Dielectric function and critical points of the band structure for hexagonal and cubic GaN and AlN

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Over the past 10 years, the group-III nitride semiconductor alloy system (In,Ga)N was intensively studied because its unique properties allows the fabrication of very efficient light emitting and laser diodes for the blue/green spectral regions. The development of deep-UV lasers however can only be achieved if GaN, AlN, and their related alloys are used. Recently, deep-ultraviolet lasing at 241 nm was reported [1]. Other applications of AlN/GaN are the development of short period superlattices as Bloch oscillators [2] or distributed Bragg mirrors with very high reflectivity [3]. For the design of such heterostructures and for the evaluation of the achieved properties detailed knowledge of the complex dielectric function (DF) over an extended energy range is essential. It turns out, however, that the current knowledge of the DF for (Al,Ga)N is rather poor. Either the studies are restricted to the transparent region below the band gap [4], or only pseudo-dielectric functions were reported [5]. Here, we report for the first time DF's for GaN and AlN with both wurtzite and zincblende crystal structure as obtained from spectroscopic ellipsometry (SE) measurements. From the data the transition energies at critical points of the band structure are extracted. Preliminary studies of hexagonal AlGaN alloys with various Al concentrations allow in addition the determination of the bowing parameters (b) characterising the deviation of the peak shifts from linear behaviour.

Hexagonal GaN (thickness 1800 nm) and AlGaN films (400 nm on a 400 nm thick GaN buffer) were grown by MOVPE on sapphire substrates. Growth details can be found elsewhere [6]. The investigated AlN layers (200 nm) were deposited by plasma-induced MBE on Si(111). Either hexagonal or cubic films were obtained depending on the carbonisation conditions prior to growth (formation of approximately 3 nm thick in 3C-SiC coverage of Si) [7]. The cubic GaN under investigation is 600 nm thick and was grown by MBE on a 3C-SiC(100) substrate. For the VUV measurements (3 to 9.5 eV), the **3m-N**ormal-**I**ncidence-**M**onochromator **1** at BESSYII was used as light source. The ellipsometric parameters Ψ and Δ were recorded at an angle of incidence of 68°. Prior to the final measurements the samples were heated up to 400 °C for 10 minutes which removes residual organic contamination as monitored by a mass spectrometer and emphasised by a comparison of the pseudo DF's. For the determination of the DF in the low-energy range we used a commercial ellipsometer (J.A. Wollam Co., Inc.).

In order to obtain 'true' DF's and not only pseudo-dielectric functions, Ψ and Δ were fitted by taking in to account the rms surface roughness (for most films below ~1 nm) as well as the interface layers. Results for the real (ε_1) and imaginary parts (ε_2) of hexagonal GaN and

AlN are shown in Fig. 1. Due to (0001) orientation of the films, the data correspond nearly to the ordinary DF. First of all, the excellent matching of the data recorded by both ellipsometers should be noted. Taking into account the exciton binding energies, we obtain at the Γ-point of the Brillouin zone values for E_0 (splitting between Γ_9^V valence and Γ_7^C conduction band) of 3.45 eV (6.25 eV) for GaN (AlN). The other critical point are found at 6.95 (7.96) eV, 7.89 (8.95) eV, and 9.08 eV. Although theoretical calculations [8] yield qualitatively the same spectral dependency, the magnitudes or peak positions differ still.
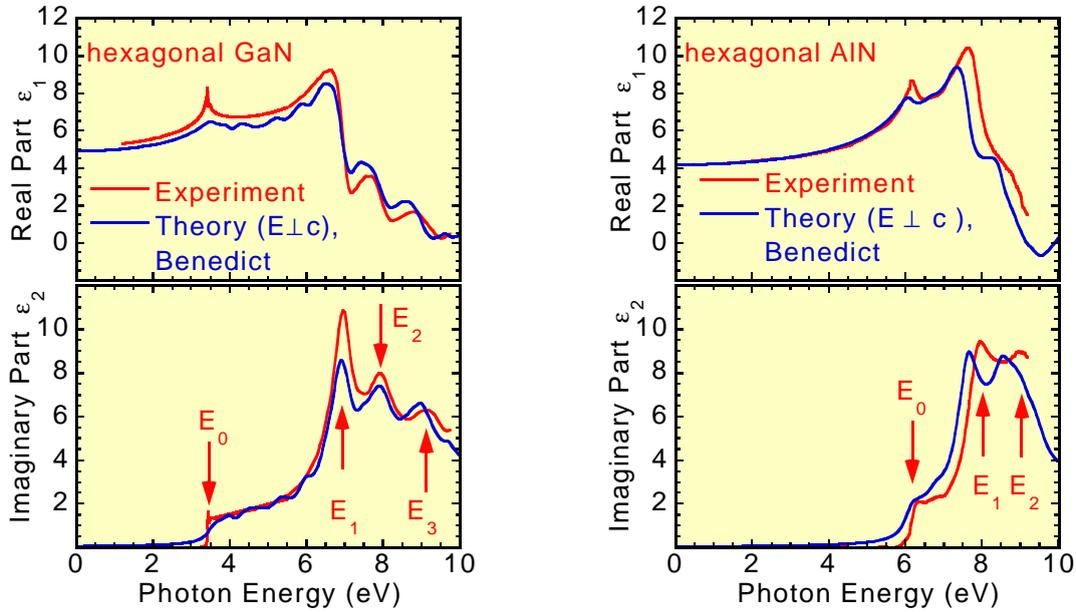
Fig. 1: Comparison of experimentally determined DF's (red) of hexagonal GaN (left) and AlN (right) with the results of theoretical calculations (blue) [8]. Critical point energies are indicated by arrows.
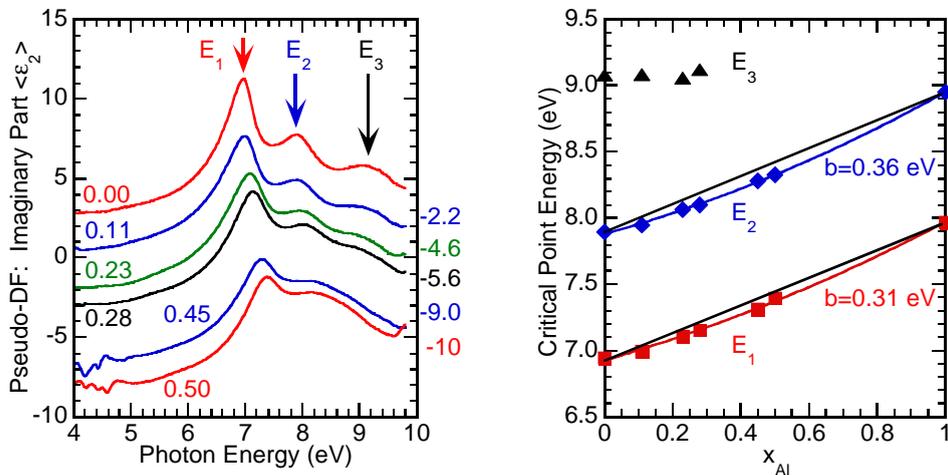
Fig. 2: Imaginary part (left) of the pseudo-dielectric functions for hexagonal $Al_xGa_{1-x}N$ alloy. Dependency of the critical point energies on the alloy composition and the fit results for the determination of the bowing parameter b are shown on the right.

Figure 2 (left) shows the imaginary part of pseudo DF's for AlGaN alloys with Al content up to 50%. Compared to previous studies [5], the critical points are much better resolved emphasising the excellent structural and surface properties of the films. In contrast to the analysis presented in Ref. 5, we find a clear deviation from linear increase of the E_1 and E_2 critical point energies with Al content (Fig. 2 right). A fit yields bowing parameters of b=0.31 eV and 0.36 eV for E_1 and E_2, respectively, while the E_0 band gap is well represented by

b=0.9 eV (not shown here). In the next step, the ellipsometric data has to be fitted in order to get the full DF's over the whole energy range.

Figure 3 shows for the first time DF's for cubic GaN (left) and AlN (right) up to 9.5 eV. Beside the E_0 band gap at 3.22 eV we determine the E_1 and E_2 critical point energies with 7.28 eV and 7.59 eV. An additional shoulder is found between 8 eV and 9 eV which is also predicted by the theoretical calculations. For cubic AlN the onset of strong absorption is found at 5.74 eV which corresponds to the valence band conduction band splitting at the Γ point of the Brillouin zone. The value is approximately 700 meV higher than reported in Ref. 9. Due to the small layer thickness it is not possible to determine the indirect band gap of cubic AlN. The other two critical points are resolved at 7.42 eV and 8.02 eV. They are only slightly shifted with respect to GaN which might be expected if previous results of low-Al content cubic layers [10] are taken into account.
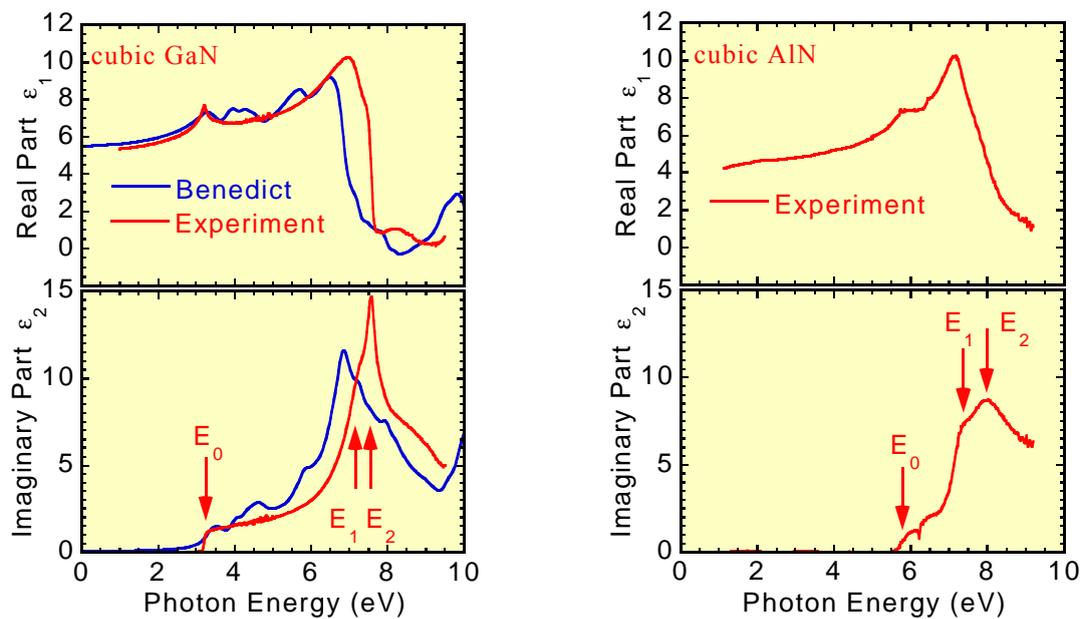
Fig. 3: Comparison of experimentally determined DF's (red) of cubic GaN (left) and AlN (right) with the results of theoretical calculations (blue) [8].

In summary, we have presented dielectric functions of hexagonal and cubic GaN and AlN as fitted from spectroscopic ellipsometry data. A large number of critical points of the band structure has been resolved. For hexagonal AlGaN alloys, the shift of the E_1 and E_2 transition energies with increasing Al content is characterised by a small bowing parameter. The direct absorption edge for cubic AlN is found at 5.74 eV which is much higher than previously reported.

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