PA02

EXAFS AS A TOOL FOR INVESTIGATION OF THE LOCAL ENVIRONMENT OF Ge ATOMS IN BURIED LOW-DIMENSIONAL STRUCTURES

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Keywords: X-ray absorption, EXAFS, TEM, low-dimensional structures, Ge thin film

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The GeSi based heterostructures with self-assembled nano-islands and quantum dots are very prospective in view of their optoelectronic applications in Si-based technology. By now, in spite of large number of articles dedicated to the investigation of GeSi islands, a lot of problems concerning growth mechanism and island composition, as well as elastic strains inside the QDs, are still unsolved.

To solve such problems, the GeSi low dimensional structures were studied by Extended X-Ray Absorption Fine Structure (EXAFS). The aim of this investigation was to get knowledge about the local structure around Ge atoms inside formed quantum dots. This structure depends on the growth temperature and the thickness of Ge layer buried in the silicon matrix. These parameters strongly influence the QDs luminescence.

Series of measurements were performed for a single Ge layer buried in the silicon matrix at A1 station at the HASYLAB/DESY (Germany) with the angle of 45^0 between the incident beam and sample surface. The fluorescence, total electron yield and the transmission modes of detection were used. The samples were grown by molecular beam epitaxy (MBE). The growth of QDs containing heterostructures (with *in situ* RHEED control) was done in "KATUN-S" MBE installations by Stranski-Krastanov mode on (001) Si substrates.

The Artemis and Athena programs using IFEFFIT data analysis package were applied for data analysis. The theoretical amplitudes and phases were calculated by FEFF8.

By using theoretical approaches in the quantitative analysis of EXAFS spectra we are able to describe the local structure of formed QDs. This analysis defines the magnitude and the sort of strain in the Ge-Ge and Ge-Si bonds. In this work it will be shown that over some critical thickness of Ge layer equal to ~10 monolayers the elastic strains decrease and the misfit dislocations appear. This sharply deteriorates the optical properties of the investigated Si/Ge/Si structures.

Our further investigation of the above structures showed that the Si atoms diffusion inside the Ge QDs depends on the Ge layer growth temperature. In the samples with a *low growth temperature* (210°C) of Ge layer, the core of formed QDs consists of pure strained germanium, so silicon atoms migrate only to the Ge/Si interfaces region. Formation of strained and relaxed monocrystalline Ge core inside the QDs was assumed on the basis of the results of EXAFS spectra analysis and from the geometrical estimation of contribution of Si atoms from the QDs surface.

Concerning the *higher temperature* of growth (500÷750°C) the diffusion of Si atoms increases inside the QDs and the Ge_xSi_{1-x} solid solution forms within the limits of x (48÷33%).

To confirm the EXAFS analysis conclusion more measurements were performed using transmission electron microscopy (TEM). The *low temperature* samples with 8÷20 ML of Ge were investigated by cross-section and plan-view TEM. The reported results of TEM studies of the local structure of germanium quantum dots (QDs) in "sandwich" Si/Ge/Si structures are in good correlation with EXAFS conclusion.

In Figure 1, the HREM image of sample Si/8 ML Ge/Si is shown. Changes of the contrast along the layer permits us to suppose the QDs formation, but they are densely populated and in projection (which we have in TEM cross-section sample) the layer appears as continuous one. This Ge layer is covered by Si capping layer. This Si layer is uniform without structural defects present and no misfit dislocations are observed at the Ge/Si interfaces.

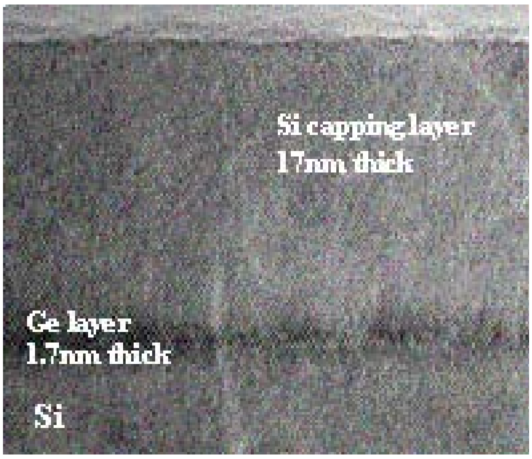

Figure 1. The high-resolution image for Si/8 ML Ge/Si sample.

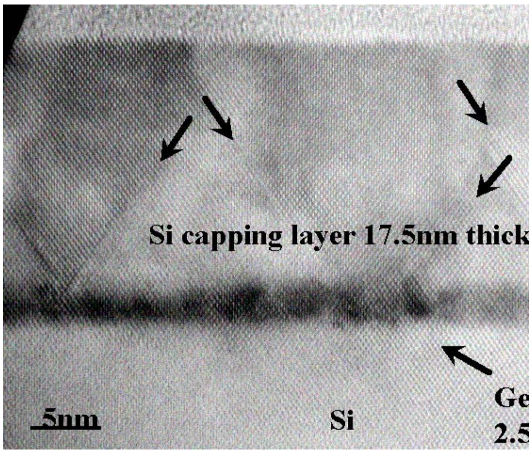

Figure 2. The high-resolution image for Si/12 ML Ge/Si sample.

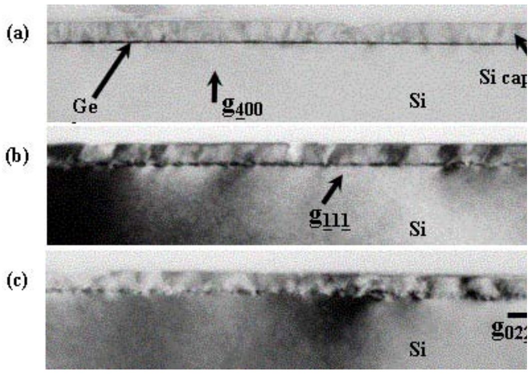

Figure 3. TEM bright field near surface images obtained in two beam conditions for Si/12 ML Ge/Si sample.

The HREM results for Si/12 ML Ge/Si sample clearly show the QDs formation (Fig. 2). The arrows mark planar defects created at the Ge layer on (111) planes in the Si capping layer. They start from the Ge layer (they are marked by arrows in Figure 2). One can see them also in low magnification images obtained under two beam conditions with ***g***-vector $\underline{1}1\underline{1}$ (Fig. 3b) and $02\underline{2}$ (Fig. 3c). These defects are stacking faults formed on {111} planes of Si. Also the misfit dislocation appear at the Ge/Si interfaces.

The formation of the QDs was also confirmed for 20 ML sample. The Ge layer in this case exhibits more dotted structure suggesting that with increasing of Ge thickness more QDs are shaped. The planar defects in the capping layer, similar to ones observed in the sample with 12 ML were visible, but in this sample the defects started at the base of QDs and propagate through the Ge layer to the sample surface.

These observations confirmed the results of EXAFS studies that after some critical thickness of Ge layer, the strains in formed QDs are relaxed by formation of misfit dislocations.

Acknowledgments: This work was partially supported by the State Committee for Scientific Research (Republic of Poland) Grant No. 72/E-67/SPB/5.PR UE/DZ 27/2003-2005 and by the IHP-Contract HPRI-CT-2001-00140 and G1MA-CI-2002-4017 (CEPHEUS) of the European Commission. TEM part of work was supported by U.S. Department of Energy under the contract DE-AC03-76SF00098.

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