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Conduction band properties of III-nitrides characterized by synchrotron ellipsometry on core level excitations

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Group III nitrides such as Ga-, Al- and In-nitride and compounds are a class of semiconductors with one of the highest technological potential today. But in contrast to the recent advances in epitaxial growth and technology, the understanding of fundamental material properties is surprisingly poor. Many questions concerning the electronic band structure are still open. A prominent example is the ongoing discussion about the exact value of the fundamental band gap of InN. A mayor problem for theoretical calculations is the correct treatment of In4d/Ga3d-core electrons, which slightly interact with the nitrogen 2s valence electrons. In GaN this interaction is much weaker than in InN. The s-d-coupling is difficult to handle, because it results also in an additional p-d repulsion effect [2]. This coupling is may be responsible for the very low band gap of InN. The determination of the relative energetic positions between the valence and conduction bands could provide already helpful information [7]. But a complete experimental analysis of electronic transitions (excitations) is mandatory for testing and validating theoretical results. Common methods are either photoemission experiments, which determine e.g. the valence band DOS with respect to the Fermi level, or optical reflection and absorption measurements, which reveal interband electronic transitions in the visible and VUV spectral range.

We use the synchrotron light at BESSY II in order to access the optical properties of GaN and InN in the far VUV spectral range by spectroscopic ellipsometry [4, 11]. This measurement technique is based on the determination of the polarization of light before and after the reflection on the sample surface under a certain angle of incidence. The measured amplitude and phase differences can be translated subsequently into the dielectric function (DF) or the commonly used refractive and absorption coefficient.

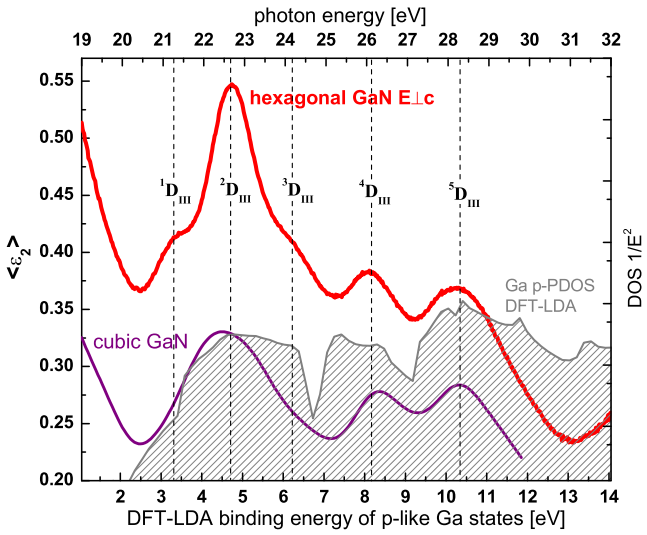

Figure 1: Imaginary part of the measured DF of hexagonal and cubic GaN (solid) in comparison to the calculated PDOS of the p-like empty states around the Ga-atoms (patterned) [10]. The Ga3d transition structures are denoted with $^1D_{III} - {}^5D_{III}$ according to the notation of Cardona et.al. [3].

Above 18 eV the DF of GaN and InN is dominated by optical transitions between the Ga3d/In4d core states and the p-like unoccupied (conduction) electron bands. Transitions to conduction states with s-character are not allowed due to the dipole selection rules. However, the localized d-states have a sharp binding energy without significant dispersion in the entire Brillouin zone. Thus, these d-levels can be used to explore the site specific density of empty states in a similar manner as known from X-ray absorption on the N1s core level edge [8]. The stable crystal structure of III-nitrides is the hexagonal wurtzite lattice where the hexagonal closed packed III-nitride layers are stacked in an ABAB... sequence. Thus, the electronic and optical properties reveal an extraordinary axis, the c-axis, parallel to the stacking sequence. All other perpendicular directions remain degenerated. The metastable cubic zincblende crystal structure of GaN was successfully stabilized

in thin films on appropriate cubic substrates [1]. The electronic as well as optical properties of this cubic material are assumed to be isotropic. However, the integrated density of conduction band states should be almost identical in both crystal structures. This is, in fact, observed in our ellipsometric measurements on a wurtzite and zincblende GaN sample. Figure 1 shows the imaginary part of the DF in the spectral range of Ga3d transitions. The DF is proportional to the number of excited electrons and should directly relate to the partial density of states (PDOS) with dominant p-character in the conduction bands. Both line shapes are almost the same. The lower overall amplitude and the broadening of transition features are related to the lower crystal quality of the cubic sample.

We compare these measurements in figure 1 also to the calculated PDOS of p-like states on the Ga site (patterned) of cubic GaN. As assumed, the DF is approximately reproduced by the calculated PDOS although excitonic effects as well as k and energy dependent variations of matrix elements could influence the DF. The DF of wurtzite GaN was determined on a c-plane sample, where the c-axis is perpendicularly oriented to the surface. In this orientation we have determined the ordinary DF, which relates to excitations with the electric field vector perpendicular to the c-axis. In order to access also the extraordinary DF we use M-plane GaN [0$\bar{1}$00] sample, where the c-axis lies in the surface plane.

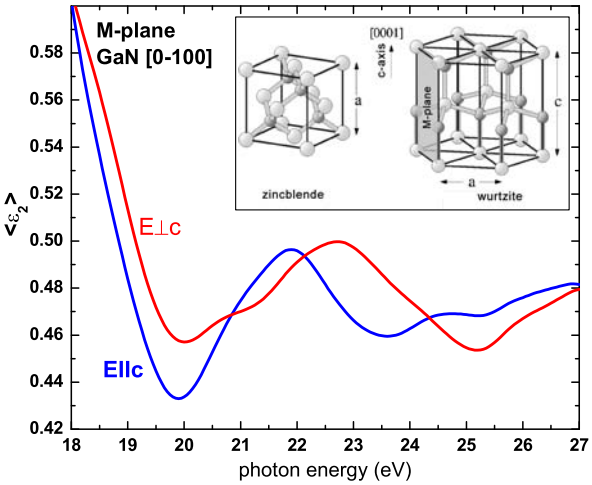

Figure 2: Imaginary part of the ordinary and extraordinary DF of GaN between 18 and 27eV measured on M-plane GaN [1-100].

By measuring in the two high symmetry orientations we can determine both dielectric tensor components which are presented in figure 2. According to these measurements we observe a reasonable shift to lower energies and a slightly different line shape of the extraordinary DF while the ordinary component is almost identical to the measurements on the c-plane sample. This shift could be explained by a distortion of the chemical bondings along the c-axis. Polarization effects as well as a charge accumulation at interfaces along the extraordinary crystal axis are already known in III nitrides.

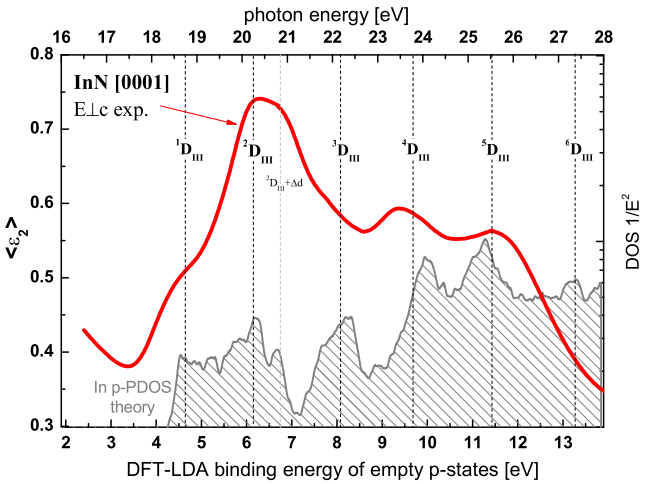

Figure 3: Imaginary part of the measured DF of hexagonal InN (solid) in comparison to the calculated PDOS of the p-like empty states around the In-atoms (patterned) [5]. The In4d transition structures are denoted with ${}^1D_{III} - {}^6D_{III}$. All these valence band characteristic features split up due to a spin orbit splitting of the In4d-states, which is notable e.g. in the ${}^2D_{III}$ and ${}^2D_{III} + \Delta d$ structure.

Figure 3 shows a comparison between the imaginary part of the ordinary DF of wurtzite InN and the calculated PDOS of p-like InN conduction band states. Between 16 and 28 eV the DF is again dominated by excitations of In4d core-states. The line shape of the DF and the assumed PDOS are nearly identical to the respective GaN measurements but shifted by about 2 eV to lower energies. This shift correlates to the lower band gap of InN in comparison to GaN. Recent photoemission experiments report a binding

energy of the $In4d_{5/2}$ electrons of 17.4±0.1 eV with respect to the valence band maximum [9]. On the other hand, we can determine the onset of In4d transitions to conduction bands at about 18 eV (fig. 3). The comparison of both measurements further support the new results about a InN band gap at 0.68 eV [6].

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