ESRF	**Experiment title:** **Intermixing and strain relaxation mechanism in self-organized Ge quantum dots in Si(111)**	**Experiment number**: SI 496
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Report:

There is recently much interest in structures and devices of reduced dimensionality, such as (1-D) quantum wires and (0-D) quantum dots, the latter being the subject of the present experiment. In a quantum dot the charge carrier confinement is in all three spatial directions. One of the methods to obtain quantum dots is that of self-organized growth of an epilayer on a lattice mismatched substrate. Ge quantum dots on Si have been obtained in this way either by Molecular Beam Epitaxy (MBE) or by Chemical Vapour Deposition (CVD). The present consensus is that the growth of Ge on Si (4.2 % mismatch) is of the Stranski-Kastanow type: a 2D pseudomorphic wetting layer of thickness ~ 4 Å initially forms, followed by the appearance of 3D islands. The degree and type of strain in these islands is a matter of current reasearch. It is generally believed that below a certain thickness the islands are coherently strained, with a degree of strain which decreases with the distance from the substrate. Above a certain thickness the appearance of misfit dislocations which decrease the strain energy has been observed e.g. by AFM. However, a clear picture of the mechanisms of strain relaxation for semiconductor dots is not yet available.

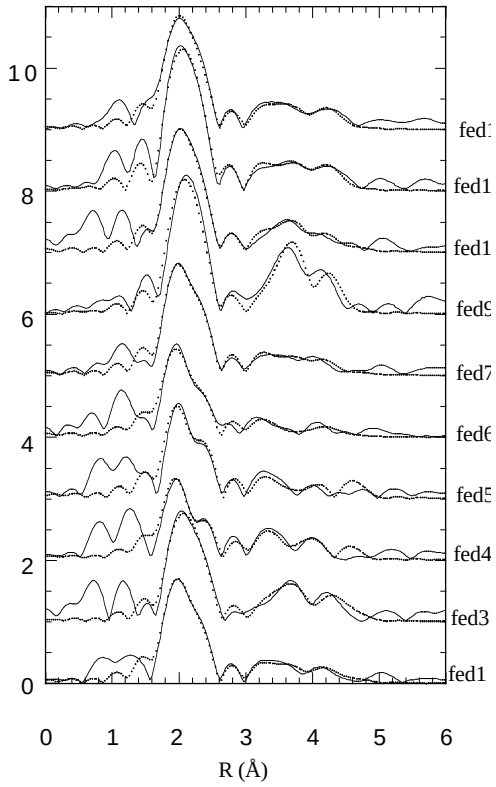
Analysis of Ge K-edge XAFS of Ge dots deposited on Si(001) by CVD lead us to the conclusion that a previously disregarded mechanism plays an important role in minimizing the strain energy: intermixing of Si atoms from the substrate into the Ge dots [1]; we proposed that the strain – enhanced diffusion was the driving force for atomic motion. Following those results we have obtained the present beamtime in order to study intermixing

in the related system of Ge dots deposited by MBE on Si(111); preliminary evidence had indicated that in the wetting layer for Ge/Si(111) there was considerable intermixing [2].

XAFS measurements were successfully performed on the GILDA beamline on fourteen samples deposited at the University of Rome "Tor Vergata". The measurements were performed in the fluorescence mode using the 13 element detector, digital electronics and the specially designed vibrating and LNT cooled sample holder. All these features allowed data with good signal - to – noise ratio to be collected on these "difficult" samples. The sample thickness ranged between 1.5 and 9 nm while the substrate deposition temperature was varied between 450 and 550 ºC.

Data has been analysed with the FEFF package up to the third coordination shell. In the figure we show a set of preliminary Fourier transforms of the data (continuous line) and the fit (dotted line). The fit has been performed assuming that each coordination shell is composed of a mixture of Ge - Ge and Ge – Si contributions, the total coordination being fixed to the value for the diamond structure; the relative number of Ge - Ge and Ge - Si contributions was equal for all shells. The fit was performed in R – space in the range 1.7 – 4.4 Å (not corrected for phase shifts) using a k^2 weight.

A detailed analysis of the fitting results including a correlation with the growth parameters is in progress. However, we can anticipate that in all the samples the Ge – Si coordination number ranges between 1.1



and 2; assuming the absence of ordering effects this implies an average Si concentration in the dots ranging between 0.25 and 0.5. This confirms and extends our previous results on the (001) substrate [1].

References

[1] F. Boscherini, G. Capellini, L. DiGaspare, N. Motta, F. Rosei and S. Mobilio, "Ge-Si intermixing in Ge quantum dots", Appl. Phys. Lett. **76**, 682 (2000).

[2] F. Rosei, N. Motta, A. Sgarlata, G. Capellini, and F. Boscherini, "Formation of the wetting layer in Ge/Si(111) studied by STM and XAFS", Thin Solid Films **369**, 29-32.(2000).