FZR ROBL-CRG	**Experiment title:** HIGH- PRECISION DETERMINATION OF ATOMIC POSITIONS IN 6*H*- AND 4*H*-SIC CRYSTALS AND INVESTIGATION OF GERMANIUM NANOSTRUCTURES ON SILICON CARBIDE	**Experiment number:** 20-02-24
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Shifts:	**Local contact(s):** Dr. Norbert Schell	*Received at ROBL:* - 3 MAR. 2000

Names and affiliations of applicants (* indicates experimentalists):

Andreas Bauer*
Dr. Günter Hess*
Dr. Jürgen Kräußlich*
Prof. Dr. Konrad Goetz
Friedrich Schiller University of Jena
Institute of Optics and Quantumelectronics
Department of X-ray Physics
Max-Wien-Platz 1
D-07743 Jena / Germany

Report:

In this period at the beamline BM 20 at the ESRF we carried out the following investigations:

(i) Completion of the measurements for the structure refinement of the silicon carbide (SiC) polytypes 6*H* and 4*H* (Ref.[1]).

(ii) Silicon and germanium nanocrystals on silicon carbide substrates.

(i): To complete previous measurements at the BM20 [1] the following measurements were done. An absolute calibration of the integrated intensities of the "quasiforbidden" reflections rocking curves required measurements on a nearly perfect silicon crystal. Selected SiC-reflections, e.g. the 00.2-reflection of the 6*H* polytype (Fig. 1) with phase invariants ϕ_3 close to 0° and 180°, respectively, were investigated. Such combinations of reflections allow a very precise determination of the phase invariant to obtain an unambiguous structure refinement model. We also measured the forbidden 6*H*-SiC 00.9 reflection (same angular position as the "quasiforbidden" 00.6-reflection of the polytype 4*H*) to ascertain the polytype-purity of the crystal. An azimuthal scan of the 00.9 reflection shows no asymmetry of the "Umweg"-reflection. More over an ω-scan displays no peak.

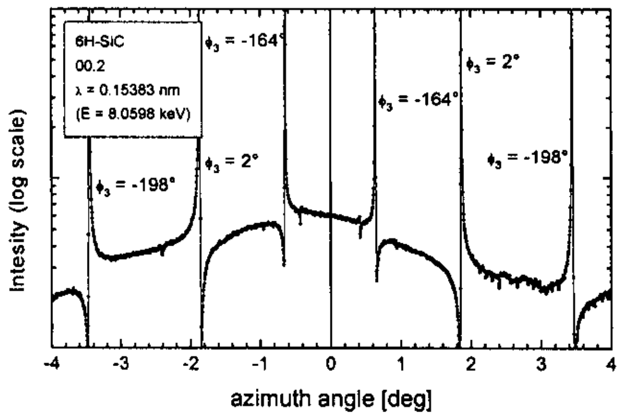

Fig. 1: Azimuth scan of the "quasiforbidden" 6*H*-SiC 00.2 reflection. The phase invariant is given by $\phi_3 = \phi_L + \phi_{H\text{-}L} - \phi_H$, were ***H*** characterizes the weak "quasiforbidden" reflection, ***L*** and ***H–L*** the two remaining strong "Umweg"-reflections.

[1] Forschungszentrum Rossendorf, Project-Group ESRF-Beamline (ROBL-CGR), Report January 1998 – June 1999, p 68.

(ii): Different SiC-surfaces were coated with thin layers of Si resp. Ge and subsequently annealed to 900 °*C* respective 600 °*C*. Such a procedure produces, according to AFM, Si- or respectively Ge-nanocrystals whose number, size distribution and shape depends on the process parameters. Three of those samples were investigated on the ROBL-beamline at the ESRF. The θ/2θ - scans show for all samples 111- and 220-reflections of Si respectively Ge (Fig. 2). This reveals unambiguously that the nanocrystals grow preferentially in two different orientations (<111>, <110>). Interestingly, for the Ge-samples those reflections are shifted towards the angular position of the respective Si-reflection. Such a peak shift could be explained by a lattice distortion due to the lattice mismatch or by the change in the lattice constant due to the formation of a Si/Ge solid solution. The lateral orientation of the (111)- and (110)-nanocrystals was investigated by comparison of theϕ-scans of an appropriate nanocrystal-reflection (220-reflection for (111)-nanocrystals and 111-reflection for (110)-nanocrystals) with an appropriate substrate-reflection (Fig. 3). This comparison showed that the (111)-nanocrystals as well as the (110)-custers grow coherently with respect to the substrate.

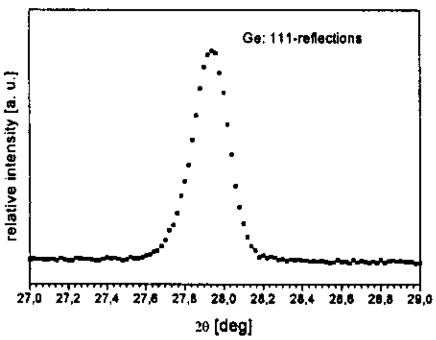

Fig. 2: θ/2θ scan of Ge-clusters on 6*H*-SiC: 111-reflections of Ge

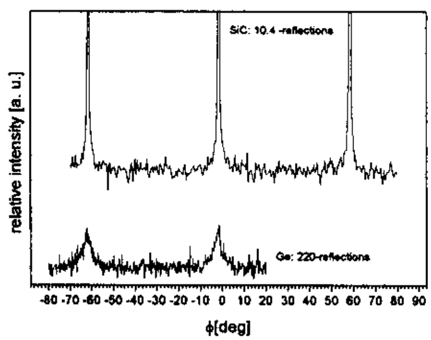

Fig. 3: Comparison of ϕ-scans of the Ge(111)-clusters (220-reflection, χ = 35.27°) with the the SiC substrate (10.4-reflection, χ = 54.79°)