Comment on "Mie Resonances, Infrared Emission, and the Band Gap of InN"

In a recent Letter [1] Shubina *et al.* carefully studied the optical properties of two representative sets of InN epilayers grown by both plasma-assisted molecular beam epitaxy (MBE) and metal-organic chemical vapor deposition on sapphire and other substrates. The authors observed a correlation between the occurrence of infrared (IR) photoluminescence (PL) and In precipitates. They concluded that the observed PL can hardly be attributed to the nearband-edge luminescence. The principal absorption edge should be situated at significantly higher photon energies. They suggested that resonances due to scattering or absorption of light in InN layers containing clusters of metallic In may have been erroneously interpreted as the IR band gap absorption in tens of papers.

A very strong argument for their conclusions and interpretation is based on the measurement of the absorption edge of a MBE sample almost free of In inclusions using thermally detected optical absorption (TDOA) at a temperature of 0.35 K [Fig. 2(c) [1]]. It was claimed that the gap energy in a TDOA spectrum corresponds to the position of the kink between the constant and the slope parts in the absorption spectrum, which is near 1.4 eV. They attempt to conclude that the true band edge of InN is somewhere here. They claim that simulations of optical absorption of InN with 2% of metallic In for various depolarization factors (Fig. 5 [1]) show that resonance absorption shifts the absorption spectrum down to the IR range.

Unfortunately the authors have overlooked or ignored arguments against their interpretation of the optical absorption and the conclusion concerning a gap of about 1 eV for InN. First, in all recent theoretical and experimental studies a characteristic line shape of the dielectric function (DF) of InN has been found [2-4]. Independent of the exact value of the calculated or measured gap, there appears a steep increase of the imaginary part from its onset to a plateau in a wide photon energy range as a consequence of the nonparabolicity of the band structure around the Γ point. It seems that this transition region in Fig. 1(c) [1] has been incorrectly identified as the fundamental gap. Moreover, the corresponding sample with a high carrier concentration up to 8.4×10^{19} cm⁻³ should exhibit a huge Burstein-Moss effect of at least 0.4 eV [5] that cuts the absorption above the fundamental gap as seen in the spectrum.

Second, in Ref. [1] the possible influence of In inclusions on the absorption line shape was modeled employing effective medium theory. The host InN material was simulated using optical data with an absorption threshold of about 2.4 eV [6]. This value contradicts the conclusion of the paper and, more importantly, gives poor agreement between measured and simulated absorption spectra in Fig. 5 [1]. We have repeated the simulation for 2% In



FIG. 1. Absorption spectrum simulated for InN with 2% metallic In (dashed line) compared with the measured spectrum (solid line) for an In-free sample [4] that is used in the effective medium theory.

contents and a depolarization factor of 0.07 using a previously reported DF of InN [4] but allowing a variation of the gap. For 2.4 and 1.4 eV we find again no agreement with the measured spectrum. However, the spectrum in Fig. 1 simulated for an onset of the InN absorption at 0.9 eV (expected for a Burstein-Moss shift due to a carrier concentration of 2×10^{19} cm⁻³) fits the TDOA spectrum in Fig. 5 [1] extremely well. The observed absorption maximum around 1 eV is indeed a consequence of metallic In inclusions.

Summarizing, we cannot agree with the identification of the kink position at about 1.4 eV in the optical absorption as the position of the fundamental gap of InN. Rather, all the absorption spectra presented in Ref. [1] can be consistently described in terms of the novel InN with a gap smaller than 1 eV.

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Received 14 May 2004; published 20 December 2004 DOI: 10.1103/PhysRevLett.93.269701 PACS numbers: 78.40.Fy, 78.20.Bh, 78.66.Fd

ACS IIUIIIDEIS. 78.40.Fy, 78.20.DII, 78.00.Fu

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- [1] T. V. Shubina et al., Phys. Rev. Lett. 92, 117407 (2004).
- [2] C. Persson *et al.*, J. Phys. Condens. Matter **13**, 8945 (2001).
- [3] F. Bechstedt et al., Phys. Status Solidi (a) 195, 628 (2003).
- [4] R. Goldhahn *et al.*, Mater. Res. Soc. Symp. Proc. **743**, L5.9 (2003).
- [5] J. Wu et al., Phys. Rev. B 66, 201403 (2002).
- [6] V. V. Sobdev and M. A. Zlobina, Semiconductors **33**, 385 (1999).