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INFLUENCE OVERGROWTH PARAMETERS ON THE LOCAL STRUCTURE IN CdSe QUANTUM DOTS STUDIED BY FINE STRUCTURE METHOD

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The II–VI quantum dots have attracted interest due to application in red, green and blue laser diodes, as well in fundamental physics [1]. The ZnSe-based laser diodes are not long-term stable under electrical operation. Nevertheless, it has been shown that such green emitting ZnSe lasers are significantly more stable when replacing the ZnCdSSe quantum well by a stack of CdZnSe/ZnSSe quantum dots [2].

CdSe quantum dots can be formed in a ZnSe matrix by molecular beam epitaxy (MBE). This system has a high lattice mismatch (~7%) resulted in self-assembled quantum dots (QDs) during epitaxial growth [3].

Since the self-organization process has a stochastic nature, the resulting nanostructures have a certain dispersion of their sizes and shapes and, in addition, the dots are chemically inhomogeneous. Therefore, a reliable and non-destructive characterization of the structure of quantum dots is of a crucial importance to improve their applicability. Several characterization techniques such as transmission electron microscopy (TEM), scanning tunneling microscopy (STM) and atomic-force microscopy (AFM) have been employed to aid the understanding of the growth mechanisms and to determine optimal growth conditions.

The structural investigations of CdZnSe/ZnSe quantum dots were mainly performed by high-resolution x-ray diffraction (HRXRD) using synchrotron radiation, high-resolution transmission electron microscopy (HRTEM) and luminescence [4, 5], yielding the structure and the correlations of the positions of CdSe quantum dots.

The capping process of quantum dots plays an important role for their optical properties; however the capping layer introduces additional strain and changes in the chemical composition by intermixing during the deposition of the capping layer. To get information about the intermixing of substrate and capped layer a key issue is to determine the optimal technological conditions in order to obtain the nanostructure with demanded optical and electrical properties.

In order to explain the influence of the overgrowth parameters on the structure of the formed CdSe quantum dots Extended X-ray Absorption Fine Structure (EXAFS) and Diffraction Anomalous Fine Structure (DAFS) were employed. Due to its selectivity for a chosen element, EXAFS is well suited to determine the bond lengths Cd-Se, Cd-Cd and Cd-Zn and atomic ordering within strained CdSe/ZnMgSSe quantum dot layers. However, the EXAFS signal provides structural information averaged over all absorber atoms selected. To obtain the bond lengths and the atomic ordering within regions with a chosen elastic strain, the DAFS technique was used. From the DAFS spectra we determined the structure of the neighborhood of absorbing atoms in a region of the dot volume with given strain (iso-strain volume). Therefore, local atomistic structural parameters for this volume are obtained as results. The advantage of the DAFS method is that the EXAFS-like information can be obtained "locally," allowing us to detect possible atomic ordering in CdSe/ZnMgSSe alloys.

A series of CdSe/ZnSe/MgS single quantum dots layers grown by molecular beam epitaxy (MBE) on GaAs(001) substrates were studied. The CdSe monolayers (ML) were embedded in a 1.4 nm ZnSe layer surrounded by 2 nm MgS barriers grown on a GaAs substrate with 50 nm ZnSe underneath and 25 nm above this dot structure. The investigated samples differ in the amount of deposited CdSe monolayers.

The EXAFS spectra at the Cd K edge (~27 keV) were collected at fluorescence mode using a multi-element Ge detector.

The DAFS spectra at the Se K-edge (~12.7 keV) 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 axis was chosen along the (h00) line (radial direction). The DAFS signal stems from an iso-strain volume, the position of which is determined by the value of the q_r coordinate, where the DAFS signal was collected. The grazing incidence geometry allowed us to reduce the contribution of the substrate to the scattered intensity and enhances the contribution of the quantum dots to the measured signal. To avoid the oxidation, the samples were kept in He atmosphere during the measurement.

The Athena program was used to subtract the pre-edge background, normalize to the experimental edge step and absorption data from the EXAFS data [6]. The DAFS spectrum $\chi(E)$ depends on the real (χ') and imaginary (χ'') parts of the anomalous form-factor of the Se atoms. The numerical Kramers-Kronig transformation was used to extract the imaginary part χ''(E) of the DAFS spectrum [7]. Then, the data were transformed to the direct R-space and both EXAFS and DAFS data were fitted in R-space to theoretical curves generated by the FEFF 8 code for the Cd-Se, Cd-Cd and Cd-Zn pairs [8]. Then, the Artemis program was used to obtain the structure parameters, *i.e*., bond lengths (R), Debye-Waller factors (σ^2) and coordination numbers (N) [9]. The EXAFS and DAFS results are discussed in details.

References

[1] T. Passow, K. Leonardi, D. Hommel, "Optical and Structural Properties of CdSe/Zn(S)Se Quantum Dot Stacks", *Phys. Stat. Sol. (b)* **224** (2001) 143–.

[2] M. Klude, T. Passow, R. Kröger, D. Hommel, "Electrically pumped lasing from CdSe quantum dots", *Electr. Lett.* **37** (2001) 1119–11120.

[3] K. Leonardi, H. Heinke, K. Ohkawa, D. Hommel, H. Selke, F. Gindele, U. Woggon, "CdSe/ZnSe quantum structures grown by migration enhanced epitaxy: Structural and optical investigations", *Appl. Phys. Lett*. **71** (1997) 1510–1512.

[4] Th. Schmidt, T. Clausen, J. Falta, G. Alexe, T. Passow, D. Hommel, S. Bernstorff, "Correlated stacks of CdSe/ZnSSe quantum dots", *Appl. Phys. Lett.* **84** (2004) 4367–1569.

[5] G. Bacher, H. Schömig, M.K. Welsch, S. Zaitsev, V.D. Kulakovskii, A. Forchel, S. Lee, M. Dobrowolska, J. Furdyna, B. König, W. Ossau, "Optical spectroscopy on individual CdSe/ZnMnSe quantum dots", *Appl. Phys. Lett*. **79** (2001) 524–526.

[6] http://cars.uchicago.edu/ifeffit

[7] M.G. Proietti, H. Renevier, J. Hodeau, J. Garcia, J. Bérar, P. Wolfers, "Diffraction-anomalous-fine-structure spectroscopy applied to the study of III-V strained semiconductors", *Phys. Rev. B* **59**, 5479 (1999); J.O. Cross, *Ph.D. thesis*, (University of Washington, Seattle, 1996); J. Coraux, V. Favre-Nicolin, M.G. Proietti, B. Daudin, H. Renevier, "Grazing-incidence diffraction anomalous fine structure: Application to the structural investigation of group-III nitride quantum dots", *Phys. Rev. B* **75** (2007) 235312.

[8] S.I. Zabinsky, J.J. Rehr, A. Ankudinov, R.C. Albers, M.J. Eller, "Multiple-scattering calculations of x-ray-absorption spectra", *Phys. Rev. B* **52** (1995) 2995–3009.

[9] B. Ravel, M. Newville, "*ATHENA*, *ARTEMIS*, *HEPHAESTUS*: data analysis for X-ray absorption spectroscopy using *IFEFFIT", J. Synchrotr. Rad*. **12** (2005) 537–541.