

Carrier-induced refractive index change in InN

C. Bulutay^{1,*} and N. A. Zakhleniuk²

¹ Department of Physics and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Turkey

² Department of Computing and Electronic Systems, University of Essex, Wivenhoe Park, Colchester, CO4 3SQ, UK

Received 2 July 2007, revised 5 November 2007, accepted 6 November 2007

Published online 18 December 2007

PACS 78.20.Ci, 78.30.Fs

* Corresponding author: e-mail bulutay@fen.bilkent.edu.tr, Phone: +90-312-2902511, Fax: +90-312-2664579

Rapid development of InN technology demands comprehensive assessment of the electronic and optoelectronic potential of this material. In this theoretical work the effect of free electrons on the optical properties of the wurtzite phase of InN is investigated. The blue shift of the optical absorption edge by the free-carrier band filling is known as the Burstein-Moss effect for which InN offers to be a very suitable candidate as has been recently demonstrated experimentally. Due to well known Kramers-Kronig relations, a change in absorption is

accompanied by a change in the index of refraction. Considering n-type InN samples with free electron concentrations ranging from 5×10^{17} to $5 \times 10^{20} \text{ cm}^{-3}$, and employing a nonlocal empirical pseudopotential band structure, it is shown that this leads to a few percent change of the index of refraction. These carrier-induced refractive index changes can be utilized in optical switches, furthermore it needs to be taken into account in the design of InN-based optical devices such as lasers and optical modulators.

© 2008 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

1 Introduction The optoelectronic applications of InN are of particular interest since the InGaN alloys are capable to cover wide range of optical spectra from blue-green to near-infrared region [1]. A common property of the grown InN films is the very high unintentional electron density that ranges from 10^{18} to mid- 10^{20} cm^{-3} [2–4]. As a direct consequence it has been shown experimentally that this gives rise to a blue shift of the optical absorption edge [5, 6]. This is known as the Burstein-Moss effect which is the increase of the effective band-gap due to Pauli blocking of the optical transitions to the filled portions of the bands. As a consequence, the high electron concentration in n-type InN samples leads to the reduction of the absorption which is described by the imaginary part of the dielectric function. According to the Kramers-Kronig relation (KKR), the real part of the dielectric function is intimately connected to its imaginary part. Hence, the refractive index of a semiconductor can be modulated by the free carriers [7]. Several types of semiconductor optical devices utilize this effect, like digital switches, phase modulators, tunable Bragg gratings in distributed Bragg reflector lasers [8].

The carrier-induced refractive index change is most pronounced in semiconductors with small effective masses and energy gaps, like n-InSb [7]. With the revised narrow band gap of InN [2], in this theoretical work we show that this carrier-induced refractive index change is particularly important for InN. As we shall show below, this is due to interesting conduction band structure where the band filling gives rise to much larger absorption band edge shifts.

2 Theoretical results For a realistic assessment, we employ a nonlocal empirical pseudopotential band structure of InN that reproduces the most up-to-date band data such as the effective masses and band nonparabolicities [9]. The corresponding density of states is shown in Fig. 1. It can be observed that due to the narrow band-gap nature of this material the low density of states prolongs to about 2 eV from the conduction band edge. This causes substantial band filling effects as illustrated in Fig. 2 which displays the *shift* in the absorption edge, known as the Burstein-Moss effect. As a word of caution, we should note that this shift is to some extent overestimated compared to the experimentally observed value [6]. This is possibly due to

accompanied red shift resulting from the band-gap renormalization [10] which is not included in this work.

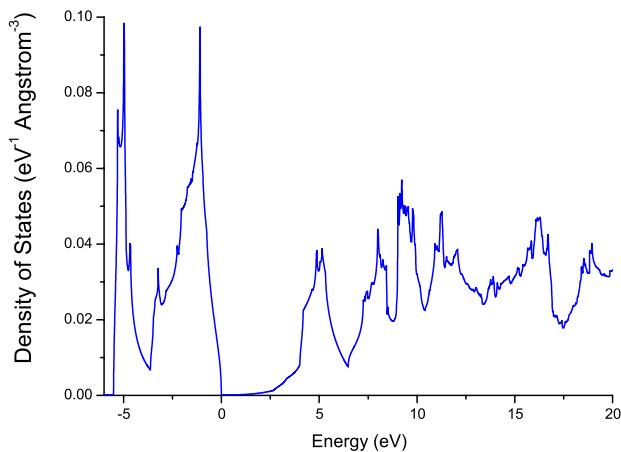


Figure 1 Computed density of states of InN; energy reference is set to valence band maximum.

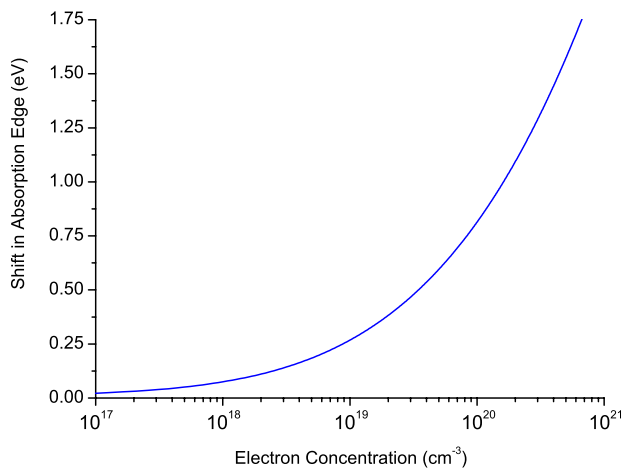


Figure 2 The shift of the absorption edge due to conduction band filling by excess electrons.

The direct consequence of this carrier-induced blue shift of the effective optical gap is the modification of the absorption profile which is described by the imaginary part of the dielectric function, as shown in Fig. 3. On the other hand, as a manifestation of the causality principle, the KKR links the imaginary and real parts of the dielectric function. In Fig. 4 we show the associated modification of the real part of the dielectric function due to excess electrons in InN. Both dielectric functions in Figs. 3 and 4 refer to

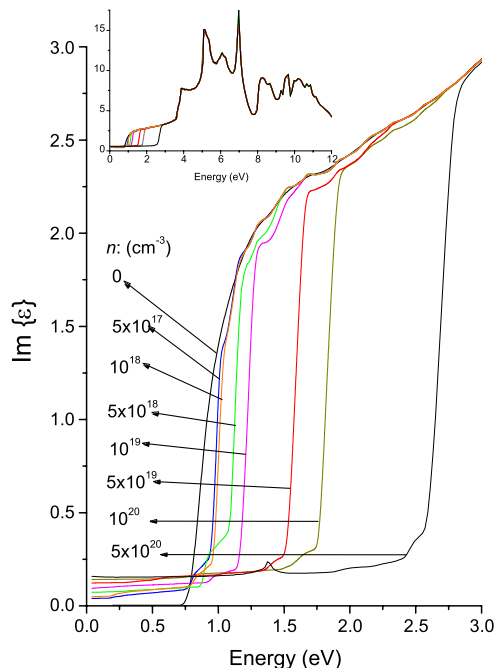


Figure 3 Imaginary part of the in-plane (perpendicular to *c*-axis) dielectric function for different excess electron densities. The inset shows the behaviour for a broader energy range.

the photon polarization perpendicular to the *c*-axis of the wurtzite crystal.

Finally, we display in Fig. 5 the dependence of the static refractive index on the excess electron density. It can be observed that this gives rise to up to few percent carrier-induced tunability of the refractive index. Already at a carrier density of a few 10^{18} cm^{-3} the predicted refractive index change reaches the level of 10^{-2} which is substantially larger than the index change produced by the Pockels or Franz-Keldysh effects under significant applied fields [7]. Undoubtedly, this is a valuable feature for optical device applications such as optical switches, phase modulators and tunable Bragg gratings in Distributed Bragg Reflector lasers.

3 Conclusion In this theoretical work, we investigate the Burstein-Moss effect in *n*-type InN based on the nonlocal empirical pseudopotential band structure. We observe substantial blue-shift of the absorption edge for the typical grown InN samples with unintentional free electron densities on the order of 10^{19} cm^{-3} . By obtaining the full energy dependence of the imaginary part of the dielectric function, its real part is also calculated through the KKR. As a result, a free carrier-induced refractive index change by few percents is demonstrated. This suggests possible InN-based optical device applications such as in the optical switches, phase modulators and tunable Bragg gratings in distributed Bragg reflector lasers. However, it

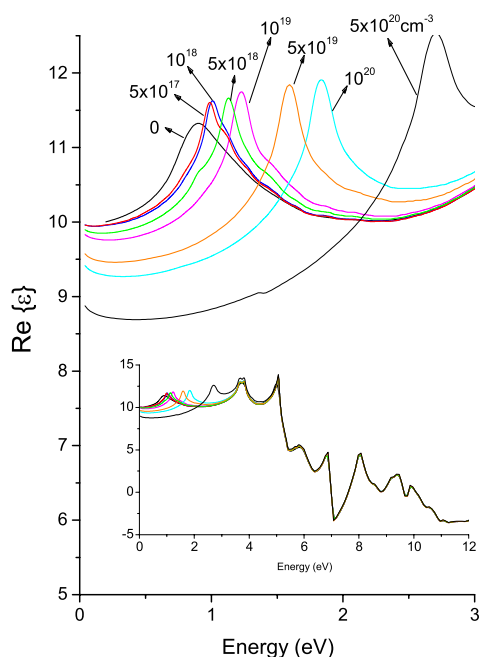


Figure 4 Real part of the in-plane (perpendicular to *c*-axis) dielectric function for different excess electron densities. The inset shows the behaviour for a broader energy range.

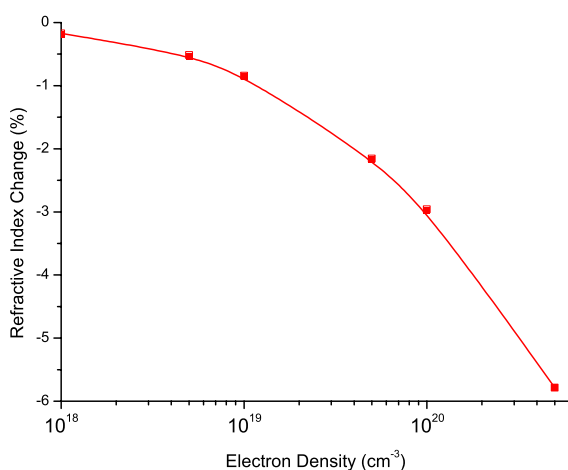


Figure 5 The percentage change of the index of refraction versus excess electron density.

should be noted that we do not include the band gap renormalization which leads to a red shift of the optical gap as the carrier density increases; this becomes quite significant at 10^{19} cm^{-3} and beyond [10] which can partially cancel the Burstein-Moss blue shift. Similarly, the free carrier ab-

sorption is not taken into account. Our primary goal here was to demonstrate the importance of the full-band calculations of the optical parameters of InN.

Acknowledgements The authors would like to thank the British Council for supporting the partnership of the Bilkent and Essex universities. The work of C.B. is also supported by the Turkish Scientific and Technical Council TÜBİTAK within the COST 288 Action.

References

- [1] J. Wu, W. Walukiewicz, K. M. Yu, W. Shan, J. W. Ager, E. E. Haller, H. Lu, W. J. Schaff, W. K. Metzger, and S. Kurtz, *J. Appl. Phys.* **94**, 6477 (2003).
- [2] J. Wu, W. Walukiewicz, K. M. Yu, J. W. Ager III, E. E. Haller, H. Lu, W. J. Schaff, Y. Saito, and Y. Nanishi, *Appl. Phys. Lett.* **80**, 3967 (2002).
- [3] V. Yu. Davydov, A. Klochikhin, V. V. Emtsev, S. V. Ivanov, V. V. Vekshin, F. Bechstedt, J. Furthmüller, H. Harima, A. V. Mudryi, A. Hashimoto, A. Yamamoto, J. Aderhold, J. Graul, and E. E. Haller, *phys. stat. sol. (b)* **230**, R4 (2002).
- [4] Y. Nanishi, Y. Saito, and T. Yamaguchi, *Jpn. J. Appl. Phys.* **42**, 2549 (2003).
- [5] A. G. Bhuiyan, K. Sugita, K. Kasahima, A. Hashimoto, A. Yamamoto, and V. Y. Davydov, *Appl. Phys. Lett.* **83**, 4788 (2003).
- [6] J. Wu, W. Walukiewicz, S. X. Li, R. Armitage, J. C. Ho, E. R. Weber, E. E. Haller, H. Lu, W. J. Schaff, A. Barcz, and R. Jakiela, *Appl. Phys. Lett.* **84**, 2805 (2004).
- [7] B. R. Bennett, R. A. Soref, and J. A. Del Alamo, *IEEE J. Quantum Electron.* **26**, 113 (1990).
- [8] J.-P. Weber, *IEEE J. Quantum Electron.* **30**, 1801 (1994), and references therein.
- [9] C. Bulutay and B. K. Ridley, *Superlattices Microstruct.* **36**, 465 (2004).
- [10] J. Wu, W. Walukiewicz, W. Shan, K. M. Yu, J. W. Ager, E. E. Haller, H. Lu, and W. J. Schaff, *Phys. Rev. B* **66**, 201403 (2002).