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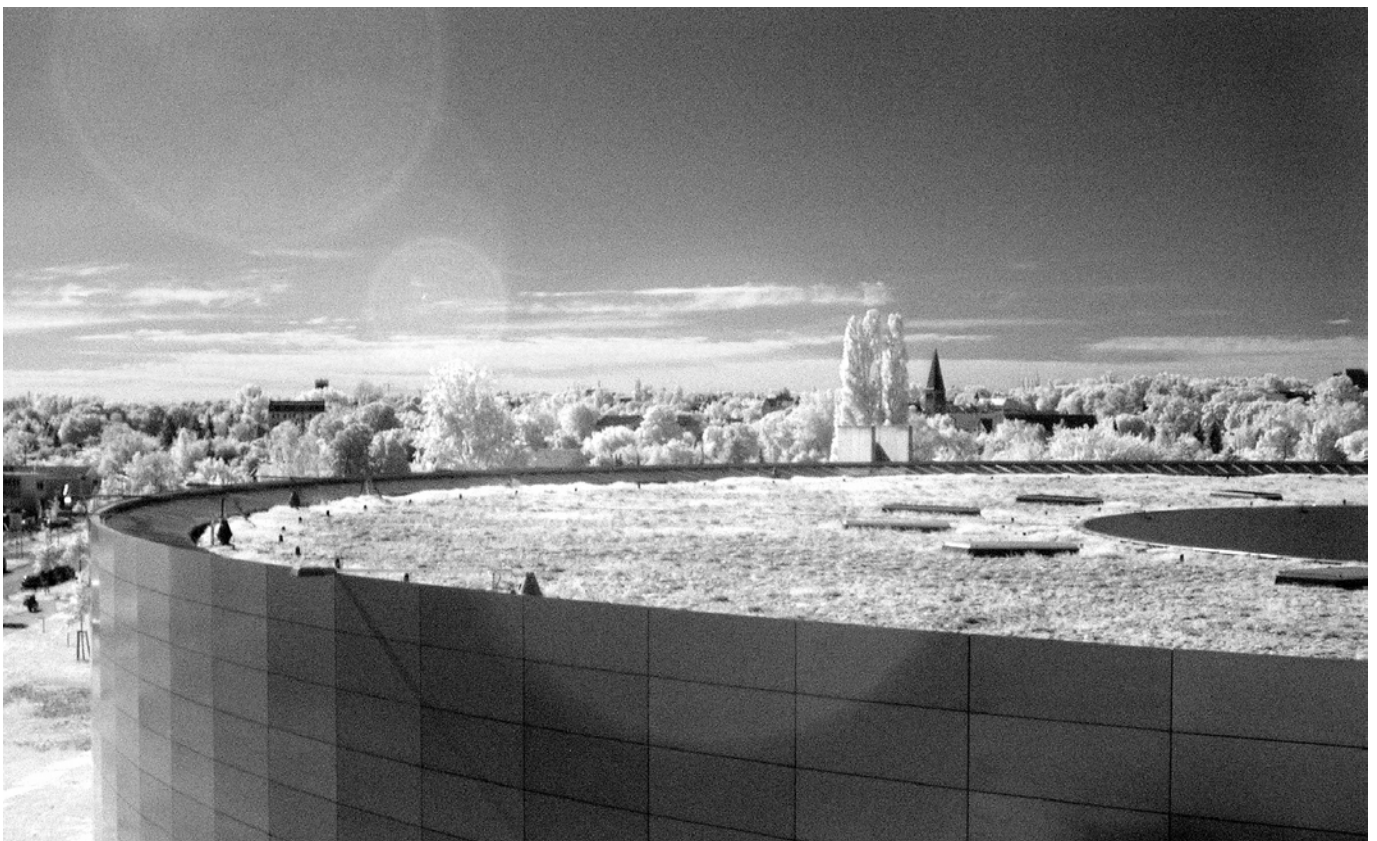
VUV-XUV Dielectric Function of InN

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VUV-XUV Dielectric Function of InN

M. Rakel[1,3], C. Cobet[1,3], R. Goldhahn[2], W. Richter[1] and N. Esser[3]

[1]Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, D-10623 Berlin
[2]Inst. f. Physik, Zentrum f. Mikro- und Nanotechnologien, TU Ilmenau, D-98684 Ilmenau
[3]ISAS- Institute for Analytical Sciences, Albert-Einstein-Str. 9, D-12489 Berlin

An ellipsometric study on InN and GaN in a spectral region from 2.5 till 30eV is presented. These nitrides crystallize in the thermodynamically stable wurtzite (hexagonal) structure and in the metastable zinc blende (cubic) structure. Especially for InN relatively few experimental studies of the optical properties have been carried out although the recently found small band gap value of 0.7 eV increases the possible emission range of III-nitride optoelectronic devices from the deep UV down to the near IR region. A further advantage of InN is the small electron effective mass what leads to a large saturation velocity. That makes InN to a promising material for high speed or high frequency electronic devices.

By taking advantage of using linear polarized light in an ellipsometric measurement, the dielectric tensor components corresponding to the electric field vectors along the crystallographic axes, can be separately examined. This allows a separation of direction dependent electronic contributions and thus a study of the anisotropy of the chemical bondings. In particular for the wurtzite structure (coordination number 4) the anisotropy in the chemical bonds along the c axis and in the plane (slightly tilted with respect to the c plane) defines the amount of optical transitions in different directions. For the ellipsometric investigation of this anisotropic electronic properties hexagonal samples are required for which the c-axis lies in the sur-

Figure 1: The imaginary parts of the ordinary ε_{o2} and extraordinary ε_{e2} DF of a-plane InN in the spectral range of interband transitions.

face plane, like in m-plane GaN (1-100) and a-plane InN (11-20). As recently reported in Ref. [6] one succeeded in depositing high quality a-plane InN on r-plane sapphire with an AlN nucleation and GaN buffer layer using plasma assisted MBE. By use of these samples measurements of the different components were realized by rotating the sample in the two high symmetry orientations were the optical axis is either parallel or perpendicular to the plane of incidence.

The ordinary and extraordinary dielectric function (DF) where determined the first time with the BESSY ellipsometer at the 3m-NIM-monochromator in the spectral range above the common band gap of about 0.7 eV [4, 5]. The imaginary parts of both components (Fig. 1) show remarkable differences. While for the ordinary component at least seven absorption structures at 4.82, 5.38, 6.18, 6.54, 7.66, 7.94 and 8.54 eV contribute to the DF, we can identify only three at 5.40, 7.61 and 9.16 eV in the extraordinary component up to 10 eV . Furthermore, correlated absorption peaks differ in the magnitude and are shifted in their energy against each other. A heuristic assignment of the different structures can be found in comparison with earlier results on wurtzite-type GaN [3] and CdS or $CdSe$ [1]. Within this assignment the cubic E_1 transitions are understood in terms of critical points (CP) or lines along the $\pm[111]$ directions of the corresponding zinc-blende Brillouin
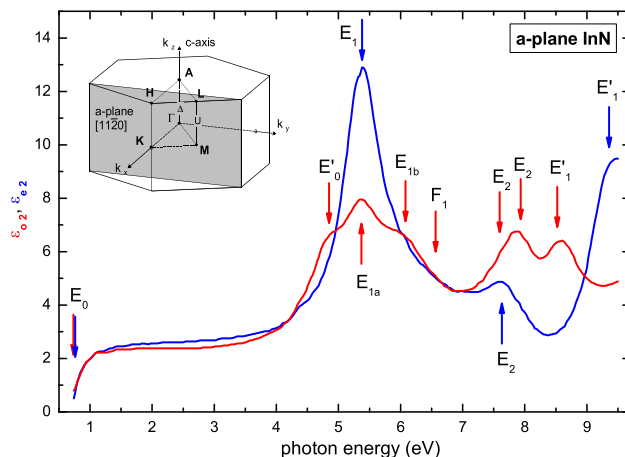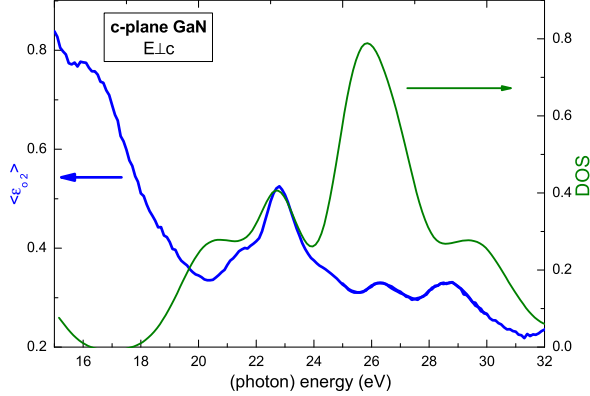
Figure 2: Imaginary part of the hex. GaN ordinary DF in comparison with the DOS of p-like conduction bands (DFT-LDA [7]). The energy position of the DOS was calculated in relationship to the Ga3d-core states and shifted by 1.5 eV.
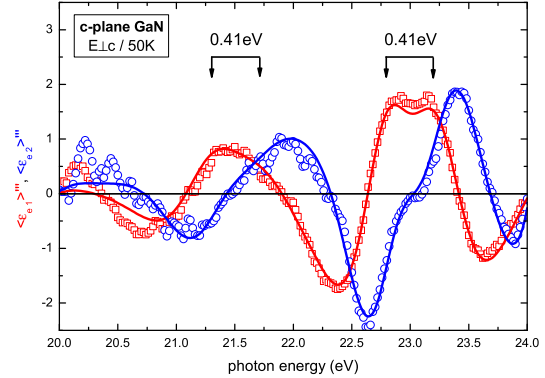

Figure 3: Third derivative of the ordinary DF of the hex. GaN. Both Ga3d valance band transitions structures show distinct a spin-orbit splitting of 0.41 eV.

zone. In the cubic crystals, these states are degenerated with the corresponding stats in the $\pm[1\overline{1}1]$, $\pm[\overline{1}1\overline{1}]$, and $\pm[\overline{1}11]$ directions. The symmetry of the $\pm[111]$ directions are very similar to that of the corresponding $\pm[0001]$ c axis of wurtzite crystals, while the other three split in wurtzite structures from $\pm[111]$ but remain degenerate with each other due to the sixfold symmetry around the c axis. Together with the corresponding cubic E'_0 CP this two CP's can be attributed to the three absorption structures at 4.82, 5.38, 6.18 eV in the ordinary component. A symmetry consideration indicates that the [111]-like singlet appears only for $\varepsilon_\parallel$ while the $\pm[1\overline{1}1]$ triplet should appear for both polarizations. According to this interpretation, the measured extraordinary component shows only one strong absorption structure at 5.40 eV where the $\pm[1\overline{1}1]$ triplet is found degenerated with the E'_0 transitions. Within this argumentation the following two major absorption structures in the ordinary component of the DF can be attributed to the cubic E_2 (located along the $\pm[111]$ direction) and E'_1 CP's. But in the hexagonal crystal structure no associate high symmetry axis could be related to the cubic $\pm[111]$ direction. Consequently, the correlated hexagonal InN E_2 CP's are found in both components of the DF while the E'_1 CP is showing again a strong anisotropic behaviour. But, in the limitation of the presented spectral range no comparable splitting in the ordinary component is found like for the E_1 transition. Anyhow, discrepancies beyond the pure symmetry argumentation can be attributed to anisotropic chemical bonds parallel and perpendicular to the c axis.

In a spectral region above 15eV the DF of GaN and InN is dominated by optical transitions between the Ga3d/In4d semicore and the p-like unoccupied (conduction) electron states. Because of the nondispersive behaviour of the d-band one gets a characteristic view of the p-like conduction bands. The electron transition is governed by the dipole selection rules what results in the fact, that a d electron can only be excited to p- or f-orbital. In the case of c-plane GaN the DFT-LDA calculations for the p-like DOS are fitting into the experimental spectra what is shown in Fig. 2. With a resolution better than 0.02eV we find also evidences for the predicted spin-orbit splitting of the d-bands. Similar to the theoretical predictions or photo emission measurements we determine a spin-orbit splitting of 0.41 eV for GaN (Fig. 3). In Fig. 4 the DF of a-plane InN is shown for both components. From the pure symmetry argumentation no principle differences are expected between the hexagonal ordinary and extraordinary or the cubic DF. But the two measured components differ considerable in the principal line shape and emphasis the assumption of a large anisotropy in the chemical bonding. For the In4d levels a somewhat higher spin-orbit splitting is predicted than for GaN. Possibly, this is not resolved due to the low crystal quality of the available samples.

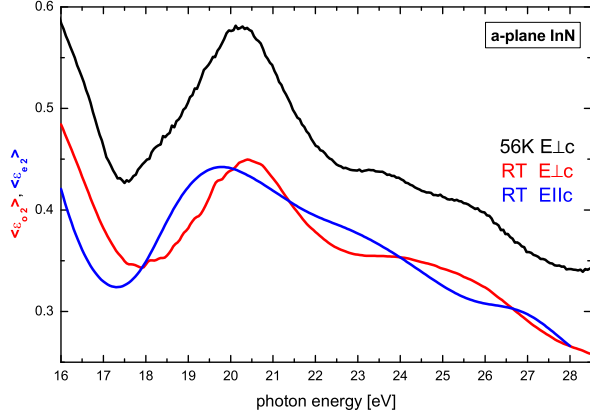For the XUV-measurements (12-30eV) the TGM-4 beamline was used as light source.

Figure 4: Imaginary parts of the ordinary ε_{o2} and extraordinary ε_{e2} effective DF of a-plane InN in the spectral range of the In4d excitations.
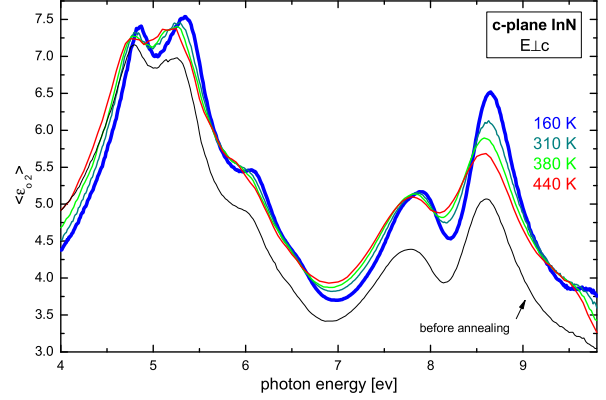

Figure 5: Imaginary part of the ordinary ε_{o2} DF function of c-plane InN at different temperatures.

Finally VUV ellipsometric measurements were also taken on c-plane MBE grown InN (1070 nm layer thickness) at the 3m-NIM1 beamline. It is assumed that InN forms a native oxide on the surface and is highly water contaminated while leaving it in air atmosphere. In order to get rid of these contaminations, the sample was annealed at 480°C for 10 min in UHV. This kind of "deoxidation" yields to a considerable change in amplitudes like shown. For temperature dependent investigations, spectra were taken between 440 K and 160 K. Fig. 5 shows a comparison with the room temperature spectra. Like expected there is a blue shift for the low and a red energy shift for the high temperature structures, whereas the low temperature spectra has a much sharper quality. After first and second derivation analysis under consideration of the Kramers-Kronig consistency we can clearly verify seven interband transition peaks for energies till 10eV as discussed above. But surprisingly, we observed remarkable variations in the amplitude behaviour for the different interband transitions, especially for the structure at 8.6 eV. The latter shows a much stronger increase of peak height with decreasing temperature than the other structures. A closed cycle cryostate will be mounted in the future in order to enhance interband transition structures and to resolve the predicted anomalous spin-orbit splittings of the top valence bands [2].

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