Local estimation of lattice parameters

T. Niermann, D. Plüschke, J.-B. Park, and M. Lehmann

Institut für Optik und Atomare Physik, Technische Universität Berlin,
Straße des 17. Juni 135, 10623 Berlin

niermann@physik.tu-berlin.de
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An essential element of many semiconductor-based optoelectronic devices like for example laser-diodes are low-dimensional heterostructures. For a deeper understanding of structure-related electronic and optic properties and a fine control of the grown structures, the assessment of composition and strain-state of such elements is inevitable.

Even if atomic resolution electron microscopy is the key technique for investigation of small structures, such quantities are not easily measured. With peak-fitting-methods [1, 2] or the geometric-phase-analysis (GPA) [3], it is possible to measure local changes of the lattice parameters, from which strain and changes in composition can be derived. However, the task of assessing the local lattice parameters remains challenging as a high accuracy is needed: in the $In_xGa_{1-x}As$-system for instance, a change of composition of 5% will result in a change of lattice parameters of only ~2 pm. Other sophisticated techniques deduce the local composition from different measurable quantities, e.g. CELFA [4] interprets the phase and amplitude of chemical-sensitive reflections in zinkblende materials.

Unfortunately, these techniques are either not applicable or are very difficult to apply on the wurtzite structure of Nitride-based semiconductors (at least for non-kinematic thicknesses). The pronounced non-centrosymmetry leads to a shift of lattice fringes in respect to the underlying lattice. This shift depends on the values of composition, thickness and defocus. Except for narrow windows of these parameters, this virtually renders peak-fitting unsuitable and causes different problems with the GPA.

The accuracy of lattice parameter estimation is ultimately limited by the instrument's resolution, the signal-to-noise ratio, and the number of pixels in the area under investigation. Since often it is sufficient to know the lattice parameters with a lateral resolution of a few nanometers, the area in which the parameters are estimated can be increased to several unit cells. This increases effectively the number of pixels analyzed.

We present a method, which is based on direct fitting of the lattice parameters of a small image region. The amplitude and phase of all reflections of the lattice are estimated for a given set of lattice parameters. These are the Fourier-coefficients of a pattern with lattice periodicity. Now the lattice parameters are varied until this pattern matches the investigated image area in a least-squares-sense. Since the information from all reflections is used, a larger accuracy is achieved compared to methods which only rely on the analysis of a single pair of reflections.

An example of such a fit of GaN is shown in figure 1. The residual, i.e. the experimental image with the fitted pattern subtracted, shows no remnants of the lattice periodicity; only the amorphous overlayers of the sample and the shot noise can be seen.

When this fit is be repeated for different (possibly overlapping) areas in the region of interest, a mapping of the local lattice parameters can be realized. Fig. 2 shows such a mapping for an $In_xGa_{1-x}N$-quantum well inside a GaN-matrix. Even if the quantum well cannot be seen in the HRTEM-micrograph by eye, it is clearly revealed by the lattice parameter analysis. Only the *c*-parameter (growth direction) is shown. The experimental image shown in both figures was obtained using a Tecnai F20 equipped with an image Cs-corrector operating at 200 kV located at the Triebenberg lab of TU Dresden.

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5. This work is performed within the DFG collaborative research center SFB 787 “Halbleiter-Nanophotonik”.

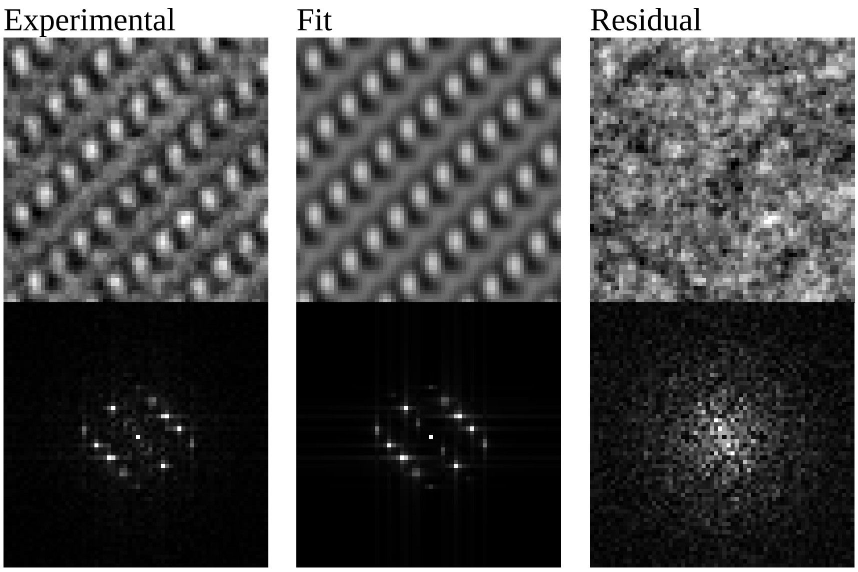

Figure 1. The upper row shows the fit area in the experimental image (see Fig. 2 for a larger region), the fitted lattice pattern and the residual of the fit. The lower row shows the respective FTs. The size of the investigated region is 2.4x2.4 nm^2. The intensities of the experimental image and of the fit are equally scaled within each row.

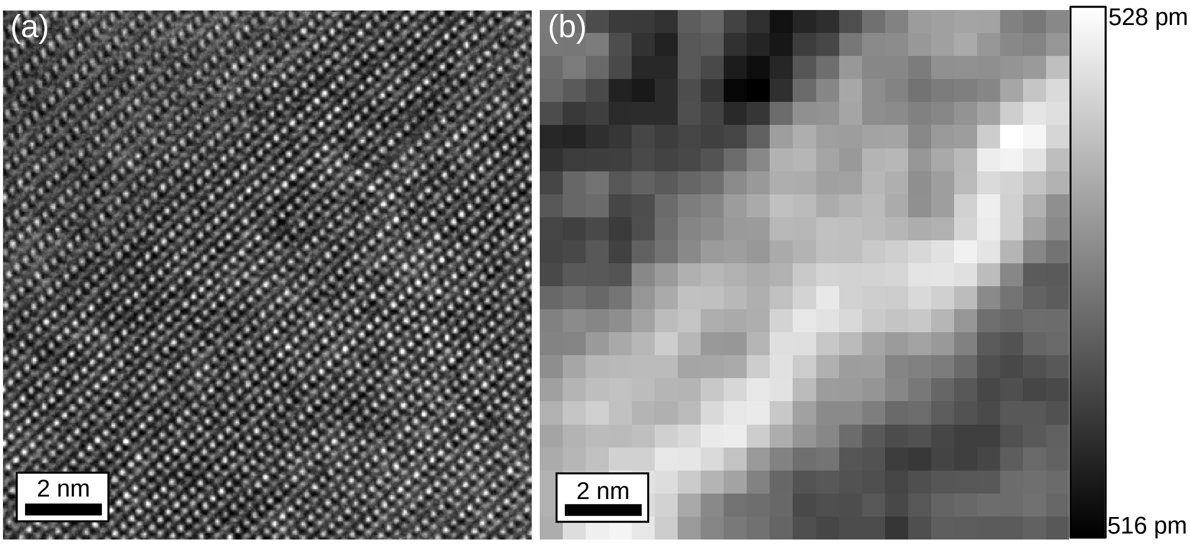

Figure 2. Lattice parameter mapping of an $In_xGa_{1-x}N$-quantum well in a GaN-matrix: (a) HRTEM micrograph; (b) lattice parameter in *c*-direction. Each point represents the result of a fit like the one in Fig. 1.

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