

## Local Structure Parameters of Ge Quantum Dots on Si(001) by XAFS Spectroscopy

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Recent studies of electronic properties of self-assembled Ge Quantum Dots (QD) on Si(001) produced by molecular beam epitaxy process have demonstrated the existence of discrete spectra of zero-dimensional hole states in the Ge clusters [1]. The heterostructures of this type naturally formed as large-scale dense arrays can be easily built into existing paradigm of silicon integrated systems for electronic memories, optoelectronic devices and for quantum transistor. Due to the 4% larger lattice constant and interatomic distances of Ge, strain evolving during growth of Ge films on Si(001) causes a series of critical morphological and some local spatial structure changes.

The local microstructure parameters of Ge were determined in Ge films on Si(001) produced by molecular beam epitaxy process at 300°C. Spatial parameters of Ge atoms surrounding were determined from GeK EXAFS (extended X-ray absorption fine structure) spectroscopy data using EXCURV92 program. XAFS measurements were performed at the VEPP-3 storage ring at the Budker Institute of Nuclear Physics in Novosibirsk. XAFS spectra were measured in surface sensitive mode based on total electron yield and fluorescent detection. The sample positions were kept to provide angles 0 and 90° between the normal of the Si(001) plane and the electric field vector  $E$  to determine structural parameters anisotropy.

Electron diffraction and scanning tunneling microscopy results analysis revealed thickness of wetting layers (4-5-monolayer thick) and average meanings in plane dimension and height of the dots formed during strained layer epitaxy (Stranski-Krastanov growth mode). Two structures were formed in parallel on two part of Si(001) substrate. Both structures contained Ge layers separated by blocking Si layers 10 nm thick and differed only in the thickness of the deposited germanium layers. The first type of the structure contains pseudomorphous 4-monolayer Ge (2D) film. The second structure type contains pyramid-like (3D) islands formed in Stranski-Krastanov growth in addition to the flat critical thickness 4-5-monolayer Ge film in order to reduce a high strain energy. This self-organized uniform Ge nanostructures have lateral sizes ~ 15 nm and height ~ 1.5 nm for the film with effective thickness equals 10 monolayers.

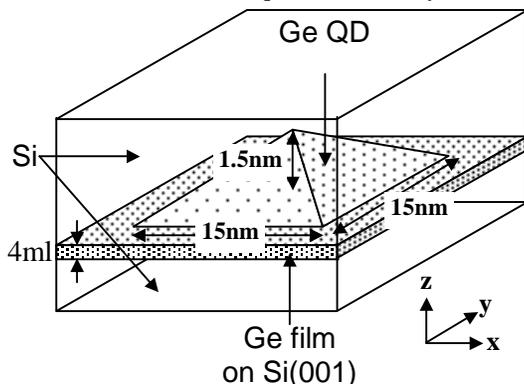


Fig. 1. Circuit of Ge nanocluster (QD) on Si(001)

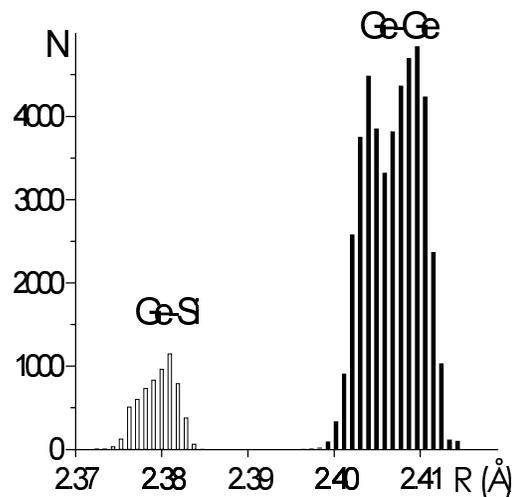


Fig.2. Bar chart of interatomic bond lengths distributions in Ge QD on Si(001) obtained by VFF method calculation. N – number of interatomic bonds, R – interatomic distances.

For analyzing the environment of Ge atoms Fourier-filtered EXAFS data  $\chi(k)$  were fitted with  $k$  and  $k^2$  weighing in the range of photoelectron wave vectors from 2.5 Å<sup>-1</sup> to 13 Å<sup>-1</sup>. The local microstructure parameters (interatomic distances, Ge coordination numbers) are linked to nanostructures morphology and adequate models are suggested and discussed.

While the experimental functions  $k\chi(k)$  of GeK EXAFS differ widely between the films of Ge<sub>x</sub>Si<sub>1-x</sub> solid solution of different stoichiometry, the function are absolutely similar for a Ge<sub>0.50</sub>Si<sub>0.50</sub> thick film and four-monolayer films. This indicates a pronounced interphase exchange of Si and Ge atoms leading to relaxation of elastic strains in the system due to the application of blocking Si layer at 500°C. It was established, that pseudomorphous 4-monolayer Ge (2D) films, as it is called, contains about 50% Si atoms. The pure Ge nanoclusters covered by 2-monolayer film with about 50% Si atoms impurity from blocking Si layers.

The EXAFS spectra for samples with pseudomorphous films and nanoclusters, measured with different  $E$  vector orientation relative to Si(001) plane, are almost indistinguishable.

Pyramid-like (3D) pure Ge islands formed in Stranski-Krastanov growth are characterized by interatomic Ge-Ge distances 2.41 Å, 0.04 Å less than in bulk Ge (2.45 Å) and Ge-Si distances 2.37 Å.

Elastic deformation spatial distribution calculation procedure of coherent strained heterostructures was developed by valence force field (VFF) method [2]. Elastic deformation spatial distributions in Ge QD on Si(001) and in their environment were obtained. The values of Ge-Ge and Ge-Si interatomic distances obtained by processing EXAFS data within the limits of experimental error ( $\pm 0.01$  Å) coincide with interatomic bond lengths obtained by VFF method calculation and allowed an understanding of previous capacitance spectroscopy results for system with QD.

Financial support from the Russian State Scientific and Engineering Program on Physics of Solid State Nanostructures (grant 99-1135) is greatly appreciated.

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2. A.V. Nenashev and A.V. Dvurechenskii, JETP, **117**(9) 570, 2000