DUBBLE	**Experiment title: Probing strain induced relaxation of surface atoms in CdSe quantum dots**	**Experiment number**: **26-01-731**
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Names and affiliations of applicants (* indicates experimentalists):

Dr. A.V. Pethukov*, Debye Institute, Utrecht University, The Netherlands

Prof. Dr. A. Meijerink*, Debye Institute, Utrecht University, The Netherlands

Report: (max. 2 pages)

Semiconductor nanocrystals or quantum dots (QDs) show optical and electrical properties that are strongly influenced by their size and surface properties. Surface capping molecules can strongly influence internal and surface structure and optical properties, but their exact role remains poorly understood. Structural phase transitions occurring in molecules at the surface of nanocrystalline semiconductors strongly affect luminescent efficiency, and this effect is anticipated to be related to surface structure changes. High resolution powder diffraction experiments were performed to probe these structural changes at the surface CdSe quantum dots. The experiments were performed at the Swiss-Norwegian beamline (SNBL) in exchange for beamtime at DUBBLE.

Experiments were performed for two highly luminescent CdSe nanocrystals (~3 nm in size) capped with different types of alkylamines and dissolved in a toluene. The phase transition temperature depends on the length of the alkyl chain of the alkylamines and increases from 240 K for C_6 to 300 K for C_{18} alkylamines. During the beamtime period the temperature dependent x-ray diffraction patterns were recorded as a function of temperature between 200 K and 320 K (20 K steps) for different samples: CdSe quantum dots capped with hexylamine (C_6), CdSe capped with hexadecylamine (C_{16}) and a background samples with same solvents and capping molecules but without the CdSe quantum dots (for background correction). The diffraction patterns showed a clear temperature dependence related to a phase transition of the capping molecules. The displacement of the surface Cd and Se atoms upon cycling through the phase transition is presently investigated by the analysis of the pair distribution function (PDF) obtained for CdSe QDs capped with the two types alkylamines. In order to obtain sufficient signal to noise ratio to observe changes in the PDF's long acquisition times were required. After the completion of the experiments for two samples and two background correction samples at various temperatures, the synchrotron suffered from a serious vacuum problem and the last days of the beamtime were lost. Nevertheless, the initial experiments were successful and allow analysis of PDF's for nanocrystals of CdSe. In the figure below the PDF's obtained from the experiments are shown for 3.1 nm CdSe quantum dots at temperatures between 200 and 310 K. Future experiments are needed to study surface relaxation for CdSe quantum dots with a wider range of capping molecules.

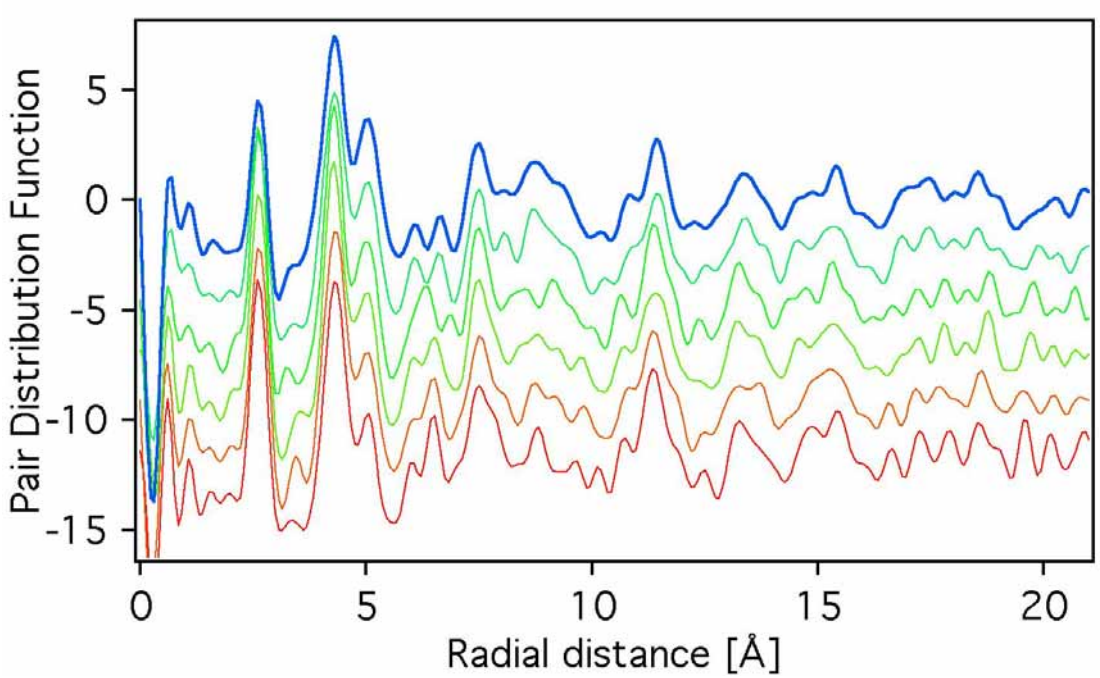

Fig. 1 - Pair distribution function for 3.1 nm CdSe quantum dots capped with hexylamine in toluene. The PDF's obtained from high resolution diffraction patterns recorded at 200 K (bottom), 220 K, 240 K, 260 K, 280 K and 310 K (top).

In addition to the main experiments on quantum dots, some high resolution x-ray diffraction patterns were recorded for anisotropic gibbsite (AlOOH) colloidal platelets. The originally grown particles (diameter of 210 nm and thickness of about 10 nm) were used as seeds for additional growing steps in order to increase the particle dimensions. Up to 4 additional subsequent growing steps have been performed. The crucial question addressed during the experiment was whether the additional layers of AlOOH are crystalline and grow epitaxially on the seed particles. The angular high resolution of the SNBL is crucial in these experiments. It allowed us to clearly resolve the width of the (002) reflection, which originates from the interplanar atomic periodicity in the direction normal to the platelets (see Fig. 2). On the other hand, the apparent width of (110) and (200) reflections, which arise from the atomic structure along the platelets, are mainly instrument-limited. These results have been included in a recent paper of J.E.G.J. Wijnhoven "Seeded growth of monodisperse gibbsite platelets to adjustable sizes" (accepted for publication in J. Colloid Interf. Sci.) along with an acknowledgement of the ESRF experiment.

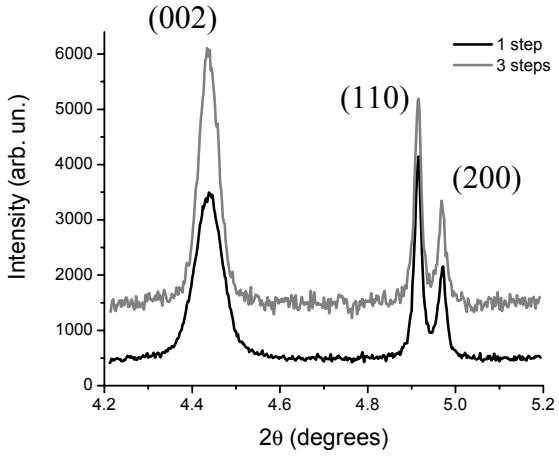

Figure 2. High-resolution XRD spectrum of gibbsite colloidal particles after one and three additional growth steps. Sharpening of the (002) reflection is clearly visible.