ESRF	**Experiment title:** X-ray diffraction studies of annealed InAs quantum dots	**Experiment number:** SI747
Beamline: ID32	**Date of experiment:** from: 03/12/2001 to: 11/12/2001	**Date of report:** 01/03/2002
Shifts: 18	**Local contact(s):** Bruce COWIE	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):
Paul Howes *, University of Leicester
Colin Norris, University of Leicester

Report:

The aim of experiment SI747 was the determination of the strain profile within and around buried InAs quantum dots as well as their shape. The samples studied were prepared by our collaborators at Sheffield University and contained 10 layers of InAs/GaAs QDs with different inter-layer separations.

Theses studies presented considerable experimental challenges. The region of interest, containing the QDs, was as thick as 1000 Å for the thickest sample, so large incident and exit angles were necessary for the x-ray beam to penetrate this depth, resulting in a high level of background scattering. In addition, the data covered a large dynamic range (8 orders of magnitude) and some time was spent in commissioning the new ID32 automatic filter system to allow measurements to be made more efficiently.

In spite of the difficulties, we measured a large, high quality data set from three multilayer samples. The inter-layer spacings were 15 ml, 30 ml and 100 ml respectively.

Summary of Data

A range of different types of data was measured from the three samples:

- High quality reflectivity scans were measured for all the samples. This data is invaluable because it probes only the vertical structure. The data show many osciallations corresponding to the different characteristic distances of the sample: the QD thickness, the interlayer spacing, the total multilayer spacing and the capping layer thickness.
- About 20 crystal truncation rod segments were also measured. These are sensitive to the 3D structure of the QDs and the resulting strain. Like the reflectivities, the CTRs also show oscillations due to the different characteristic distances in the samples.

- Diffuse scattering was measured in the region of "weak" Bragg peaks such as the $(0,\overline{4},2)$ where the contribution from the GaAs is almost absent. These measurements give information about the lateral strain. The InAs is compressed because it is embedded in the GaAs matrix which has a smaller lattice constant. The GaAs between the dots is likewise compressed whereas that above and below the dots is expanded. This leads to a spectrum of diffuse scattering concentrated mostly inbetween the GaAs and InAs Bragg peak positions.

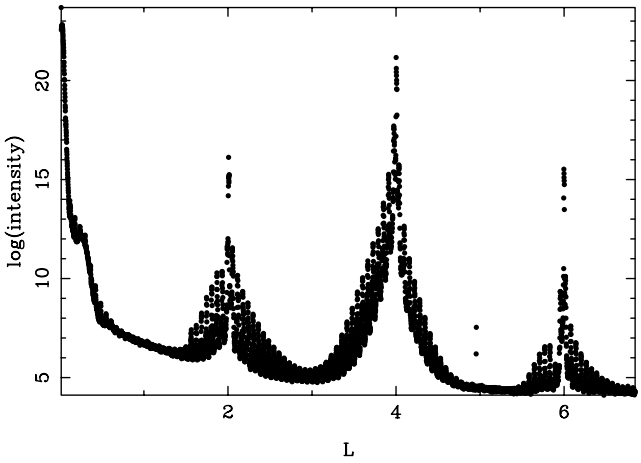


Figure 1: measured reflectivity for a sample with 10 layers of stacked QDs

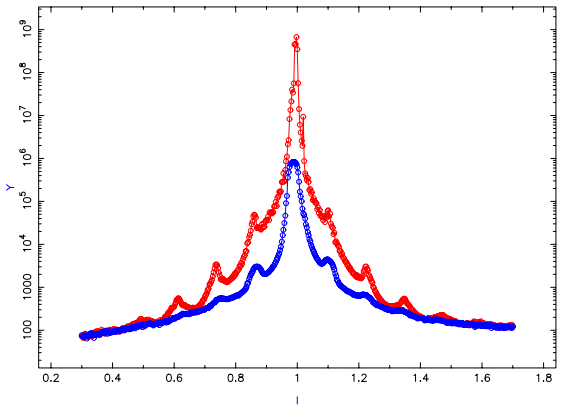


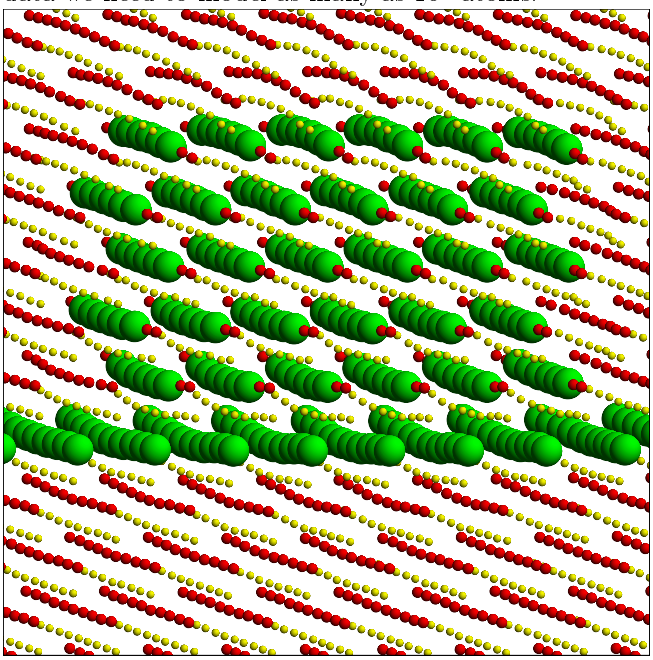
Figure 2: A typical CTR scan for a sample with 10 layers of stacked QDs. Both the signal and background are plotted.

Analysis

The analysis of the x-ray scattering data is difficult because the structures are extremely large by surface x-ray diffraction standards. A single QD may contain 30 000 atoms and the strain field extends for many nm. Also the shape, composition profile and strain all contribute to the x-ray scattering.

In spite of this, we have made *signicant progress*. We have developed a model of the QDs that uses the minimised Keating valence force field energy to calculate the relaxed positions of all the atoms given only the size and shape of the dot. This allows us to calculate the x-ray scattering at any point in reciprocal space and to simulate our data. The diffuse scattering is straightforward to simulate. The CTR and reflectivity scattering can be calculated by adding the contribution from a semi-infinite GaAs bulk crystal. Since the Keating model guarantees that the strain is physically realistic the data analysis is reduced to finding the size and shape (including fuzzy edges in the case of diffusion) of the dot.
As the data were measured only two months ago, the analysis is at an early stage but it is progressing rapidly. We are able to calculate the relaxed structure of rectangular QDs embeded in a substrate with a total of 600 000 atoms.

A small rectangular QD with its wetting layer relaxed to minimise the Keating energy. To simulate the measured data we need to model as many as 10^6 atoms.



We anticipate that the data analysis will be largely completed within 6 months and that a major publication will follow.