ESRF	**Experiment title:** Investigation of the local structure around Cd atoms in CdSe and CdTequantum dots	**Experiment number**: **HS-3599**
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Report:

The 7% lattice mismatch of the CdSe/ZnSe system causes the formation of zero-dimensional islands. The CdSe nano-objects are only observed when a special capping procedure is applied or when migration enhanced epitaxy for the cap is used to enhance the Cd surface segregation [1, 2]. It is therefore essential for the CdSe dot formation that they are embedded in a ZnSe matrix. During the grow process the intermixing between CdSe and ZnSe can occure. In the literature high-resolution x-ray diffraction (HRXRD) using synchrotron radiation, high-resolution transmission electron microscopy (HRTEM) and luminescence [3, 4] investigations concerning CdZnSe/ZnSe quantum dots are reported. These investigations considered the structure and the correlation behavior of CdSe stacks in ZnSSe barriers. In order to explain influence of the overgrowth parameter on the structure of the formed CdSe quantum dots the Extended X-ray Absorption Fine Structure (EXAFS), as complementary method was used. EXAFS is selectivity for a chosen element; therefore the local atomic ordering present in the CdSe/ZnSe can be determined.

The purpose of proposed experiment was to measure the EXAFS spectra at the Cd K edge (~27 keV) of a series samples grown by molecular beam epitaxy on (100) GaAs substrate covered with a GaAs buffer layer and 50 nm ZnSe. The quantum dots were embedded in 1 nm MgS and 1.4 nm ZnSSe surrounding the 3 monolayers CdSe active quantum dot (QD) region. Finally a ZnSe cap of 25 nm was deposited. The enhanced vertical and lateral confinement was successfully realized by this ZnSSe/MgS barrier combination. Due to this additional confinement for the first time the emission of a single CdSe quantum dot could be observed up to room temperature [5].

The EXAFS spectra were collected at fluorescence mode using a multi-element Ge detector. The Athena program was used to subtract the pre-edge background, normalize to the experimental edge step and absorption data [6]. The theoretical scattering signals for the Cd-Se, Cd-Cd and Cd-Zn pairs were generated using FEFF 8 code [7], respectively. The Artemis program was used to obtain the structure parameters, i.e. bond lengths (R), Debye-Waller factor (σ^2) and coordination number (N) [8]. The best fit of the two

coordination shell at the Fourier transform (FT) for the CdSe/ZnSe/MgS single quantum dots layer and standard sample are presented in Fig. 1 a, b and c. From the quantitative analysis follow:

- intermixing between capped ZnSe and CdSe QDs layer
- the local structure around Cd atoms in QD layer is similar to the structure of the standard sample that contain a Cd concentration of 50 % on cationic sites. This confirms that the thin MgS barriers do not influence the quantum dots itself.
- the bond lengths Cd-Se, Cd-Cd and Cd-Zn in QD layer slightly differ from the standard.

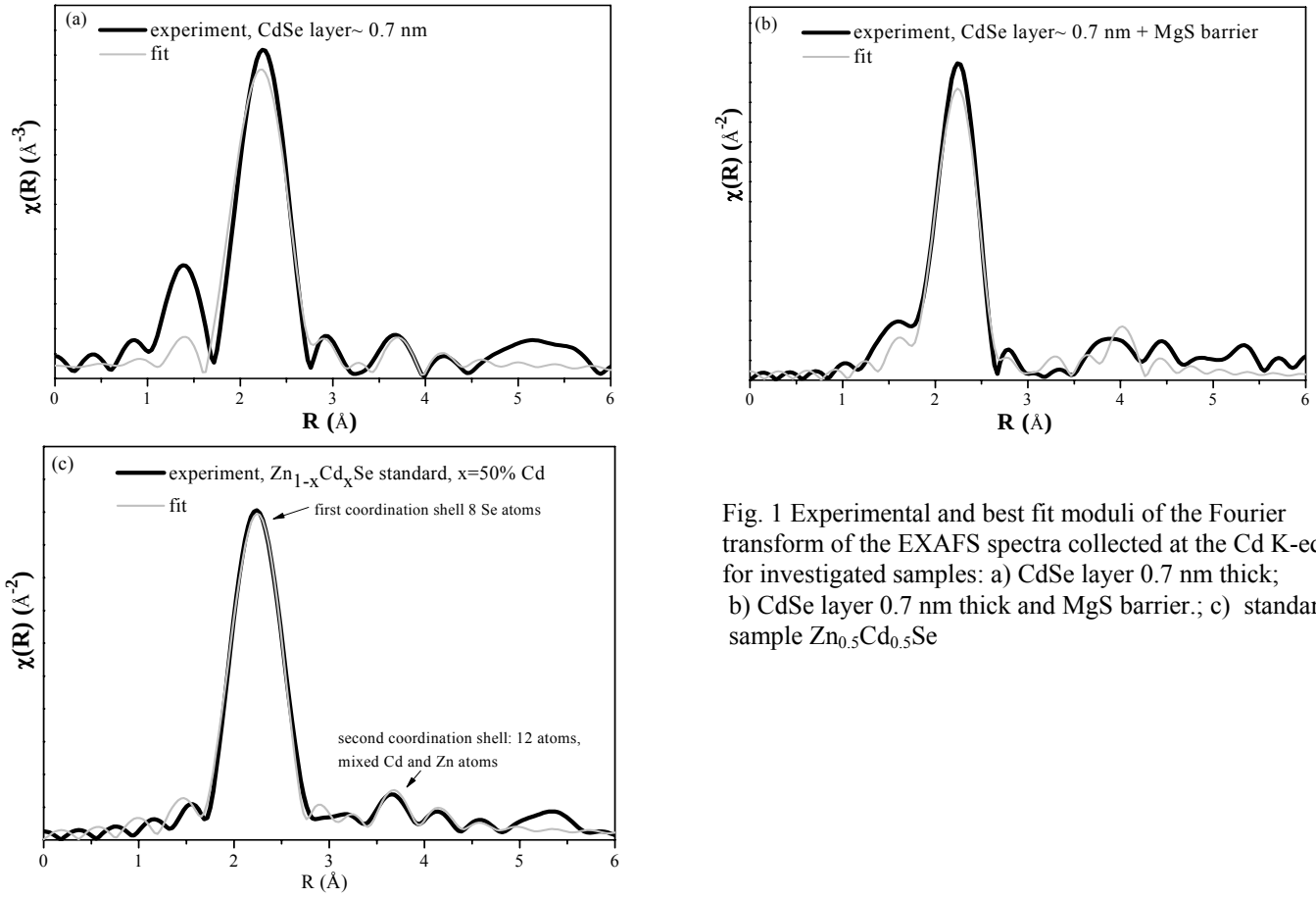

Fig. 1 Experimental and best fit moduli of the Fourier transform of the EXAFS spectra collected at the Cd K-edge for investigated samples: a) CdSe layer 0.7 nm thick; b) CdSe layer 0.7 nm thick and MgS barrier.; c) standard sample $Zn_{0.5}Cd_{0.5}Se$

The local atomic structure around Cd atoms in the nominal CdSe quantum dots were resolved using EXAFS technique we resolved the local structure. In order to get more insight into the overgrowth process, which is known to have a significant impact on the nanostructural properties the DAFS method also was applied (propsal HS-3498). The results are reported.

References

[1] D. Litvinov, A. Rosenauer, D. Gerthsen, P. Kratzert, M. Rabe, F. Henneberger, Appl. Phys. Lett. 81, (2002) 640.
[2] T. Passow, H. Heinke, T. Schmidt, J. Falta, A. Stockmann, H. Selke, P. L. Ryder, K. Leonardi, and D. Hommel, Phys. Rev. B **64** (2001) 193311
[3] Th. Schmidt, T. Clausen, J. Falta, G. Alexe, T. Passow, D. Hommel, S. Bernstorff, Appl. Phys. Lett. 84, (2004) 4367.
[4] T. Schmidt, E. Roventa, T. Clausen, J. I. Flege, G. Alexe, S. Bernstorff, C. Kübel,
A. Rosenauer, D. Hommel, and J. Falta, Phys. Rev. B 72 (2005) 195334.
[5] R. Arians, T. Kümmell, G. Bacher, A. Gust, C. Kruse, and D. Hommel, Apll. Phys. Lett. 90 (2007) 101114
[6] http://cars.uchicago.edu/ifeffit
[7] S. I. Zabinsky, J. J. Rehr, A. Ankudinov, R. C. Albers, M. J. Eller, Phys. Rev. B 52, 2995- 3009 (1995).
[8] B. Ravel, M. Newville, J. Synchrotron Rad. 12, 537- 541 (2005).