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Shifts: 18	**Local contact(s)**: Vincent Jacques (email: vincent.jacques@u-psud.fr)	*Received at ESRF:*

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Report:

Highly-perfect epitaxial semiconductor layer stacks are quintessential for many low-dimensional quantum structures such as ultrafast transistors, solid state lasers and detectors. Since dimensional scaling in the CMOS technology is approaching fundamental limits, the use of other semiconductor materials on the Si platform with superior optical and electrical properties is one promising method to achieve the so-called functional scaling. Combining Si with other semiconductor materials raises, however, serious concerns about processing compatibilities, since in general these materials are neither lattice-matched to the Si substrate, nor are they likely to exhibit similar thermal properties. Consequently, defect formation and wafer bowing are serious obstacles.

Faced with the task of producing very thick crystalline active layers made from Ge for high-efficiency and high-resolution X-ray detectors monolithically grown on Si CMOS substrates, we have shown that these problems can be solved by replacing continuous layers with arrays of closely spaced individual crystals. These crystals are deposited on deeply patterned Si substrates by low-energy plasma enhanced chemical vapor deposition (LEPECVD) using a new mechanism of self-limited lateral expansion. Since the interpretation of high-resolution X-ray diffraction experiments performed with a laboratory source on such arrays was complicated by the averaging over thousands of crystals, we have performed scanning nanodiffraction in order to locally map the strain status and crystal quality of a single crystal. X-ray scanning (115) nanodiffraction was performed on individual Ge crystals at the ID01 beamline using a tightly-focused beam (X-ray energy 11.07 keV) down to ~500×300 nm produced by Fresnel zone plates. In order to avoid signal contributions from adjacent scatterers, chosen crystals were isolated by etching and subsequent removal of their nearest neighbours, see **Fig 1a**. By scanning along their heights, we showed that the plastic strain generated by the large mismatch of the lattice

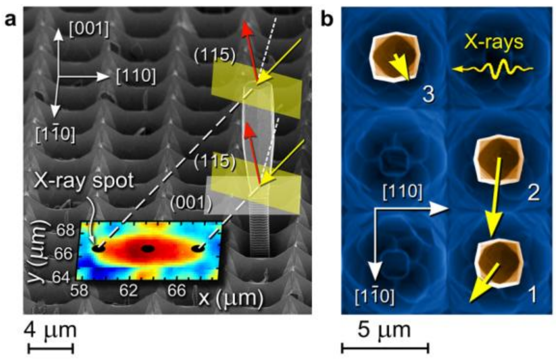

Fig. 1: *(a) Scanning X-ray nanodiffraction of an isolated, 11-µm-tall Ge crystal. The color map represents the scattered intensity collected around the Ge(115) peak when the incident beam was scanned along the crystal. (b) Top-view SEM micrograph of three Ge crystals showing schematically their tilt enhanced by a factor of 500.*

parameters between Si and Ge causes these crystals to be slightly tilted with respect to each other, see **Fig 1b**. Hence, the apparent mosaicity of the order of 0.1°, previously measured with laboratory sources, could be explained in terms of individual tilts of thousands of crystals. An example of 3D reciprocal space maps (RSM) projected onto Q_xQ_z for Ge and Si is shown in **Fig 2**.

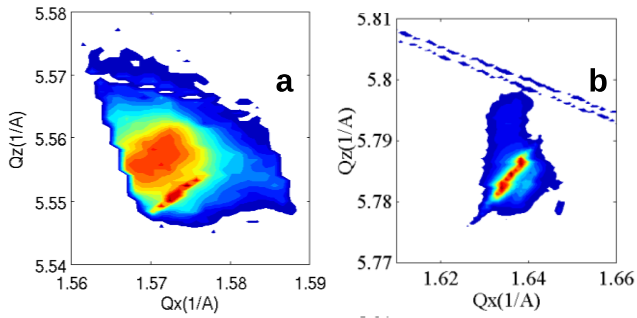

Fig. 2: *Reciprocal space map around (115) for beam in the middle of the pillar: (a)signal from Ge - the narrow oblique peak is from crystal and the broad diffuse scattering originate from Ge in trenches, (b) signal fom Si substrate.*

By scanning the crystal quality along the vertical growth direction, we have found that, after reaching sufficient height, the Ge crystals become indistinguishable from defect-free single crystals, see **Fig 3**. The Ge crystal peak shape coincide with the Si substrate peak within the experimental resolution.

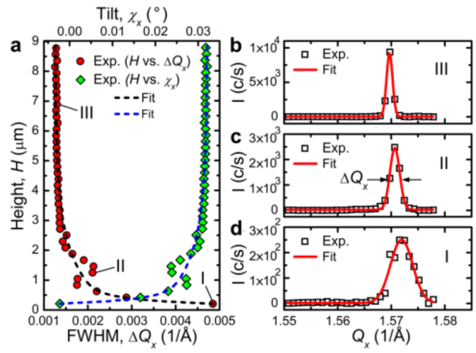

Fig. 3: *(a) Full-width-at-half-maximum (FWHM) of the Ge(115) peak and tilt along the Qx direction vs. crystal height. (b–d) Cross-sections through the Ge(115) peak along Q_x at 3 different crystal heights (e.g. I, II and III) depicted in (a).*

As the second sample we have investigated a similar isolated SiGe crystal, see **Fig 4a**, but covered by multiple quantum well structure on top. 3D RSMs were recorded at every point of the mesh, scanning the area around the crystal. Collecting a range of interest around selected superlattice satellites, we were able to reconstruct top crystal facets. Scanning diffraction micrograph in **Fig 4b** corresponds well to SEM image in **Fig 4a**. Selected isolevel plot of 3D RSM is demonstrated in **Fig 4c**. **Fig 4d** shows the 2D Q_xQ_z projection of 3D RSM for the middle part of the crystal top. The shape of the superlattice satellites demonstrates that the MQW structure on top is defect free as well, as the buffer crystal.

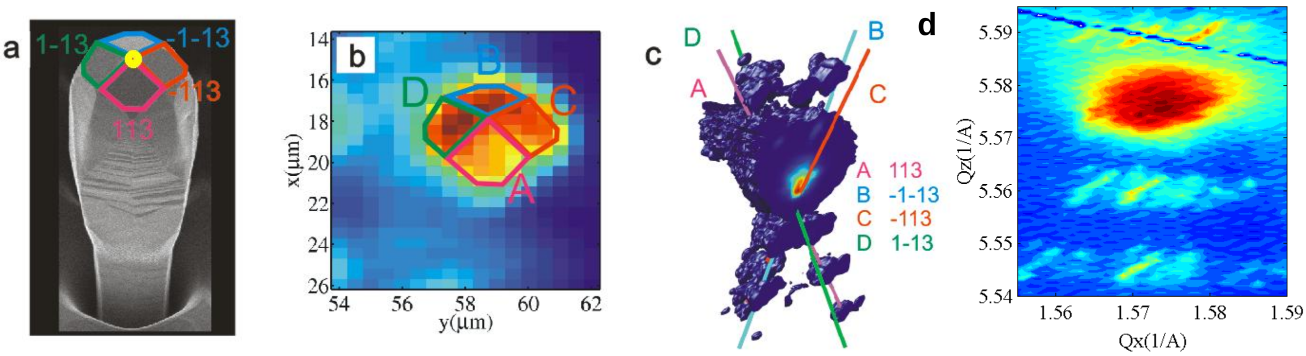

Fig. 4: *(a)Perspective view SEM micrograph of a 8 μm tall SiGe crystal with crystallographic facets, (b) the intensity maps scanned over the surface for all SL-1 peaks, the crystal facets shape is reconstructed, (c) 3D RSM around (115) reciprocal space point as iso-level surface plot recorded in the middle of the crystal. (d) example of the 2D RSM at selected point (yellow).*

This first demonstration of perfect strain-free single crystals evolving from a heavily distorted interface with a mismatched substrate could pave the way for device applications hampered so far by dislocations, substrate bending and layer cracking. Especially the fabrication of high-brightness light-emitting diodes, radiation detectors, power transistors and multiple-junction solar cells might profit from the elimination of mismatch related defects.

[1] C. V. Falub, et al, ESRF Highlights 2013 p. 96.

[2] C. V. Falub, M. Meduňa, D. Chrastina, F. Isa, A. Marzegalli, T. Kreiliger, A.G. Taboada, G. Isella, L. Miglio, A. Dommann, and H. von Känel, *Scientific Reports* **3**, 2276, (2013).

[3] C.V. Falub, T. Kreiliger, F. Isa, A.G. Taboada, M. Meduňa, F. Pezzoli, R. Bergamaschini, A. Marzegalli, E. Müller, I. Giovanni, D. Chrastina, A. Neels, P. Niedermann, A. Dommann, L. Miglio, and H. von Känel, *Thin Solid Films* **557**, 42 (2014).