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Report:

X-ray Diffraction Anomalous Fine Structure method combines x-ray diffraction (XRD) and absorption spectroscopy (XAS) [1]. In this method, the diffracted intensity is measured as a function of x-ray energy close to the absorption edge of a given element. DAFS signal is collected at the given scattering vector q_r , i. e. the signal stems from the volume of quantum dots with a given strain (iso-strain volume). Therefore, as results local structural parameters for this volume are obtained. The advantage of this method in comparison to the grazing-incidence diffraction (GID) consists in the fact that the diffracted radiation depends only on the neighboorhood of a given atom *in the given iso-strain volume* the spectrum is not infuenced by structural defects in the crystal lattice.

The aim of the experiment HS3498 was to measure the DAFS spectra at the Cd K-edge (27 keV) for CdSe/ZnSe/MgS quantum dots grown by molecular beam epitaxy (MBE) on the GaAs(001) substrate. Due to the technical difficulties we performed the measurements at the Se K-edge (~12.7 keV) instead of the Cd K-edge. The DAFS spectra were collected in grazing-incidence geometry at different positions in reciprocal space near the (800) diffraction spot (for various deviations q_r from the reciprocal lattice point) in order to obtain local chemical information and information on the atomic ordering in a particular iso-strain volume. The q_r has chosen along the (h00) line (radial direction). By changing q_r the iso-strain volume was changed. The graizing incidence geometry allowed us to reduce the contribution of the substrate to the scattered intensity and enhances the contribution of the quantum dots. To avoid the oxidation the samples were kept in He atmosphere during the measurement.

Figure 1 demonstrates a radial scan from a sandwich structure, in which the CdSe dot layer (nominal thickness 1.0 nm) was surrounded by a pair of ZnSe layers (1.4 nm each). This ZnSe/CdSe/ZnSe tri-layer was surrounded by two thin MgS barriers (2 nm) and ZnSe buffer layers (50 nm in the bottom and 25 nm on the top). The whole stack was deposited on a (001)GaAs substrate [2]. The resulting DAFS spectra colectted at different h positions indicated at Fig. 1 are plotted in Fig. 2 after subtraction of a fluorescence background. Since the DAFS spectrum $\chi(E)$ depends both on the real (χ ') and imaginary (χ '') parts of the anomalous form-factor of the Se atoms, we have extracted the imaginary part χ ''(*E*) of the DAFS spectrum by numerical Kramers-Kronig transformation [3]. The χ ''(*E*) spectrum was then converted to the χ ''(*k*) dependence, where

k is the length of the wave-vector of the photoelectrons depending on the difference $E-E_K$ (E_K is the energy of the absorption edge) Figure 3 presents the extended oscillation contribution $k^*\chi''(k)$ extracted from the raw DAFS spectra.

Then, the DAFS oscillation were transformed to direct (R)-space (Fig. 4) in order to obtain the local environment of the Se atoms, as well as the Cd concentration and atomic ordering in different iso-strain volumes of the quantum dots. The first peak signed (first coordination shell) as 1 at the Fourier transform (FT) that contain mixed Cd and Zn atoms at the position h_1 is shifted to low *R*. From that we can conclude that at this case the first cordiantion shell is dominated by Zn atoms and the distance tends to the Se-Zn. This results was expected since the h_1 -value was choosen close to the ZnSe substarte. The h_2 position corresponds to the volume of CdSe QDs. The concentarion of Cd is higer than Zn atoms. A significant change at the second coordiantion shell from which the Se atoms contribute are not expected.

DAFS experiments were combined with EXAFS measurements at the CdK absorption edge, perfomed at the beamline BM08 (see report HS359).

The results achieved from the DAFS and EXAFS analysis represent a valuable contribution to the understanding of the structure of CdSe/ZnSe/MgS and CdTe/ZnTe systems. They will help to optimise the growth process in order to obtain the quantum dots-based devices with the best optical properties.



Fig. 1 Diffraction profile in radial (800) direction. 1- ZnSe substrate; 2- the CdSe quantum dots. The DAFS data were colleted at the position incicated by h_1 and h_2 .



Fig. 3 The oscillation $k^2\chi(k)$ extracted from DAFS data shown on the fig. 2 for two different value of h.



Fig. 2. Raw DAFS spectra collected at two different value of h, namely h_1 =7.999, h_2 =7.975.



Fig. 4 The magnitude of the Fourier transform of the oscillation presented on the fig. 3

Refernece:

 $k^2 \chi(k)$

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