Microscopic mapping of the full strain tensor, local orientation and composition in an In$_x$Ga$_{1-x}$N heterostructure via scanning X-ray diffraction

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The growth of single-crystalline thin films is the basis for many modern semiconductor devices, such as LEDs, laser diodes, transistors etc. Lattice strain caused by a mismatch of lattice constants or thermal expansion coefficients between film and substrate is an important consequence of the growth and a major factor to influence the electronic band structure and optical properties of the device. Therefore, strain engineering of the crystal lattice by geometrical relaxation or constraints is an established route to tune these properties. However, an accurate microscopic characterization of strain not done routinely. Here we present the developments of the “strain microscope” beamline ID01 of the ESRF aiming to tackle this problem by means of X-ray diffraction microscopy.

X-ray diffraction is frequently used to determine the unit cell dimensions of epitaxially grown films which allows to evaluate growth parameters such as lattice perfection, strain, composition, mosaicity and thickness averaged over the X-ray beam footprint. However, microscopic resolution is required to study the origins of deviations in these parameters. While some techniques provide access to such information (e.g. transmission electron microscopy, Raman spectroscopy), scanning diffraction X-ray microscopy (SDXM) proposed here has advantages being non-destructive, model-free and having high strain sensitivity. The spatial resolution is determined by the beam size and can reach values below 100nm at ID01. 3D Reciprocal space maps are obtained for each point on the 2D surface by rocking the sample around the Bragg angle finally resulting in a 5D dataset $I(x, y, q_x, q_y, q_z)$. Combining three of such datasets from non-coplanar reflections yields microscopic maps of local orientation and the full strain tensor $\varepsilon_{ij}$. From the lattice dimensions, the local stoichiometry can be derived on knowledge of the elastic coefficients of the material.

The technique is applied to an In$_x$Ga$_{1-x}$N heterostructure which is used as a template for growth of a multiple quantum well for LED applications. High In-content is desired as it leads to a red-shift of the emission in In$_x$Ga$_{1-x}$N LEDs that otherwise perform very well in the blue region of the visible spectrum. This could become one way to close the “green gap” existing in the efficiency of monolithic white light emission devices. Our sample consists of a first In$_x$Ga$_{1-x}$N layer that has been grown on a Sapphire substrate. Subsequent photolithography patterning is used to produce sub-mm structures and facilitates a stress-release after lifting off the InGaN film from the substrate. This way, another In$_x$Ga$_{1-x}$N layer of higher (here nominally 5%) In-content and lower mismatch strain can be grown on top. The strain relaxation induced by patterning and the thereby induced variations of In-content are the target of this study. Fig. 1 shows maps of the extracted lattice parameters of the regrown top-layer. These show variations on 1um lengths scales. The lattice tilts and in-plane parameters between lower and top layer correlate. In contrast, out of plane lattice parameter and In-content show rather different distribution.

**Fig. 1:** Variation of lattice parameters of the regrown In$_x$Ga$_{1-x}$N film in a 30x30 um$^2$ region close to the corner of a square pad that is obtained by photolithography patterning. Strain relaxaton at the edges is clearly seen.