(\omega) + k_{\parallel}(\omega))/3$) part of refraction index. The $n(\omega = 0)$ is about 2.40 and 2.39 for the Non-SOC and SOC calculations, respectively. It is in good agreement with other researchers results [14-16]. The SOC only slightly affects the complex refraction index, which shifts the result little. The peak is shifted by 30 meV for refractive index, and 70 meV for the extinction coefficient.

The optical reflectivity for NonSOC and SOC calculations is shown in **Figure 6**. The measurement is rare for the compound $CuIn_{0.5}Ga_{0.5}Se_2$. However, the $CuInSe_2$ is calculated as well using the same method, which has good agreement with experimental measurements [17]. Therefore, our calculation result is reliable in that sense. The $R(\omega = 0)$ is 0.17 for both of NonSOC and SOC calculations. The difference between NonSOC and SOC is small. However, SOC shifts the result about 70 meV.

4. Conclusion

In this work, the band structure and many optical properties of $CuIn_{0.5}Ga_{0.5}Se_2$ are calculated without and with considering the spin-orbit coupling. The software program Wien2k is utilized. The band structure is influenced

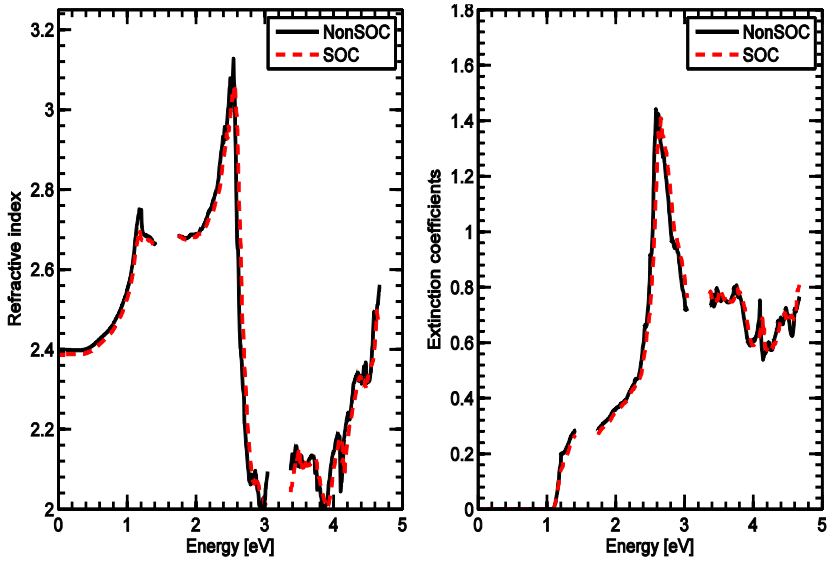

Figure 5. **The average real and imaginary part of refractive index (left panel and right panel) is shown.**

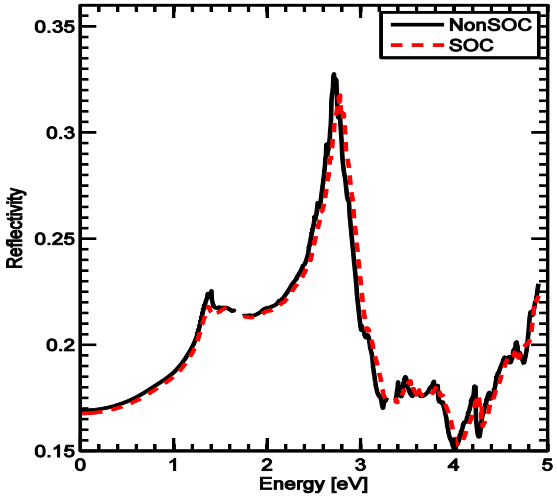

Figure 6. **The average reflectivity is shown in the energy range of visible sunlight spectrum.**

strongly by the SOC, especially the VBs near the Γ point. The main shape of optical properties such as the dielectric function, the absorption coefficient and others show the similarity in both NonSOC and SOC calculations. However, the SOC causes more peaks in the dielectric function, and the shape of most optical properties is shifted slightly by the effect of SOC. Our result is in good agreement with results from earlier experiments and simulations.

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