Simultaneous measurement of In and N concentration maps and profiles in InGaNAs from a single TEM lattice fringe image

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In the field of optoelectronic devices such as lasers and solar cells, semiconductor nanostructures play a central role since decades. The applicability of such devices is determined by controlling structural, chemical and geometrical properties on atomic scale. For example, the tailoring of ternary $In_xGa_{1-x}As$ quantum wells embedded in GaAs barriers in the high In content range is strongly limited by the strain originating from the large lattice mismatch between InAs and GaAs. A recent approach is the inclusion of nitrogen to allow for a nearly lattice-matched epitaxial growth of $In_xGa_{1-x}N_yAs_{1-y}$ on GaAs substrates.

In this work, we introduce a new method to measure both *x* and *y* locally from a single high-resolution transmission electron microscopic (TEM) image. Our technique basically combines two approaches that have successfully been applied to ternary zinc blende structures in the past: First, the composition evaluation by lattice fringe analysis (CELFA [1]) uses the chemical sensitivity of the 200 beam to form lattice fringe images of the (200) lattice planes via a two beam imaging condition. Then, the local fringe contrast is a fingerprint of the local concentration *x*, which is derived by comparison with Bloch wave simulations. Second, analysis of the strain state is based on a measurement of the local lattice parameter, which can be converted to the local chemical composition [2] using Vegard's law.

For the quaternary system, we demonstrate 2 methods to derive local strain as well as local (200) fringe contrast from a single high-resolution TEM image recorded on a C_S corrected Titan80/300 facility: The easiest approach is to measure both local strain and local contrast from (200) lattice fringe images alone. In this case, the resulting composition maps shown in Figure 1 are representative for specimen regions with little compositional fluctuation, such as the inner quantum well region. This is because the 200 beam phase depends on the chemical composition, thus strain measurement can be erroneous at sharp interfaces. To overcome this problem, we also used a 3-beam imaging condition using the beams 000, 220 and 200. Here, contrast of the 200 fringes is evaluated as before, but strain is measured from the 220 fringes, because the phase of the 220 beam is robust against concentration gradients. In general, care must be taken in the selection of beams which pass the objective aperture. Our 3-beam condition assures that the 220 and the 200 sine-type oscillations in the image are not coupled by means of nonlinear imaging.

We demonstrate the essence of a detailed error analysis for quantitative work. As to the experimental conditions, a centre of Laue circle of (030) should be used in the 3-beam case to excite both the 200 and the 220 reflections strong enough, and to minimize the influence of unknown specimen thickness at the same time. Concerning the theoretical data which enters the Bloch wave simulation of the composition dependent 200 beam amplitude, our focus is on the effect of the redistribution of electrons due to chemical bonding on structure factors. In quantum wells grown by metal-organic vapour phase epitaxy (MOVPE)

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with nominal concentrations of *x = 8%* and *y = 0-3%*, the use of isolated atom scattering data [3] leads to absolute errors of 3% and 1% for the evaluation of the In content *x* and N content *y*, respectively. In contrast, the use of modified atomic scattering amplitudes (MASA [4]) obtained from density functional theory calculations reproduces the nominal compositions, which have additionally been confirmed by X-ray diffraction.

Our results exhibit In segregation profiles as known from the ternary system. However, no evidence for a significant enrichment of N at the interfaces can be observed as published in [5].

Even if the use of MASA includes chemical bonding effects, $In_xGa_{1-x}N_yAs_{1-y}$ alloys are expected to be governed severely also by the effect of static atomic displacements (SAD) originating from the large difference in the atomic radii of N and As. Valence force field approaches are currently performed to calculate the SAD. Consequently, their influence on the structure factors and thus on the compositional analysis will additionally be discussed.

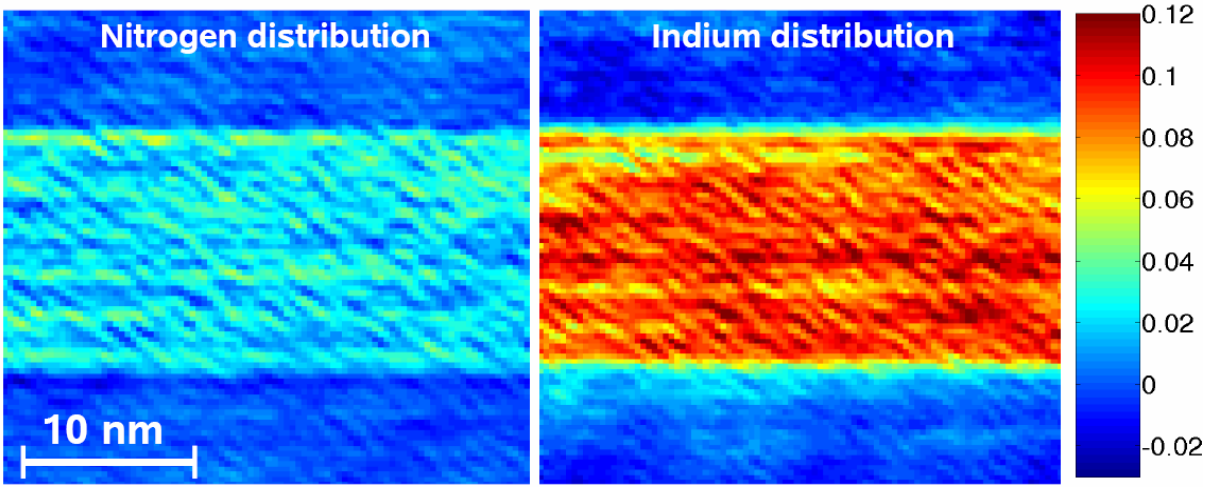

Figure 1. Local distributions of Nitrogen content y (left) and Indium content x (right) in an $In_xGa_{1-x}N_yAs_{1-y}$ quantum well. Both strain and contrast were measured from a single (200) lattice fringe image.

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