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Report:

Integration of optoelectronic and photonic devices with Si microelectronics technology has been a long-standing goal and an active research area for many years. Yet, the key challenge is the integration of crystalline materials with dissimilar lattice parameters and thermal properties on top of each other. We have recently demonstrated that exceptionally thick (> 50 μ m) Ge-layers can be monolithically integrated onto a Si CMOS platform despite the lattice mismatch of ~ 4% and thermal residual strain induced upon cooling. Dislocations, layer cracking and wafer bowing could all be eliminated by a novel mask-less process wherein high-quality Ge towers are epitaxially grown on micron size elevated structures on a clean, Si-wafer patterned by standard optical lithography and dry etching. X-ray diffraction (XRD) measurements with a laboratory diffractometer (Cu K α , FWHM ~ 1 mm) showed that the Ge heterostructures were fully relaxed, and that the width of the coherent diffraction Ge peak was very sharp along Q_z direction, as sharp as a Ge wafer. In addition, a diffused scattering around this peak in the Q_x direction was observed. Therefore, it was essential to study local crystalline properties (i.e. strain, defects, etc.) of our Ge heterostructures by means of a focused x-ray beam as the one available at the ID01 beamline.

In this experiment we aimed for the high-resolution XRD measurements (x-ray energy 11.07 keV) in coplanar geometry around the symmetric (004), and the asymmetric (115) and (206) reflections. Samples investigated consisted of ~ 10×10 mm chips containing a 8×8 mm² patterned area, which were cleaved from 4" Si(001) wafers on which epitaxial Ge layers were deposited by the LEPECVD method. Germanium layer thickness ranged from 1 up to 8 μ m, and different patterns were explored consisting of Ge towers and ridges grown on 8 μ m tall Si structures separated by 1 μ m, with ~ 2×2 μ m² footprint area (for towers) and width of 2 μ m (for ridges). Germanium ridges oriented along both [110] and [100] directions were



Fig. 1: Schematics of the (004) scattering geometry for 1 µm Ge towers grown on Si pillars.

investigated. The x-ray beam profile after the Fresnel zone plate had a FWHM $\sim 500 \times 300$ nm, which was small enough to scan the strain relaxation across a single Ge tower/ridge. Depending on the scattering geometry, however, the profile on the sample was slightly larger. Moreover, in view of the penetration depth of the x-rays a few neighboring pillars/ridges were contributing to the diffraction patterns (Fig. 1). Due to the hard limits of the goniometer and the photon energy used, the (224) reflection that would have allowed us to scan a single pillar/ridge, i.e. almost normal incidence and grazing exit, was not accessible. Both patterned and unpatterned areas of the samples were investigated. In order to measure the strain and tilt of the Ge heterostructures, we rocked the incidence angle in both symmetric and asymmetric configuration while

moving the beam across the sample. Since a 2D pixel detector was used, 3-dimensional RSMs could be constructed for each (x,y) position of the x-ray beam on the sample (see Fig. 2).

A first important issue which had to be checked was whether the Ge heterostructures were indeed tilted with respect to each other. In order to do that, we also measured the total intensity of a certain reflection at each (x,y) position. In spite of the multiple reflections caused by the incoming x-ray beam we were able to resolve the Ge on Si heterostructures as shown in Fig. 3. On the one hand the position sensitive XRD intensity maps of the Si(004) and Si(115) reflections for the patterned samples were quite regular (Fig. 3a), as expected, since the Si pillars and ridges were etched into the Si wafer. On the other hand, since the Ge towers and ridges sit on distinct networks of dislocations, they were tilted with respect to the (001) plane for



Fig. 2: Sliced 3D (h,k,l) RSM around the Ge(004) reflection for a 8 μ m thick Ge film on Si(001).

which the sample alignment was performed, as shown by the irregular position of the maximum intensity of the Ge(004) reflection (Fig. 3b).



Fig. 3: Position sensitive XRD intensity maps for the 1 µm Ge towers shown in Fig. 1: a) Si(004) reflection; b) Ge(004) reflection.

Strain information for both Ge towers and ridges were extracted from the (004) and (115) scans. At each position the (115) reflection was corrected for the corresponding (004) tilt. It was shown that the strain oscillates with a period of ~ 3 μ m, similar to the pattern period.



Fig. 4: Position sensitive XRD intensity maps for 1 μ m Ge ridges grown epitaxially on 8 μ m tall Si ridges parallel to [110] for Ge(004) (a) and Ge(115) (b) reflections. c) Perpendicular (ε_{\perp}) and parallel (ε_{II}) components of the strain across the Ge ridges.

In conclusion, the results of our experiments show that we were able to resolve the micron-size Ge heterostructures grown epitaxially on patterned Si(001) wafers, and that both tilt and strain distribution could be determined from the 3D RSMs. Similar analyses will be performed for all the samples investigated during this beamtime and the results will be compared with finite element simulations.