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Anisotropy of the dieletric function for hexagonal InN

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Among the group-III nitride semiconductor compounds, the physical properties of InN are known rather poorly. This is mainly attributed to the difficulties in growing high-quality crystals. Currently, the debate focuses on the question concerning the band gap of InN. Interband optical absorption measurements of sputtered polycrystalline InN films yielded a band gap of E_g~1.9 eV. This value has been accepted for a long time and was frequently used as the end-point value for the extrapolation of the band gap in $In_xGa_{1-x}N$ alloys. Studies of epitaxial layers grown by MBE or MOVPE, however, revealed a much narrower gap of E_g~0.7 eV (for a recent review see e.g. Ref.1). Recently, we compared the DF's for both types of films, as obtained from spectroscopic ellipsometry (SE) measurements in the energy range from 0.7 eV up to 5.5 eV, with the results of *first-principles* calculations. It was demonstrated [2] that only the DF of MBE-grown films exhibits the characteristic features being expected for wurtzite InN. Therefore, it was concluded that the band gap is only E_g~0.7 eV.

Calculations predict for hexagonal InN a pronounced optical anisotropy in the range of the higher-energetic critical points [3], i.e. the ordinary ε_o and extraordinary ε_e dielectric tensor components corresponding to the electric fields perpendicular and parallel to the *c*-axis, respectively, differ appreciably. Here we demonstrate for the first time that MBE-grown InN shows this characteristic behaviour.

The optical response of absorbing materials, measured by SE, depends mainly on the in-plane tensor components but only weakly on the component normal to the surface. Therefore, in order to get access to both tensor components, samples are required for which the *c*-axis lies in the surface plane. We succeeded recently in depositing high-quality InN on *r*-plane sapphire substrates with an AlN nucleation layer and GaN buffer using plasma-assisted MBE. The InN film with a thickness of 460 nm was identified to be non-polar *a*-plane which follows the *a*-plane GaN buffer (thickness of 160 nm). Further growth details as well as results of the structural, electrical and optical characterisation has been published elsewhere [4]. The ellipsometric parameters Ψ and Δ were determined for *c*-axis orientation either parallel or perpendicular to the plane of incidence. For the VUV measurements (3 to 9.5 eV), the **3m-N**ormal-**I**ncidence-**M**onochromator **2** was used as light source. The data refer to an angle of incidence of 68.7°.

In order to obtain ε_o and ε_e and not only pseudo-dielectric functions, Ψ and Δ were fitted by taking in to account the sample orientation as well the rms surface roughness of ~6 nm. The corresponding results for the real (ε_1) and imaginary parts (ε_2) of ε_o and ε_e are shown by the full lines in Fig. 1(a) and (b), respectively. First of all, the excellent matching to the data recorded with a commercial ellipsometer (J.A. Wollam Co., Inc.) in the energy range from 0.7 up to 4.5 eV should be noted. At second, the low-energy results prove that the band gap of the *a*-plane InN film does not differ to the previous results for *c*-plane MBE-grown films and is

~0.7 eV (coinciding with the strong increase of ε_2 at this energy followed by nearly constant value up to 3.5 eV).

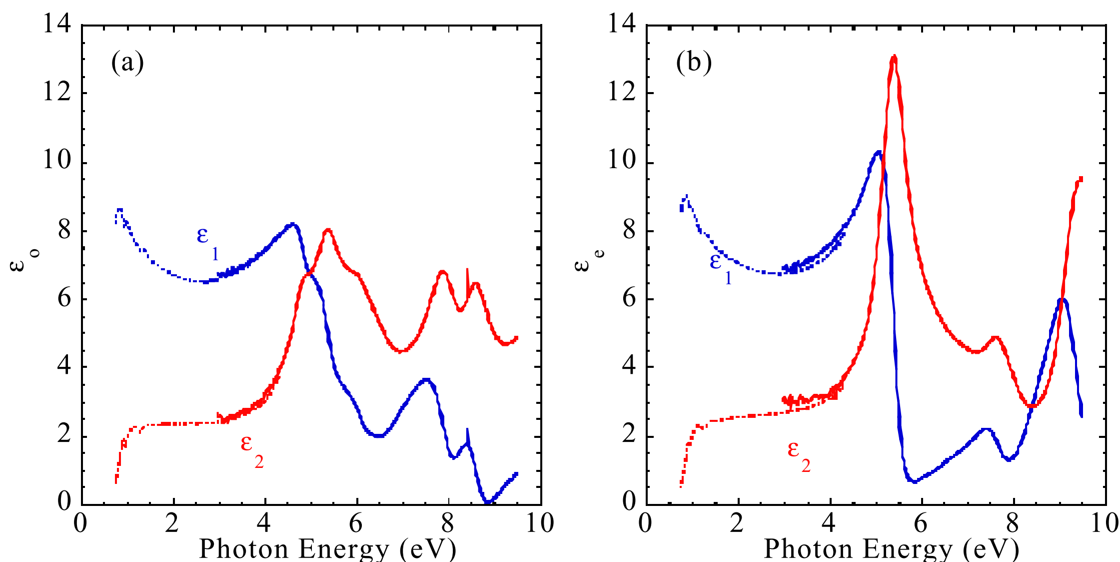

Fig. 1: Real (blue) and imaginary (red) part of the ordinary (a) and extraordinary(b) dielectric tensor components for wurtzite InN. The full lines refer to measurements at BESSy II while the dashed lines were obtained from studies using a commercial ellipsometer.

A comparison of Fig.1 (a) and (b) evidences that the ordinary and extraordinary dielectric tensor components differ appreciably in the range of the higher-energetic interband transitions. The imaginary part ε_2 of ε_o shows peaks at 4.88, 5.38, 6.02, 7.86, and 8.6 eV which are related to the critical points of the band structure. For the extraordinary component, however, only three peaks are resolved at 5.38, 7.63, and 9.44 eV. Furthermore, the magnitude of the peak found for both polarisation directions at 5.38 eV is much larger if the electric field is parallel to the *c*-axis. The qualitative shape of ε_o and ε_e as well as the intensity ratio agrees excellent with theoretical calculations [3]. It emphasises our conclusion that the low band gap (~0.7 eV) materials represent bulk-like InN with wurtzite structure.

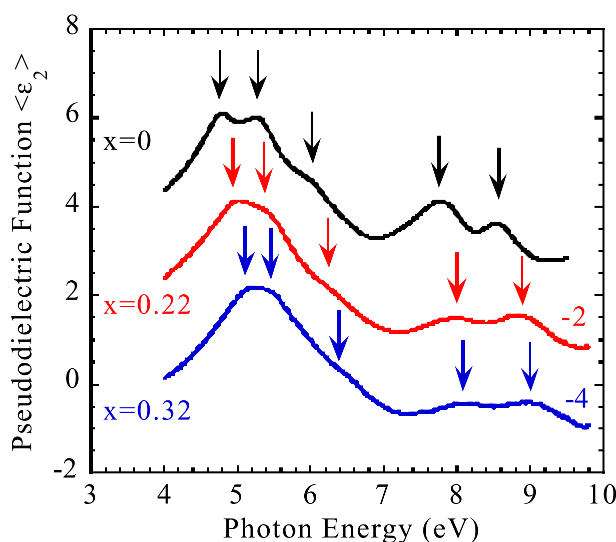

Fig. 2: Imaginary part of the pseudodielectric functions for $In_{1-x}Ga_xN$ alloys corresponding to electric field polarisation perpendicular to the c-axis. The lower curves are shifted for sake of clarity as indicated. The arrows mark the critical points of the band structure.

Studies of In-rich $In_{1-x}Ga_xN$ alloys provide further insight into the general behaviour, although only films with *c*-axis orientation normal to the surface are available until now, i.e. only the ordinary tensor component can be evaluated. Results for the low-energy range has

been reported in Ref. 2. Here we present preliminary data for the VUV range. Fig. 2 compares the imaginary part of pseudodielectric functions for two alloy layers with Ga contents of 22% and 32% with InN. As for InN, five critical points are clearly resolved demonstrating the high structural quality of the films, and as expected they shift continuously to higher energies with increasing Ga concentration. In the next step, the data have to be corrected for surface roughness allowing a comparison with the results of Fig. 1.

In summary, we have reported for the first time the ordinary and extraordinary dielectric tensor components for InN. The observed anisotropy agrees excellent with theoretical calculations, and transition energies for the critical points of the band structure have been determined.

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