Analysis of TEM diffraction contrast of (In,Ga)N/GaN nanostructures

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Nanostructures of III-N semiconductors have a great commercial potential due to their optoelectronic properties. The structural and chemical characteristics of such structures determine the performance of the light-emitting devices. Transmission electron microscopy can be used to determine these characteristics at a nanometer scale. For determination of the chemical composition several analytical methods available in transmission electron microscopy (TEM) can be applied. Here we focus on the evaluation of the composition utilizing chemical sensitive TEM diffraction contrast imaging.

The applicability of the method was tested using (In,Ga)N/GaN nanostructures generated by a two-step growth procedure. First a GaN buffer layer was grown by metal organic chemical vapour deposition on sapphire (0001). In a second step 7 (In,Ga)N layers of a nominal In content of 27 at.% were grown by molecular beam epitaxy. The nominal thickness of the (In,Ga)N quantum wells (QWs) was 3 nm separated by a 7 nm thick GaN barrier layer. The growth temperature for the (In,Ga)N QWs and the GaN barriers was 600 °C. Finally the structure was capped by a 30 nm thick GaN layer.

The sample was prepared for TEM by mechanical preparation comprising face-to-face gluing, formatting, mechanical polishing, dimpling, and final ion milling. Structural analysis was performed on a TEM Hitachi H-8110 operating at 200 kV. The values of the intensity of the diffracted beams were simulated using the EMS-online software (Stadelmann) choosing as parameters the In concentration of the (In,Ga)N and the sample thickness.

Experimental TEM dark-field images alternatively using the 0002 (Fig. 1a) and 0001 (Fig. 1b) reflections show a striking different contrast behaviour for (In,Ga)N which has wurtzite structure. This behaviour is similar to that of sphalerite materials like (In,Ga)As where a chemically-sensitive 002 and a strain-sensitive 004 reflection exist. In order to understand the different contrast regimes in case of wurtzite materials, one has to calculate the intensity I_g of the different diffracted beams g by means of the kinematical theory which is analogous to the square of the structure factor [1]. I_0002 being a function of the sum of the squares of the atomic scattering amplitudes of the group III and the group V element is found to be strain-sensitive. Inspecting the 0002 dark-field image (Fig.1a) it is obvious that the image intensity is dominated by the strain. The undulated strain contrast of the QWs hints to the formation of quantum dots (QDs).

Although the 0001 beam is forbidden according to the kinematical theory, it is dynamically excited. The dark-field image of Fig. 1b clearly shows the contrast behaviour of a chemical sensitive reflection. The QWs appear brighter, indicating an In enrichment compared to the GaN spacers. The inhomogeneities of the In distribution in the QWs are visible as well. The strain contrast is suppressed.

For explaining the contrast behaviour of the 0001 beam, its intensity in dependence on the In content was calculated for different sample thickness by the Howie-Whelan equation (Fig. 2a). It was found, that there is a strong dependency of the 0001 intensity of both composition and thickness. All of the curves shown in Fig. 2a exhibit an intensity maximum which is advantageous for quantitative composition analysis. For a clearer visualization, these findings were applied to a virtual (In,Ga)N layer containing 16 at.% of In embedded in GaN. Moreover, a Gaussian distribution of the In composition was taken into account. In Fig. 2b the
0001 intensity profiles across the layer are presented. The thickness ranges from 20 to 120 nm for the different curves. The profiles exhibit a transition from double maximum to single maximum shape and to double maximum again.

Conclusively, the In content of (In,Ga)N layers embedded in GaN can be determined from a series of 0001 dark-field images for different thickness.

![Diffraction contrast imaging of multiple (In,Ga)N quantum wells](image.png)

**Fig. 1:** Diffraction contrast imaging of multiple (In,Ga)N quantum wells:
a) strain-sensitive 0002 dark-field image, b) composition-sensitive 0001 dark-field image.

![Diagram of the simulated intensities of the 0001 beam of (In,Ga)N](image.png)

**Fig. 2:** Diagrams of the simulated intensities of the 0001 beam of (In,Ga)N:
a) 0001 intensity as a function of the In concentration for different sample thickness, b) simulated thickness series of 0001 intensity profiles across the (In,Ga)N layer with a nominal In content of 16 at. %.

References:

The authors are grateful to the EU Marie Curie Research Training Network "PARSEM" for financial support as well as J. Kozubowski and J. Smale-Koziorowska for provision of sample.