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## Report:

## Anomalous Scattering from InGaAs Quantum Dots

The aim of the proposed experiment was the structural investigation of self-organized $\mathrm{In}_{0.40} \mathrm{Ga}_{0.60}$ As quantum dot (QD) superlattices, with special emphasis to (i) the lateral ordering of extended QD-chains running along the [110]-direction, and (ii) the strain and Indium composition profiles inside and in the vicinity of the InGaAs QDs. It was planned to cover the latter point by performing anomalous scattering at different scattering geometries. For that reason experiments close to the As K-edge were performed in order to maximize the contrast between InGaAs and GaAs. This is demonstrated in Fig. 1 (right hand side) for the weak 006 reflection. We have chosen $E_{1}=11.850 \mathrm{keV}$ (just below As K-edge) and $\mathrm{E}_{2}=12.400 \mathrm{keV}$.


Fig.1: Radial scans in the vicinity of the 020 reciprocal lattice point for two different x-ray energies. Comparing the intensities at $\mathrm{E}_{1}=11.850 \mathrm{keV}$ (just below the As K-edge) and at $\mathrm{E}_{2}=12.400 \mathrm{keV}$ (above the As K-edge) the contrast is expected to be maximum. Please note that the two rocking curves have been normalized such that the QD peaks located at $\mathrm{q}_{\text {radial }}=22.9 \mathrm{~nm}^{-1}$ appear at the same intensity.

Unfortunately, it turned out that the samples were not suitable in order to achieve the goals mentioned above. The contrast achieved by tuning the x-ray energy to $E_{1}$ and $E_{2}$ was too small as to be able to evaluate
the In composition profile within the QDs. This can be exemplarily inspected in Fig. 1 (left and middle) where two radial scans ( 020 reflection) recorded at $E_{1}$ and $E_{2}$ are shown.

## Grazing Incidence Diffraction from GaAs Quantum Dot Bimolecules

During the last two days of our beam time we alternatively investigated a sample containing free-standing semiconductor quantum dot molecules ( QDM ). These quantum dot clusters are of high scientific relevance and have been extensively investigated in the last years. We have investigated freestanding GaAs QDMs grown on a strained AlGaAs layer which itself was grown on a GaAs (001) substrate, thus ensuring strainfree growth of the quantum dot molecules (QDMs) on top of the AlGaAs layer. An AFM micrograph of the sample investigated is shown in Fig.2(left).

In order to structurally characterize the sample (shape, size, ordering, strain), we have applied triple crystal grazing incidence diffraction. The scattering geometry has been chosen such that the [110] axis of the QDM is collinear with the strain-insensitive angular direction $\mathrm{q}_{\text {ang }} \equiv \mathrm{q}_{110}$. This enables accurate determination of the QDM size and inter-dot distance, independent of the strain state of the QDMs. On the other hand, the scattering geometry enables to probe strain perpendicular to the axis of the QDM, i.e., along the [110] direction. Strain would lead to a small shift of the overall diffuse intensity distribution with respect to the strong substrate reflection which is located at $\mathrm{q}_{\mathrm{rad}}=31.436 \mathrm{~nm}^{-1}$. However, no such shift could be observed neither around the 220 nor the $2 \underline{2} 0$ reciprocal lattice point proving that the QDMs are completely free of strain.


Fig.2: (a) AFM micrograph of sample under investigation; X-ray diffuse intensity distribution in the vicinity of the 220 in-plane reciprocal lattice point. (b) experimental data, (c) corresponding simulation, (d) real space model that was used in the simulation.

Fig. 2 b shows the experimental x -ray diffuse scattering from the ensemble of quantum dot molecules in the vicinity of the 220 reciprocal lattice point. Distinct intensity oscillations are observed in the $\mathrm{q}_{110}$-direction. However, the in-plane envelop function of the experimental data exhibits rotational symmetry, indicating that the shape of the individual QDs within the QDM has rotational symmetry with the symmetry axis oriented along the vertical [001] direction. The observed intensity distribution can be qualitatively explained within the kinematical scattering approach where the scattered amplitude of a non-strained homogeneous object is given by the Fourier transform of its shape function. Consequently, the amplitude of the scattered wave from a single rotational-symmetric quantum dot can be described by a corresponding rotationally-shaped distribution in $q$-space, with a central maximum at $q_{\|}=0$ and a corresponding width of $\Delta q_{\|}=2 \pi / R$ with $R$ being the characteristic radius of the dot. The scattered amplitude of the entire QDM is then given by coherent superposition of the two scattered waves from the two individual dots. Since all QDMs are oriented
along the [110] direction the corresponding interference phenomena lead to pronounced maxima in the diffuse intensity for $\mathrm{q}_{110}=2 \pi \cdot \mathrm{n} / \mathrm{d}$ where d is the distance of the two dots within the QDMs and $\mathrm{n}= \pm 1, \pm 2, \ldots$. Thus, the size of the individual dots and their spacing within the QDM can be unambiguously distinguished and evaluated independently: Using the given formulas we can extract $\mathrm{d} \approx 140 \mathrm{~nm}$ and $\mathrm{R} \approx 35 \mathrm{~nm}$ from the experimental intensity distribution shown in Fig.2b.

A more detailed, quantitative evaluation can be performed by comparing the experimental intensity distribution with corresponding simulations of diffuse scattering (Fig.2c). Respective sections of experiment (open circles) and simulation (solid line) through the central peak in Fig.2b,c are displayed in Fig.3. It is interesting to note that - in accordance with the atomic force micrograph displayed in Fig.2a - a satisfactory simulation can be only achieved by taking into account, that the QDMs are grown on an elongated flat hill of about $\mathrm{H}=5 \mathrm{~nm}$ height and $\mathrm{W}_{110}=400 \mathrm{~nm}$ and $\mathrm{W}_{110}=700 \mathrm{~nm}$ base widths. This leads to a prominent peak (feature ' P ' marked in Fig.3a and 3b) of diffuse scattering in the immediate vicinity of the 220 reciprocal lattice point at $\mathbf{q}_{\|}=\left(\mathrm{q}_{110}, \mathrm{q}_{110}\right)=(31.436,0) \mathrm{nm}^{-1}$. The diffuse intensity apart from feature ' P ' is solely related to the QDMs. In particular, the foot slope of the curve (feature ' $F$ ' marked in Fig.3b) is sensitive to the base widths and shape of the individual dots. On other hand, the behavior (position and intensity decay) of the side maxima (features ' O ' marked in Fig.3a) of the intensity distribution on the curve foot allow for evaluating the spatial dot-dot correlation parameters within the QDM. Excellent agreement between experiment and simulation is achieved when the QDMs are assumed as two flat domes (see real space model in Fig.2c) exhibiting a base radius of $R=40 \mathrm{~nm}$ and a height of $\mathrm{h}=5 \mathrm{~nm}$, separated by $\mathrm{d}=135 \mathrm{~nm}$. These parameters are in correspondence with the surface morphology as revealed by AFM (Fig.2a).


Fig.3: Sections through the intensity distributions shown in Fig.2., simulations (solid lines), experimental data (open circles). (a) Along the QDM axis ( $\mathrm{q}_{110}$-direction) intensity oscillations $(\mathrm{O})$ are observed, which are caused by interference between the scattered waves from each individual dot. (b) Perpendicular to the QDM axis ( $\mathrm{q}_{110}$-direction) extended diffuse scattering shows up ( F ), which is caused by the shape function of an individual dot. The prominent central peak $(\mathrm{P})$ is due to scattering from an elongated flat hill $\left(\mathrm{W}_{110}=400\right.$ $\mathrm{nm}, \mathrm{W}_{110}=700 \mathrm{~nm}, \mathrm{H}=5 \mathrm{~nm}$ ) located below the QDM. For the simulations the real space model depicted in Fig.2c was used.

Finally, we would like to note that, in the simulations a small fluctuation ( $\sigma=8 \mathrm{~nm}$ ) of the QDM extension along [110] was assumed while the shape and size of the single dots of the QDMs are kept fixed. The resulting good agreement between simulation and experiment is a strong indication that the QDMs are highly monodisperse in size and shape. On the other hand, the experimental data show that the positions of the QDMs are - despite their unique size, shape, and orientation - not correlated but are randomly distributed across the surface.

