Report on experiment 02-02-788

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Stability of 3C-SiC upon ion-irradiation

In a previous experiment (02-02-763) preliminary experiments have been conducted in order to analyze the radiation effects in (001)-oriented cubic (3C) and hexagonal (6H) SiC single crystals. These experiments revealed that upon 100 keV Fe ion-irradiation a thin (< 100 nm) damaged layer is formed at the surface of the single crystals. Moreover, it appeared that the scattering from the damaged layer was 10^4 to 10^8 weaker than the diffraction from the single crystal. The obtaining of high quality data hence implies a dynamic range of at least 8 orders of magnitude, a range that can only be obtained at synchrotron sources, especially if high resolution is also required.

The aim of the present proposal was (i) to record a consistent set of high-quality data in order to complete the data obtained from the preliminary experiments and confirm the first results and (ii) check whether ion-irradiation leads to a destabilization of the cubic phase. Such ion-irradiation - induced destabilization have been observed in the structurally similar GaN compound and it is known that 3C-SiC is easily destabilized, for instance upon thermal annealing.

7 3C-SiC and 8 6H-SiC single crystals (irradiated at increasing fluence) have been analyzed. We recorded data from the (004) reflection of 3C-SiC and from the (00 12) reflection of 6H-SiC. For each reflection, we recorded high resolution θ-2θ scans and θ-scans through the Bragg peak and through the peak emanating from the damaged region. Reciprocal space maps were also recorded from selected samples in order to check for the presence of star-like diffuse streaks characteristic of the presence of stacking faults and indicative of the destabilization of the 3C phase.

The θ-2θ scans are displayed in figure 1. At low fluences, a peak appears in the low angle region indicative of a dilatation gradient in the crystals. For increasing fluence, this peak is broadened and shifted towards lower angles whereas interference features are progressively blurred out. The simulation of the data with a specifically developed model [1] allows to clarify this behavior and provides important indications concerning damage build-up in SiC crystals. The simulations allowed to determine (i) the thickness of the damaged layer, (ii) the strain profile and (iii) the damage profile (through the static Debye-Waller factor) within the layer (figure 2).

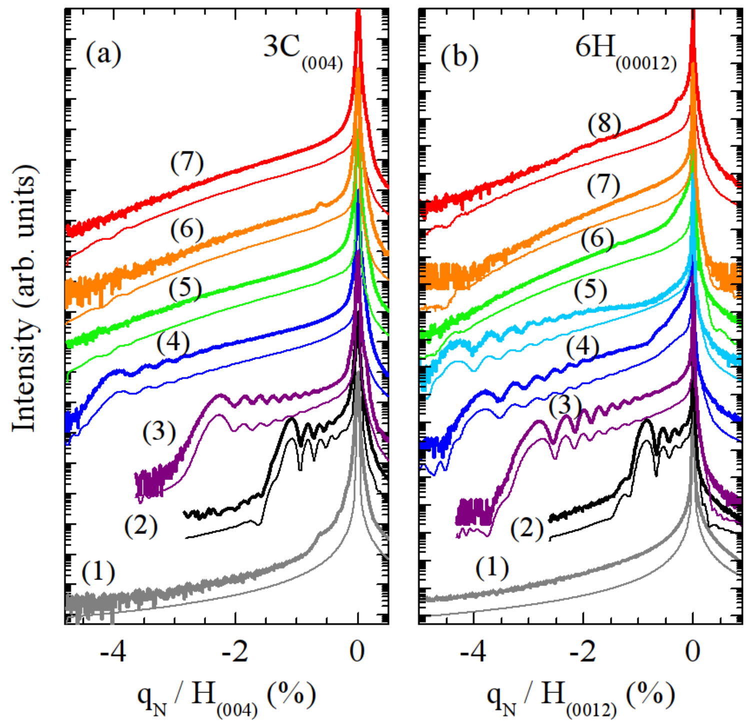

Figure 1: experimental (bold lines) and simulated (thin lines) θ-2θ profiles recorded from 3C-SiC (a) and 6H-SiC (b) for increasing fluence.

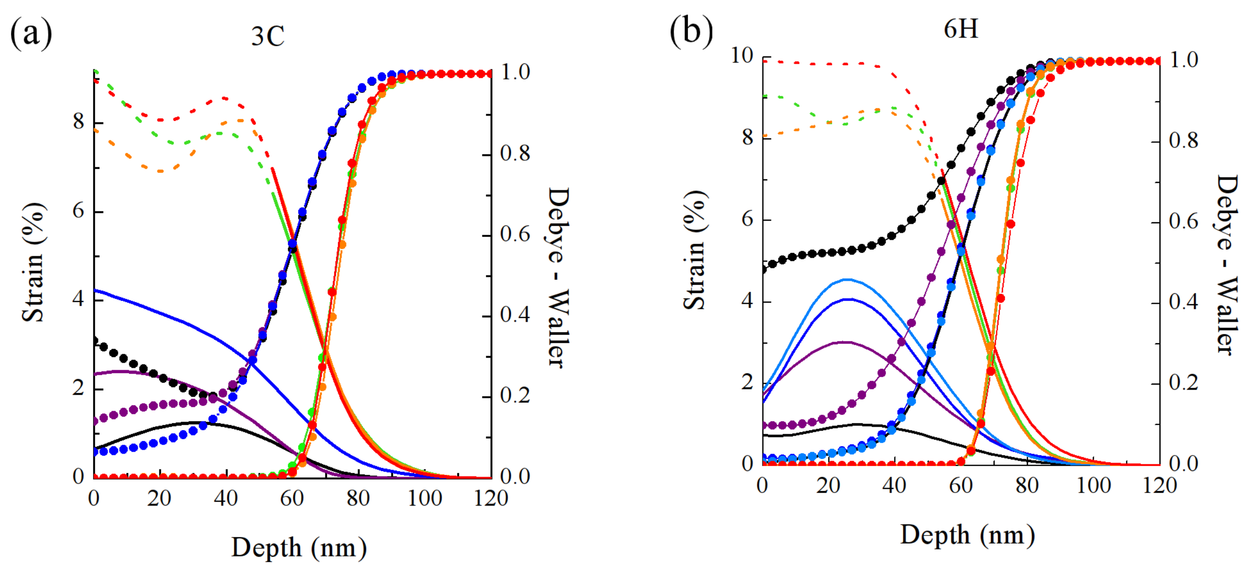

Figure 2 : strain and damage profiles obtained for 3C (a) and 6H (b) SiC (lines : strain, circles : Debye-Waller factor)

Upon ion-irradiation, a 80 nm – thick damaged layer is formed in which both the lattice parameters and static atomic displacement are significantly increased as compared to the bulk crystal. Huge strain values (up to 7%) are measured in such layers. For strain values higher than ~ 7% the corresponding elastic energy is relaxed by a catastrophic amorphization (DW = 0) of the SiC lattice. Surprisingly this amorphization occurs without the contribution of any extended defect. The Bragg peaks remain extremely sharp in the in-plane direction (all measured crystals exhibited the same behavior) and no sign of diffuse scattering can be observed. The understanding of this amorphization process is not yet complete. Simulations are currently carried-out and further experiments are required ; in particular a structural investigation of the damaged region (using in-plane diffraction) will allow to get further insights on the evolution of the structure during these stages.

[1] A. Boulle, A. Debelle, J. Appl. Cryst. 43, 1046 (2010)