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Report:

Diffraction anomalous fine structure (DAFS) is a new method combining the well-known x-ray absorption spectroscopy (methods EXAFS and XANES) and high-resolution x-ray diffraction [1]. In this method, intensity diffracted from a sample with a given scattering vector \vec{Q} is measured as a function of the energy of the primary beam close to the absorption edge of a chosen element. From the fine structure of the measured energy spectrum one can determine the local neighborhood of the chosen atom in a part of the sample having a given strain status (determined by the scattering vector \vec{Q} chosen). In several papers, the DAFS method has been used for the investigation of semiconductor heterostructures such as epitaxial layers [2] and quantum wires [3,4]. In our work, we have used this method for the investigation of the atomic arrangement in uncapped self-organized InGaN quantum dots grown by molecular-beam epitaxy on GaN(0001) templates. We have measured the DAFS spectra around the GaK absorption edge (10.36 keV) in grazing-incidence geometry (GID) at different positions \vec{Q} in reciprocal space near the (300) diffraction spot. We have chosen these positions along the (h00) line (radial direction), so that changing \vec{Q} we change the iso-strain volume of the quantum dots where the DAFS signal is coming from.

Figure 1 shows a radial scan around (300) taken in a symmetric grazing-incidence geometry (GID). The figure also indicates the values of Q used in the DAFS scans. The measured DAFS scans (after subtraction of a fluorescence background) are plotted in Fig. 2. The measured data were fitted to theoretical DAFS spectra; these spectra were simulated using the distorted-wave Born approximation and taking into account several scattering processes taking place in a system of free-standing quantum dots (see [5] for more details).



Fig. 1: Typical diffraction profile in radial (h00) direction. Left to the GaN diffraction spot at h = 3, the peak arising from the InGaN islands at $h \approx 2.87$ is clearly resolved. At the positions indicated by the arrows, DAFS scans were performed.

In this simulation, we have neglected the oscillatory parts χ' and χ'' of the dispersion corrections of the atomic scattering factors of Ga.

In the next step of the data evaluation we have applied an iterative procedure using a Kramers-Kronig analysis of the difference between the measured and fitted DAFS spectra. This procedure yielded the energy profiles of χ' and χ'' ; examples of the results are shown in Fig. 3. A Further step of the data treatment will comprise the conversion of these energy spectra to k-space and an inverse Fourier transform in order to get the inter-atomic distances in particular iso-strain volumes. We also intend to compare the $\chi'(k)$ and $\chi''(k)$ functions with ab-initio simulations using the FEFF software package. The publication of the results is expected in the next few months.



Fig. 2: DAFS spectra recorded at different scattering conditions (see Fig. 1). The solid lines are fits based on gas phase values of the scattering amplitudes.



Fig. 3: Real part χ' and imaginary part χ'' of the oscillatory contribution to the dispersion correction, as extracted from the DAFS scans and fits shown in Fig. 2.

References

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