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First principles study of electronic and optical properties of InAs

Research Article

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Abstract: The electronic and optical properties of InAs in core-level spectra are calculated using the full-potential linearized augmented plane wave plus local orbitials (FP-LAPW+lo) method. The real and imaginary parts of the dielectric function $\varepsilon(\omega)$, the optical absorption coefficient $I(\omega)$, the reflectivity $R(\omega)$, the refractive index $n(\omega)$, and the extinction coefficient $k(\omega)$ are calculated. All these values are in good agreement with the experimental data. The effect of spin-orbit coupling on optical properties is also investigated and found to be quite small.

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Keywords: FP-LAPW+lo • electronic structure • optical properties

1. Introduction

InAs has assumed increasing importance in recent years as a result of its potential applications in long-wavelength optoelectronic and high-speed electronic devices, as electron quantum well materials for both AlSb/InAs/AlSb-based electronic devices and spintronic devices [1–5]. With regard to experimental study, Ley L *et al.* surveyed the total valence band via X-ray photoemission spectra of InAs [6]. Aspnes *et al.* measured the values of pseudodielectric functions using spectroscopic ellipsometry, obtaining several other optical constants [7]. Moreover, Lacroix Y *et al.* studied the optically-excited luminescence as well as the reflectance and transmittance of epitaxial InAs at low temperature [8, 9]. With regard to theoretical study, the structural and electronic properties of InAs have been investigated using the full-potential linearized augmented plane wave (FLAPW) method and pseudopotentials by Massidda *et al.* [10]. Rhim *et al.* calculated optical properties of III-V semiconductors, including InAs, using the full-potential linearized augmented-plane-wave method with screened-exchange local density approximations [11]. A. H. Reshak has investigated optical properties of InAs with the LDA method [5]. However, the results were not in agreement with the experimental data. Thus far, the fundamentals of the observed spectra of InAs remain unclear. In order to better understand the optical properties, then, it is necessary to calculate its electronic structure.

In this work, we have calculated the electronic structure and optical properties of InAs using an accurate full-potential linearized augmented plane wave plus local orbitials (FP-LAPW+lo) method—a method based on density functional theory and implemented in WIEN2K

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code [12]. Local orbitals can improve upon the linearization (increasing the flexibility of the basis) and make possible a consistent treatment of the semicore and valence states in one energy window. The core states were treated altogether relativistically while, for the valence states, a scalar-relativistic treatment without spin-orbit coupling was employed. We have used the generalized gradient approximation (GGA) for the exchange and correlation effects [13]. The underestimation for the energy band gap by GGA was corrected by the scissor approximation technique.

2. Calculation method

Under normal conditions, InAs is a direct, narrow-band-gap semiconductor with zinc-blende crystal structure. The muffin tin radius was taken as 2.00 a.u. for both atoms. The convergence parameter RK_{max}, which controls the size of the basis sets in these calculations, was set to 10 and gives about 913 plane waves for the valence and semicore states. We have chosen 17 local orbits for In p and d, As s, p and d states. In the following, we have distinguished the In($[Ar]3d^{10}4s^2$) and As($[Ne]3s^23p^6$) inner-shell electrons from the valence band electrons of the In($4p^64d^{10}5s^25p^1$) and As($3d^{10}4s^24p^3$) shells. We have used the experimental values of the lattice parameter. Brillouin zone (BZ) integrations within the self-consistency cycles were performed via a tetrahedron method, using 56 k-points in the irreducible BZ. For the calculation of the optical properties (for the imaginary part of the dielectric tensor), a denser sampling of the BZ was needed, using 1015 k-points. An energy convergence of 0.0001 Ry was selected.

The dielectric function $\varepsilon(\omega)$ is a very important parameter for materials because it is the fundamental feature of the linear response to an electromagnetic wave and because it uniquely determines the propagation of the radiation within the material. The optical properties of matter are determined by the dielectric function $\varepsilon(\omega)$ given by $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$. The imaginary part $\varepsilon_2(\omega)$ of $\varepsilon(\omega)$, is calculated directly from the electronic structure through the joint density of the states and the momentum matrix elements between the occupied and unoccupied eigenstates:

$$\varepsilon_2(\omega) = \frac{Ve^2}{2\pi\hbar m^2\omega^2}\int d^3k \sum_{nn'} \left|\left\langle \vec{k}n \left|\vec{p}\right|\vec{k}n' \right\rangle\right|^2 f(\vec{k}n)(1-f(\vec{k}n'))\delta(E_{\vec{k}n} - E_{\vec{k}n'} - \hbar\omega). \quad (1)$$

Here, $\vec{p}$ is the momentum operator, $\left|\vec{k}n\right\rangle$ is the eigenfunction with eigenvalue $E_{\vec{k}n}$, and $f(\vec{k}n)$ is the Fermi distribution function. The evaluation of the matrix elements of the momentum operator in Eq. (1) is done over the muffin tin and interstitial regions separately. A full detailed description of the evaluation of these matrix elements is given in Ref. [14].

The real part $\varepsilon_1(\omega)$ of the dielectric function is computed from $\varepsilon_2(\omega)$ using the Kramers-Kronig relation as follows

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi}\int_0^\infty \frac{\varepsilon_2(\omega')\omega' d\omega'}{\omega'^2 - \omega^2}. \quad (2)$$

All other optical constants–including the reflectivity $R(\omega)$, the absorption coefficient $I(\omega)$, the refractive index $n(\omega)$, and the extinction coefficient $k(\omega)$—can be calculated from $\varepsilon_2(\omega)$ and $\varepsilon_1(\omega)$.

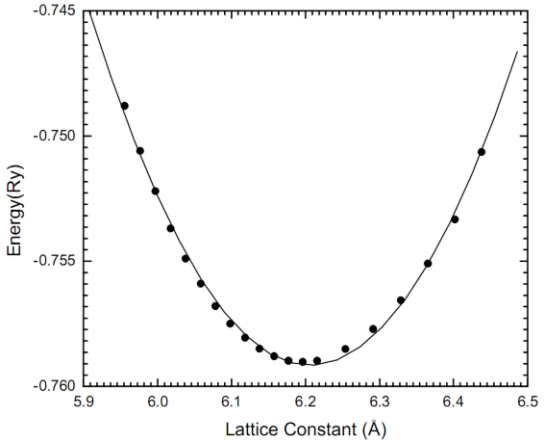

Figure 1. Calculated total energies (relative to E_0= -16288 Ry) as a function of lattice constants for InAs presented. The continuous line is the Murnaghan fit.

3. Results and discussions

3.1. Structural parameters

The equilibrium lattice constant a_0 has been determined by calculating the total energy at many lattice constants around the experimental value. The fitting of these to the Murnaghan equation of state is shown in Fig. 1. The calculated equilibrium lattice parameter is 6.191 Å, a value that is 2.2% larger compared with the experiment. The bulk modulus B_0 is 48.68 Gpa while the first pressure derivative, the bulk modulus B′, is 4.06. These results compare very well with previous pseudopotential calculations [10].

3.2. Electronic structure

The density of states (DOS) and electronic band structure for InAs are given in Figs. 2(a) and 2(b), respectively. The

Fermi level is set to zero energy. The lower valence band formed by the As 4s states is about 11.86 eV below the Fermi level with a bandwidth of 2.03 eV and the peak position at –9.94 eV. The bandwidth of As 4s is consistent with results found by X-ray photoemission spectroscopy (1.71 eV) [6], and is much better than the pseudopotential results (1.18 eV) [10]. The binding energy of the As 4s bands is consistent with most *ab initio* calculations but is usually underestimated by about 0.7 eV when compared to experimental results. This disagreement probably results from the electronic relaxation effects that, as Glassford and Chelikowsky [15] pointed out, are typically around 1 eV. The middle valence band arises from the In 5s states. The binding energy of the In 5s is 5.61 eV while experimental results show 5.82 eV [6]. The upmost valence bands formed by As 4p are located at 0 and –3.16 eV. The conduction band is mainly composed of In s and As p states.

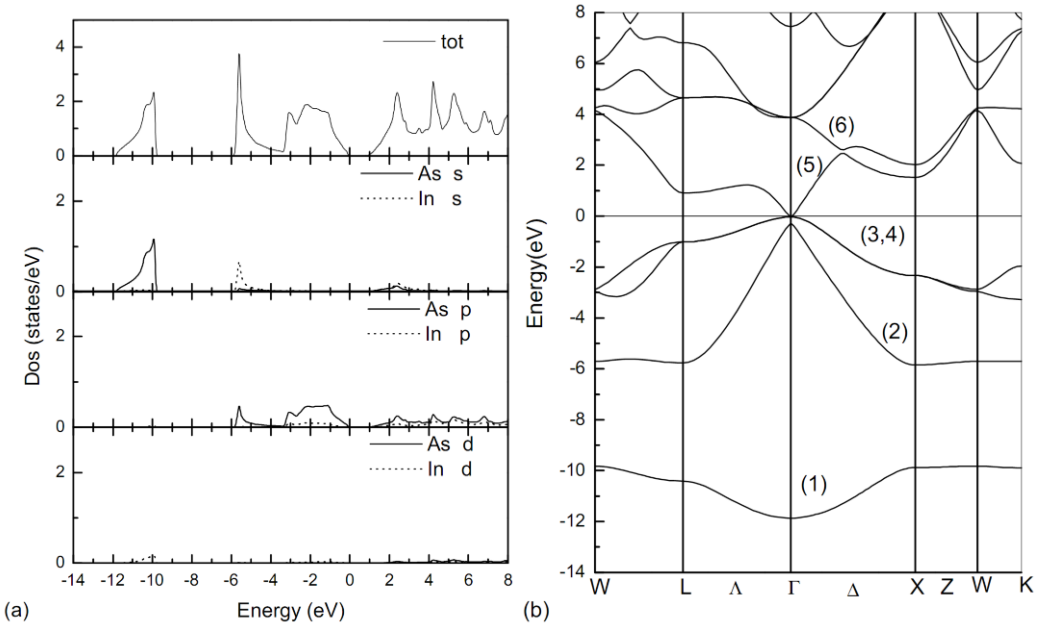

Figure 2. (a) Density of states (DOS) and (b) energy band structure along the high symmetry points in the Brillouin zone for InAs.

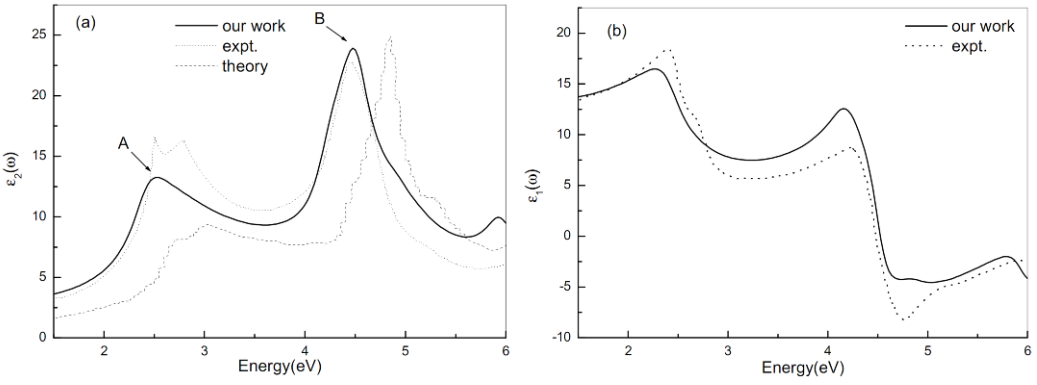

Figure 3. (a) The imaginary part $\varepsilon_2(\omega)$ and (b) real part $\varepsilon_1(\omega)$ of the dielectric function $\varepsilon(\omega)$ of InAs as a function of the photon energy along with experimental data [6] and previous theoretical results [10].

Our calculated direct band gap at asymmetry Γis 0 eV, which is much closer to the experimental value 0.417 eV [9] than to the calculated value of band gap –0.51 eV found by using the FLAPW method [10]. It is well known that the LDA and the GGA usually underestimate the energy gap [16]. This is primarily a result of the fact that they have simple forms with insufficient flexibility for accurately reproducing both exchange-correlation energy and its charge derivative. Engel and Vosko [17], in response to this shortcoming, constructed a new functional form of the GGA that has been shown to improve the results for quantities that depend on the energy eigenvalues, including the band gap [16]. Our calculated direct band gap of 0.34 eV was found by using Engel and Vosko's generalized gradient approximation (EV-GGA). One can see that the values of the calculated band gaps with EV-GGA provide a significant improvement over the earlier results based on GGA and are much closer to the experimental values.

3.3. Optical properties

The real and imaginary parts of the dielectric function for InAs are shown in Figs. 3(a) and 3(b) along with experimental data and previous academic work, respectively. The scissor operator makes a 0.417 eV rigid shift of the conduction band toward higher energies, reproducing the experimental band gap 0.417 eV as compensation for the systematic error of the generalized gradient approximation (GGA). It is apparent from the figure that our calculated results are in good agreement with the experimental data. For the imaginary parts of dielectric function, there are two peaks in our results, located at 2.50 (A) and 4.47 eV (B), respectively. Our calculated peaks' positions are much closer to experimental data (2.52 and 4.40 eV) [7] than the calculated values (2.83 and 4.61 eV) [11] found by using the FLAW method. The result is also better in comparison with Δ_{GGA}=4.47-2.50=1.97 eV, Δ_{exp}=4.40-2.52=1.88 eV [7], and Δ_{LDA}=4.80-2.47=2.33 eV [5]. Peak A (2.50 eV) corresponds primarily to the interband transitions from (3, 4) to (5) along the L direction. The interband transitions from (2, 3 and 4) to (5, 6) are responsible for critical point B resulting from transition along directions Γ, Δ, and X. It is observed that the theoretical peak A at 2.50 eV is lower in amplitude than the experimental one. This could be interpreted as a result of neglecting excitonic and local field effects or lifetime broadening in our calculations. The effect of the spin-orbit coupling (SOC) on the optical properties was also investigated and found to be quite small. This result confirms that the spin-orbit coupling has a minor influence on the optical properties for semiconductor materials [18]. However, Rhim *et al.* found SOC has significant effect on the optical properties for InAs [11].

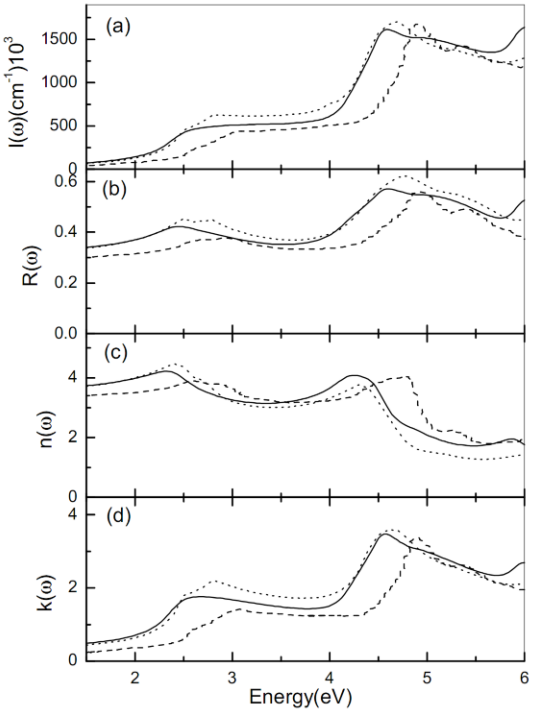

Figure 4. The calculated optical parameters of InAs as a function of the photon energy (eV). $I(\omega)$ (a), $R(\omega)$ (b), $n(\omega)$ (c), and $k(\omega)$ (d) stand for absorption coefficient, reflectivity, refractive index, and extinction coefficient, respectively. The solid lines (——) stand for our work, the dotted lines (· · ·) stand for experimental data [6] and the dashed lines (- - -) stand for previous results [10].

Fig. 4a-e shows the calculated results on the extinction coefficient $k(\omega)$, the refractive index $n(\omega)$, the absorption coefficient $I(\omega)$,and the reflectivity $R(\omega)$, respectively. One can see that our calculated results show good agreement of the peak positions with experiments, much better than previous work.

4. Conclusions

In summary, we have calculated the electronic band structure and optical properties of InAs by using the FP-LAPW+lo method. The scissor approximation makes CB an up shift of 0.417 eV toward higher energy, compensating the error by GGA. We found the effect of the spin-orbit coupling on the optical properties to be quite small. Our calculated results show that the complex dielectric function and optical constants are in good agreement with experimental data.

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