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First-principle calculations of the dielectric function of zinc-blende and wurtzite InN

C Persson[1,3], R Ahuja,[1] A Ferreira da Silva,[2] and B Johansson[1]

[1] Department of Physics, Box 530, University of Uppsala, SE-751 21 Uppsala, Sweden
[2] Instituto de Fisica, Universidade Federal da Bahia, 40210-340 Salvador, Bahia, Brazil

E-mail: clas.persson@fysik.uu.se (C Persson)

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Abstract
The imaginary part of the dielectric function of zinc-blende and wurtzite InN has been calculated using a full-potential linearized augmented plane wave method. We show that the exchange potential of Engel and Vosko gives an insulating ground state for both structures. The real part of the dielectric function has been obtained from the Kramers–Kronig dispersion relations, assuming a quasi-particle band-gap correction according to Bechstedt and Del Sole. We have found that it is necessary to have a good account of the band gap in order to derive the low-frequency optical properties. We present the longitudinal as well as the transverse components in wurtzite InN, showing that the anisotropy is small.

1. Introduction

InN is the least studied of the group III nitrides, primarily because the band gap is about 2 eV, and semiconductor technology already exists for this part of the electro-magnetic spectrum. However, the material is suitable for alloying with GaN and AlN. Knowledge of the optical properties of InN is of great importance for future technological applications [1]. Theoretically, one can investigate the optical properties by means of electronic structure calculations, which normally are based on the local density approximation (LDA) or the generalized gradient approximation (GGA). However, it has been found that both the LDA and GGA describe InN as metallic [2]; this results in an incorrect low-frequency dielectric function.

In the present work we perform calculations of the electronic structures of zinc-blende (zb) and wurtzite (wz) InN, using two different LDA exchange-correlation potentials. The exchange-correlation potential of Perdew and Wang (PW) [3] gives a metallic ground state, whereas using the exchange potential of Engel and Vosko (EV) [4] a semiconductor phase is found for both crystal structures, although the band gap is underestimated. The band gap

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[3] Author to whom correspondence should be addressed.

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has been improved according to a quasi-particle correction. We present the partial density-of-states (DOS) as well as the dielectric function. Furthermore, we also investigated the effects on the low-frequency dielectric function due to the inclusion of electron–optical phonon interactions.

2. Computational method

The computational method is based on a relativistic, full-potential linearized augmented plane wave (FPLAPW) method [5]. We have chosen the experimental values of the lattice constants and the internal lattice parameter [6]. The exchange-correlation potential is treated within the LDA using the potential of PW [3]. Since this potential gives a metallic ground state for InN, we have also used the GGA exchange potential of EV [4], and we show that this potential produces a non-zero band gap.

The applied basis set consists of about 450 (750) plane waves in the interstitial region for the zb (wz) structure. In the atomic regions, the basis set consists of spherical harmonics with azimuthal quantum number $l \leqslant 12$ and a non-spherical contribution with $l \leqslant 4$. The charge density is constructed of the plane waves and spherical harmonics with $l \leqslant 6$, and a $\boldsymbol{k}$-space matrix of 300 $\boldsymbol{k}$ points in the first Brillouin zone. Since calculations of the optical properties require a more dense $\boldsymbol{k}$-space matrix, we use 6000 (7000) $\boldsymbol{k}$ points for the zb (wz) structure in the calculations of the dielectric function.

The imaginary part of the dielectric function, $\varepsilon_2(\omega)$, in the long-wavelength limit, is obtained directly from the electronic structure using the joint DOS and the optical matrix overlap. The real part of the dielectric function, $\varepsilon_1(\omega)$, is calculated from the Kramers–Kronig dispersion relations. For the hexagonal structure, the longitudinal ($\|$) and the transverse ($\perp$) dielectric functions were calculated separately, where the longitudinal direction is along the c-axis.

3. Results

3.1. Energy band gap

The LDA/GGA is known to underestimate the band gap E_g for semiconductors. Earlier published calculations on InN show a metallic ground state (various calculations are presented in [2]). Using the PW potential, we also obtained a zero band gap for both zb- and wz-InN. However, the EV potential gives $E_g = 0.15$ eV in zb-InN and 0.36 eV in wz-InN. The value of the band gap for wz-InN is much too low compared to the experimental value of 2.11 eV [6]. To the best of our knowledge there are no experimental values for E_g in zb-InN. Because of the incorrect band gap one cannot guarantee that the calculations yield an accurate dielectric function. However, it has been shown by Del Sole and Girlanda [7] that the LDA combined with the scissors-operator approximation describes the optical spectrum rather well. We have therefore made an estimate of the correction Δ_g to the band gap by using the quasi-particle method proposed by Bechstedt and Del Sole [8]. Their model for the correction is based on the difference in self-energies obtained from the LDA and the GW approximation. The correction is given by

$$\Delta_g = \frac{e^2 q_{TF}}{2\pi\varepsilon(0)} \int_0^\infty \frac{1}{1+t^2}((1-\alpha_p) f(q_{TF} r_A t) + (1+\alpha_p) f(q_{TF} r_B t))^2 \, \mathrm{d}t \tag{1a}$$

$$f(x) = \frac{1 - 10x^2/3 + x^4}{(1+x^2)^6} \qquad r_A = \frac{a}{4\pi 1.6} \qquad r_B = \frac{a}{4\pi 1.8} \tag{1b}$$

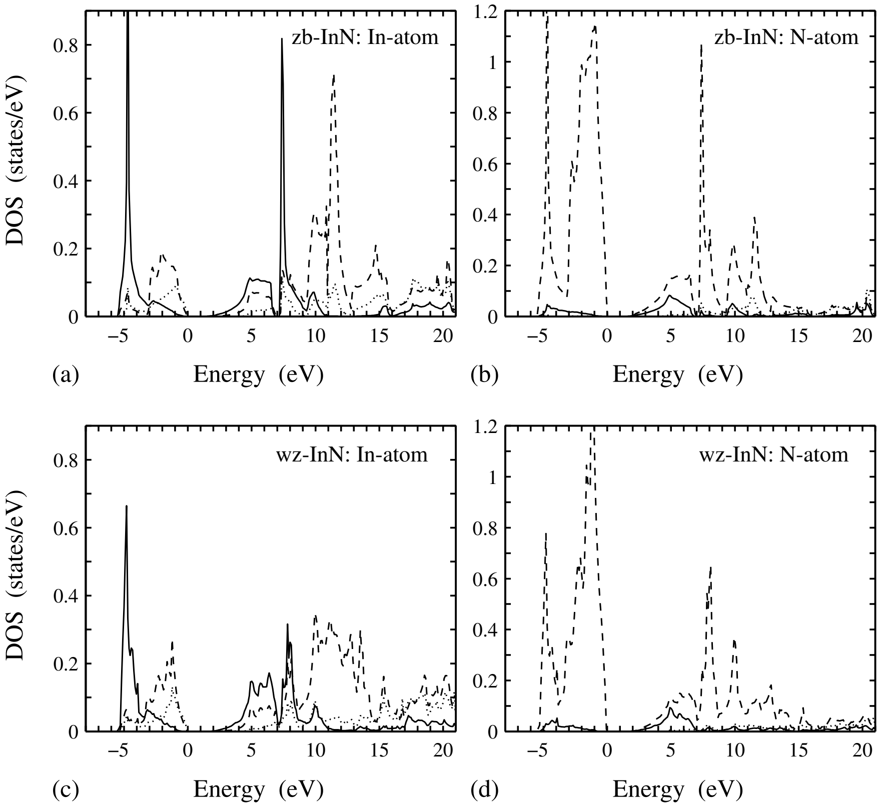

Figure 1. Partial DOS for (a) an In atom in zb-InN, (b) a N atom in zb-InN, (c) an In atom in wz-InN, and (d) a N atom in wz-InN, obtained from the EV potential. The full, dashed, and dotted curves represent s-, p-, and d-like states, respectively. The band-gap correction is included, and the zero of the energy scale is set at the valence band maximum.

where q_{TF} is the Thomas–Fermi wavenumber, $\varepsilon(0)$ is the static dielectric function and α_p is the polarity of the interatomic interaction [8, 9], calculated to be 0.767 for both crystal structures. The correction was derived for cubic structures with lattice constant a and a scalar dielectric function. We have used the above equation also for the wz structure, taking the average dielectric function $\varepsilon(0) = [2\varepsilon_{\perp}(0) + \varepsilon_{\parallel}(0)]/3$, $a = 4/\sqrt{3}$ times the average distance between the nearest neighbours, and in conjunction with the calculated values of the static dielectric function obtained from the present FPLAPW calculation (see section 3.3).

With the correction, the calculated band gap is greatly improved, but is still underestimated. This is in contrast to the case of GaN and AlN, where the corresponding correction leads to good agreement between calculation and experiment [10, 11]. The corrected band gap in zb-InN is $E_g + \Delta_g = 1.03$ (0.59) eV and in wz-InN $E_g + \Delta_g = 1.39$ (0.67) eV for the EV (PW) potential. Since the FPLAPW calculation with the PW potential gives a metallic ground state, the correction was obtained with an estimate of the low-frequency limit of the dielectric function.

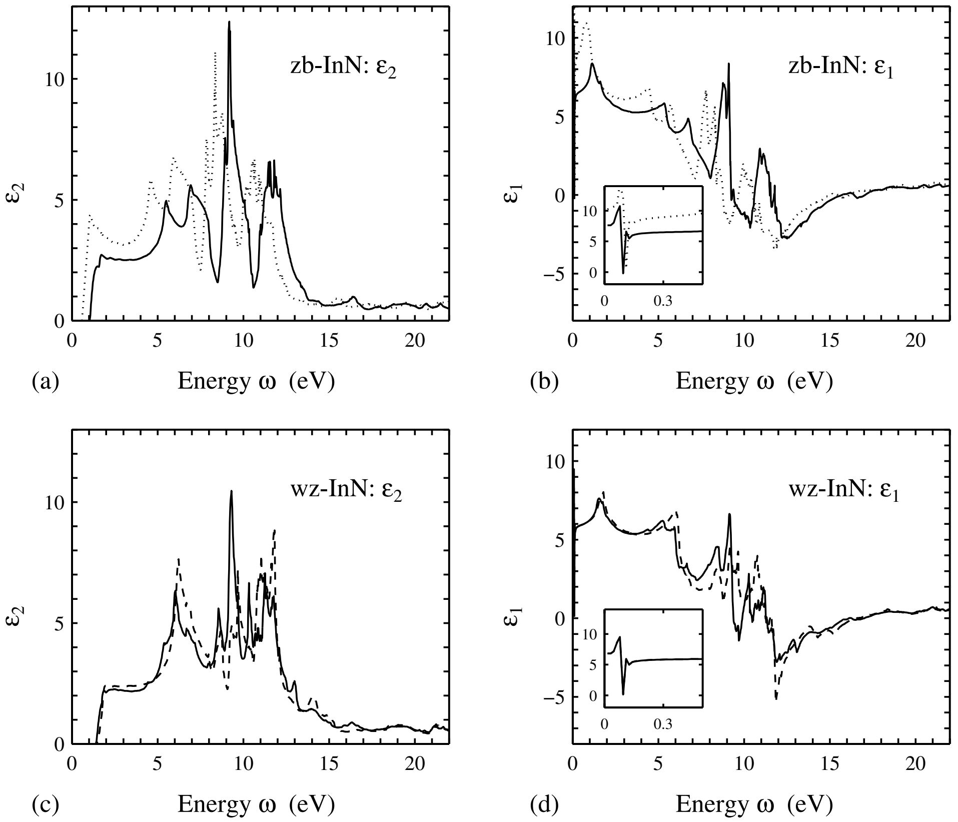

Figure 2. Imaginary part (a) and real part (b) of the dielectric function in zb-InN, using the EV potential (full curves) and the PW-potential (dotted curves). Imaginary part (c) and real part (d) of the dielectric function in wz-InN, calculated with the EV-potential, where full and dashed curves represent the transverse and longitudinal directions, respectively. The band-gap correction is included.

3.2. DOS

The calculated partial DOS for the s-, p-, and d-like states for zb-InN and wz-InN is presented in figure 1, including the band-gap correction. From figure 1 one can observe that the valence-band maximum is dominated by the p states of the N atoms. There is a relatively strong contribution of the d states on the In site, compared to that found in GaN [10]. The conduction-band minimum is almost equally predominated by s and p states.

3.3. Dielectric functions

The complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + \mathrm{i}\varepsilon_2(\omega)$ is presented in figure 2. The imaginary part is obtained directly from the electronic structure calculations, and the onset for absorption has been shifted by Δ_g. From the result, the real part $\varepsilon_1(\omega)$ is determined using the Kramers–Kronig dispersion relation. Another way of taking into account the gap correction would be to shift the conduction bands before calculating $\varepsilon_2(\omega)$. However, good arguments have been given that it is more appropriate to add the shift to $\varepsilon_2(\omega)$ for LDA calculations [7], and therefore that method has been applied.

The electronic structure calculations do not include electron–phonon interactions. However, in polar materials optical phonons play an important role in the low-frequency dielectric function. The screening from the electron–optical phonon (superscript *ep*) interaction can be taken into account through a delta function in $\varepsilon_2(\omega)$ at the transverse phonon frequency ω_{TO} [12]:

$$\varepsilon_2^{ep}(\omega) = \delta(\omega - \omega_{TO})\pi\varepsilon_1(\infty)\frac{(\omega_{LO}^2 - \omega_{TO}^2)}{2\omega_{TO}} \tag{2}$$

where $\varepsilon_1(\infty)$ is the 'high-frequency' dielectric constant, i.e. the static dielectric constant when the electron–optical phonon interaction is excluded. We will use experimental values [1] of the optical phonon energies: $\hbar\omega_{TO} = 59.3$ meV, $\hbar\omega_{LO} = 86.0$ meV in wz-InN, and assume the same values for zb-InN.

By adding $\varepsilon_2^{ep}(\omega)$ to $\varepsilon_2(\omega)$, still including Δ_g, and thereafter calculating $\varepsilon_1(\omega)$ through the Kramers–Kronig dispersion relation, we obtain a more realistic dielectric function at low frequencies. The influence of the electron–optical phonon interactions on $\varepsilon_1(\omega)$ is shown in the insets of figure 2. In table 1 we present the static $\varepsilon_1(0)$ and the high-frequency $\varepsilon_1(\infty)$ dielectric constants. The anisotropy of the dielectric function is very small in wz-InN. When both the phonon contribution and the band-gap correction are neglected, we obtain $\varepsilon_1(\infty) = 8.74$ (12.91) for zb-InN and $\varepsilon_{1,\perp}(\infty) = 7.47$ (11.63) for wz-InN using the EV (PW) potential. Thus, the effects of the band-gap correction are strong in InN.

Table 1. The static $\varepsilon_1(0)$ and high-frequency $\varepsilon_1(\infty)$ dielectric constants obtained from the EV and the PW potentials.

	PW	EV
zb-InN		
$\varepsilon_1(0)$	10.24	7.51
$\varepsilon_1(\infty)$	8.88	6.51
wz-InN		
$\varepsilon_{1,\perp}(0)$	9.51	6.72
$\varepsilon_{1,\parallel}(0)$	9.41	6.73
$\varepsilon_{1,\perp}(\infty)$	8.21	5.87
$\varepsilon_{1,\parallel}(\infty)$	8.11	5.88

4. Conclusions

We have calculated the dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ of zb- and wz-InN, using a FPLAPW method. Although we use different exchange-correlation potentials, the resulting dielectric functions are similar in the high-frequency regime. It is however crucial to have a correct treatment of the band gap and to include screening of the optical phonons for calculating the low-frequency optical properties. We calculated the longitudinal and the transverse parts of the dielectric function separately, showing that the anisotropy is small in wz-InN.

We have shown that the exchange potential of EV gives non-metallic ground states for both zb- and wz-InN, although the band gap is underestimated. Even with the quasi-particle band-gap correction, the calculated band gap is too small. The real part of the dielectric function was determined with the correction.

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