Advanced Structural Investigation of SiGe Heteroepitaxially Grown Crystal Arrays

I. Marozau, F. Isa •, A. Jung • T. Kreiliger •, G. Isella ••, H. von Känel •, P. Niedermann, O. Sereda

Imaging sensors directly coupled to readout units form are an area of growing technological interest. One example concerns devices for X-ray imaging and inspection, ranging from medical diagnostics and cancer therapy to non-destructive testing of all kinds of goods (quality assurance, security). A new approach towards X-ray detector fabrication, based on epitaxially grown Ge and SiGe crystal arrays, has helped to overcome the problems of crystal defects, layer cracks and wafer bowing. High resolution X-ray diffraction is a powerful tool to investigate the structural quality and strain condition in the three-dimensional SiGe crystal arrays heteroepitaxially grown on Si.

Monolithic integration of SiGe semiconductors on Si substrates is an easy and efficient way to combine specific optical and electronic properties of SiGe with the advantages of Si-based CMOS technology. This approach requires fabrication of high-quality dislocation-free heteroepitaxial SiGe layers on Si, which is a very challenging task due to the relatively large lattice mismatch between Ge and Si of about 4%. To overcome this difficulty, it was recently proposed to use pillar-patterned Si substrates for the growth of three-dimensional micron-size Ge and SiGe crystal arrays, which have been shown to be almost dislocation-free [1, 2] (Figure 1).

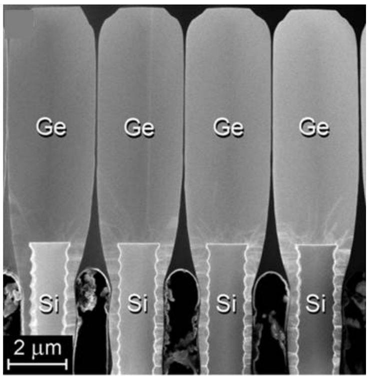

Figure 1: Cross-section view SEM micrograph of Ge three-dimensional crystal array grown on pillar-patterned Si substrate [2].

High resolution X-ray diffraction (HRXRD) was applied to study the epitaxial quality and strain state of such SiGe crystal arrays, in which the Ge content gradually increased from 0.5 at.% at the interface with the substrate to 40 at.% at the surface. Utilization of parallel monochromatic X-ray beam and narrow-acceptance-angle analyzer in combination with the high resolution goniometer, enables very precise analysis of tiny crystal lattice distortions by HRXRD. In particular, reciprocal space mapping of asymmetric crystallographic reflections allows a separate determination of in-plane and out-of-plane unit cell parameters and calculation of the corresponding strains in epitaxial samples.

An analysis of the $\omega/2\theta$ diffraction patterns (shown in Figure 2) and the corresponding rocking curves suggests that the SiGe crystals are epitaxially grown on Si substrates and exhibit a high structural quality. The crystals reveal a small tilt of up to ~ 0.1° with respect to the surface normal, which is probably due to slightly eccentric deposition geometry. The Ge content of 40.9 at. % was calculated for the top SiGe layer from the position of its crystallographic reflection (Figure 2). This value is in a good agreement with the expected target value of 40 at. %. Figure 3 shows an example of a reciprocal space map (RSM) around the asymmetric (115) reflection. A comparison of the experimentally acquired data with the theoretical calculations reveals that the crystals are fully strain-relaxed through their whole height of ~30 µm. The calculated in-plane and out-of-plain strain values for the top $Si_{0.6}Ge_{0.4}$ layer are very small (~ 0.01%).

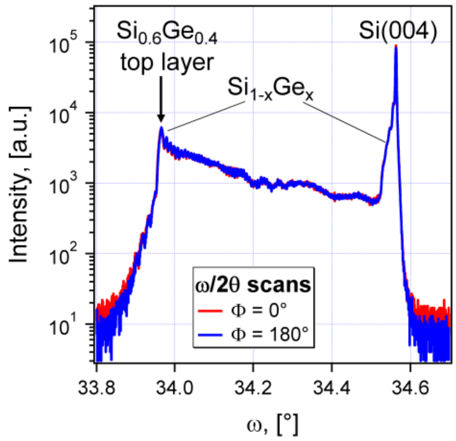

Figure 2: $\omega/2\theta$ XRD patterns of graded SiGe crystals on Si. Two measurements were performed at different Φ angles to account for the crystals tilt effect for calculation of the Ge content.

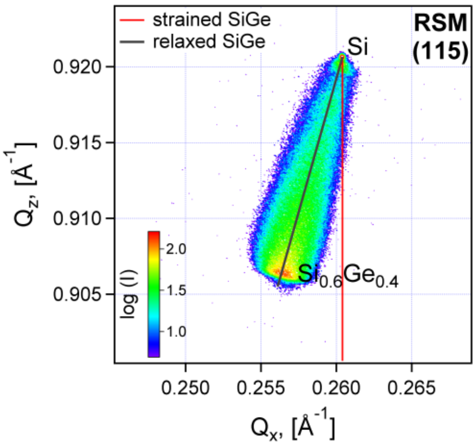

Figure 3: Reciprocal space map measured around the (115) asymmetric Bragg reflection. The theoretically calculated evolution of the reciprocal lattice parameters in case of fully strained and fully relaxed SiGe is shown with red and dark grey lines, respectively.

Performed structural analysis of the SiGe crystals provides valuable information for understanding the performance of this functional component for the development of a novel X-ray detector.

• Laboratory for Solid State Physics, ETHZ, Zurich, Switzerland
•• L-NESS, Como, Italy

[1] C.V. Falub, *et al.*, Science, 335 (2012) 1330-1334
[2] C.V. Falub, *et al.*, Thin Solid Films, 557 (2014) 42–49