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Transition energies and bowing parameters for In-rich InGaN and InAlN alloys

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Growth and characterization of In-rich InGaN alloys has attracted much interest recently. It arises from the band gap correction for InN from the long time accepted value of 1.9 eV down to only about 0.7 eV. Due to the reduced band gap a renewed evaluation of many material parameters of InN and their compositional dependence for (In,Ga)N and (In,Al)N alloys is mandatory. For this aim, determination of the dielectric function (DF) by spectroscopic ellipsometry (SE) has become one of the most powerful methods for studying absorption related properties of In-compounds both around the band gap as well as in the range of the high-energy critical points (CP) of the band structure [1-3]. For example, the experimentally determined shape of the DF and the optical anisotropy of InN [1] has been theoretically reproduced recently [4]. Here, we report ordinary DF's up to 9.5 eV for In-rich InGaN and InAlN alloys and their analysis, i.e. transition energies for the CP's and their compositional dependences (bowing parameter). The latter data were determined by fitting the third derivatives of the DF.

The DF's of three $In_xGa_{1-x}N$ films (x=0.67, x=0.69, x=0.77) with ~300 nm thickness and three $In_xAl_{1-x}N$ films (x=0.91, x=0.83, x=0.71) with ~400 nm thickness were determined. Samples were grown on (0001) sapphire by plasma-induced molecular beam epitaxy (MBE) using either GaN or AlN buffer layer. Further growth details as well as results of the structural, electrical and optical characterisation has been published elsewhere [2,5].

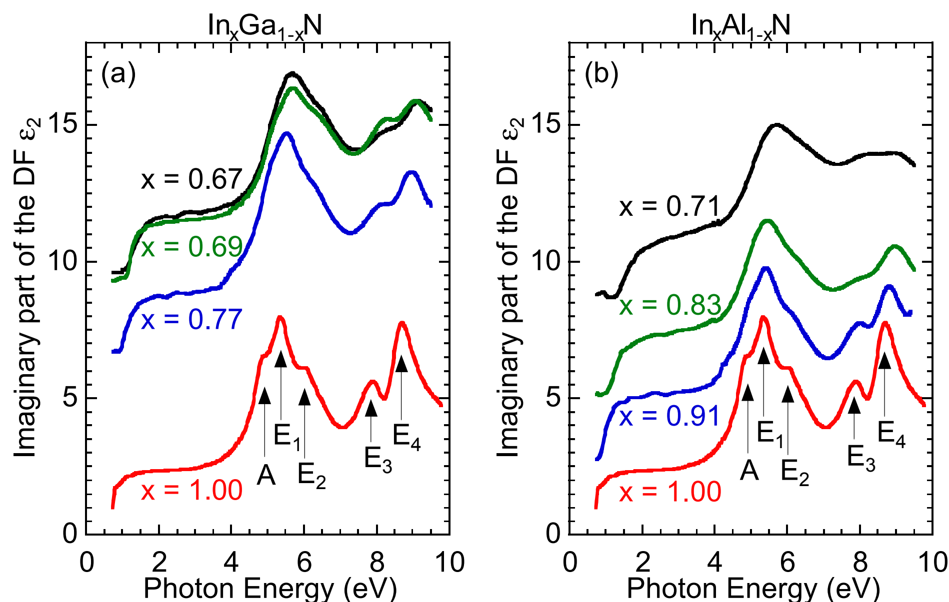

Fig. 1: Imaginary parts of the DF of $In_xGa_{1-x}N$ (a) and $In_xAl_{1-x}N$ (b) alloys obtained from fitting ellipsometric data **Y** *and* **D**. *The alloy data are vertically shifted for sake of clarity according to the Indium content.*

Figure 1 shows the imaginary part of the DF's for the InGaN (a) and InAlN (b) alloys and in comparison to the data of InN over the whole investigated range from 0.74 eV up to 9.5 eV. Due to the c-axis orientation normal to the surface, these data correspond to the ordinary dielectric tensor component [3]. The data above 4 eV were obtained from the BESSY ellipsometer at the 3m-NIM-monochromator, the excellent matching to the data recorded with a commercial ellipsometer (J.A. Wollam Co., Inc.) in the energy range from 0.74 up to 4.5 eV should be noted. Beside the gap structure in the low-energy range, the shape of the ordinary tensor component is strongly influenced by contributions arising from at least five critical points of the band structure in the energy range above 4.5 eV. All of them are clearly resolved for the alloys despite a larger broadening compared to InN. It confirms the good crystalline quality of the InGaN and InAlN films. As expected for an alloy system, they undergo a continuous shift to higher energies with increasing Ga(Al)-content.

For a high-resolution determination of the transition energies of the critical points following accurate approach was used. One calculate the third derivative of the point-by-point obtained DF (after surface roughness correction) multiplied by the square of the photon energy E. The resulting spectra can be fitted [6] via

$$\frac{d^3}{dE^3}\left(E^2\bar{\boldsymbol{e}}\right) = \sum_{j=1}^{5} e^{i\cdot \boldsymbol{f}_j} \cdot \frac{C_j}{\left(E + i\cdot\Gamma_j - E_j\right)^{n/2}} \quad , \qquad (1)$$

where $\boldsymbol{f}_j$, C_j, $\boldsymbol{G}_j$, and E_j denote the phase angle, the magnitude, the broadening energy, and the transition energy of the j-th CP, respectively. With n=6 corresponding to a two-dimensional critical point, we obtain excellent agreement to the experimental data which is exemplarily demonstrated for $In_{0.77}Ga_{0.23}N$ and $In_{0.91}Al_{0.09}N$ in Fig. 2(a) and (b), respectively.

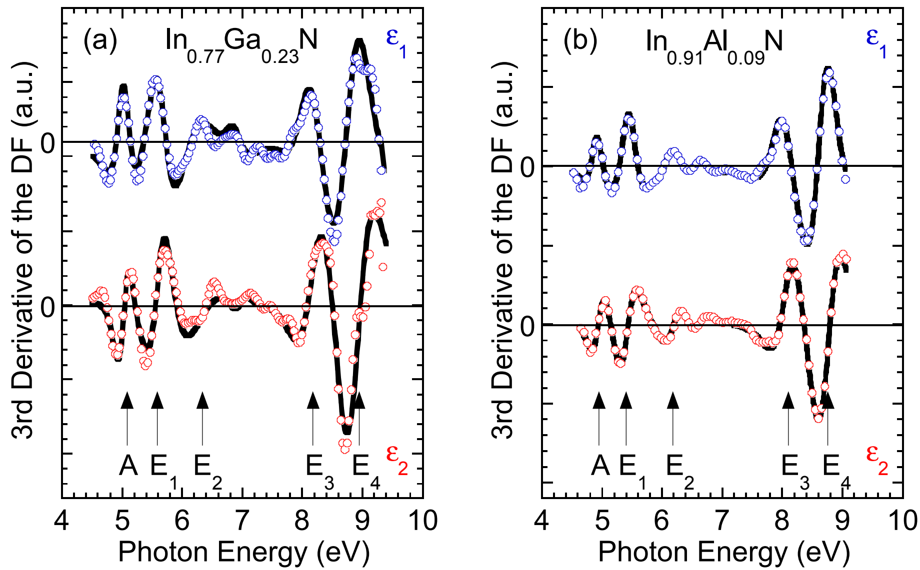

Fig. 2: Fit of the third derivative of the DF for the $In_{0.77}Ga_{0.23}N$ (a) and the $In_{0.91}Al_{0.09}N$ (b) sample. The circles represent the experimental data, and solid lines are the best fit. The transition energies of the critical points are marked by arrows.

Figure 3(a) displays all fitted critical point energies for InGaN alloys. They amount for InN: 4.86 eV (A), 5.44 eV (E_1), 6.06 eV (E_2), 7.99 eV (E_3), and 8.59 eV (E_4). With the values for GaN of 7.00 eV (E_1), 7.96 eV (E_2), 9.25 eV (E_3) bowing parameters of b=0.44 eV (E_1), 1.33 eV (E_2), and 0.83 eV (E_3) are obtained. For the determination of the band gap values, carrier induced band gap renormalization and Burstein-Moss shift was taken into account [2]. Taking the values for InN of E_0=0.68 eV [2] and for GaN of E_0=3.45 eV the fit yields b=1.77 eV for the fundamental band gap bowing, which is in good agreement with the previously published value of 1.43 eV [7]. Figure 3(b) evinces the results for InAlN alloys. With the

values for AlN of 6,30 eV (E_0), 7.97 eV (E_1) and 8.95 eV (E_2) bowing parameters of b=4.0 eV (E_0), 1.8 eV (E_1) and 2.7 eV (E_2) are obtained. No estimations can be made for the other critical points due to the lack of corresponding data for AlN.

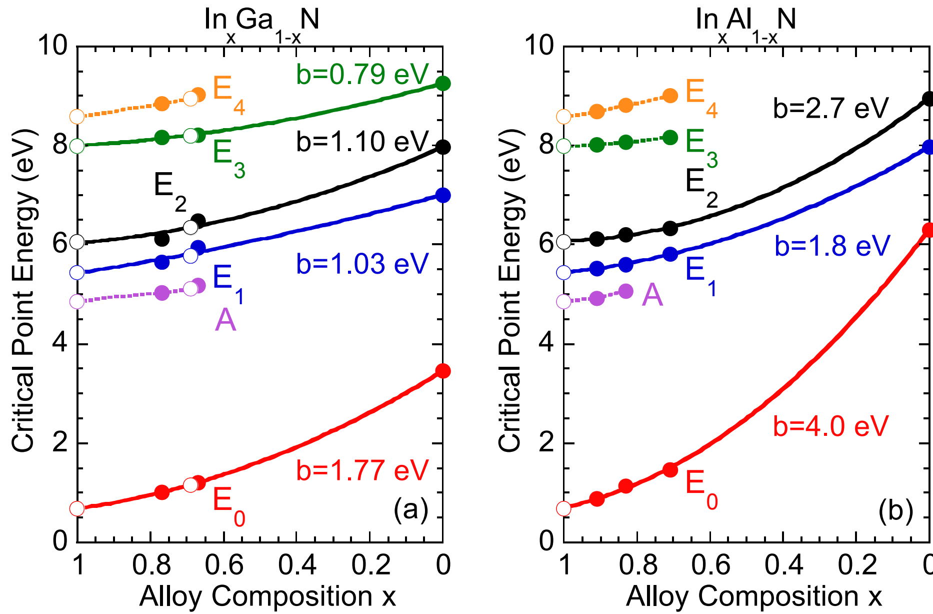

Fig. 3: Resulting critical point energies of InGaN (a) and InAlN (b) alloys as a function of composition. The open and full circles refer to the samples grown on GaN buffer and on AlN buffer, respectively. The solid lines represent the fit results.

In summary, we have determined the DF's of InGaN and InAlN alloys in the energy range from 0.74 eV up to 9.5 eV. Applying a third derivative based DF line shape fitting procedure yields the transition energies in the range of the critical points of the band structure with highest resolution. From the transition energies the bowing parameters for the compositional dependence of four and three critical points for InGaN and InAlN alloys, respectively, are derived.

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