	Experiment title: **Strain analysis in ion-beam induced lateral nano-structures in silicon using forbidden Bragg reflections**	**Experiment number**: SI-1379
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Report:

The formation of periodic ripples in the nanometer length scale at the metal and semiconductor surfaces has become a topic of intense research [1]. Such ripples are produced due to of the interplay between a roughening process by ion beam erosion (sputtering) and smoothening processes caused by thermal or ion-induced surface diffusion. In the previous investigations we considered the ripple formation and the amorphization of a Si (100) substrate depending on implantation dose and energy [2]. Samples with optimized values of irradiation angle at 60° and an irradiation energy of 60 keV (Ar^+ ion-beam) and high dose of implantation (7×10^{17} ions/cm^2) were studied. The surface ripples pattern was characterized by depth resolved x-ray grazing incidence diffraction (GID) and by atomic force microscopy (AFM) [2].

Synchrotron-radiation measurements of forbidden reflection in silicon have been performed from early 80s [3]. Some x-ray reflections that are forbidden by the symmetry of the lattice become observable after the keV energy range Ar ion irradiation of Si. The symmetry of the crystal is then modified by the irradiated ions that cause an increase of the structural factor of forbidden reflections.

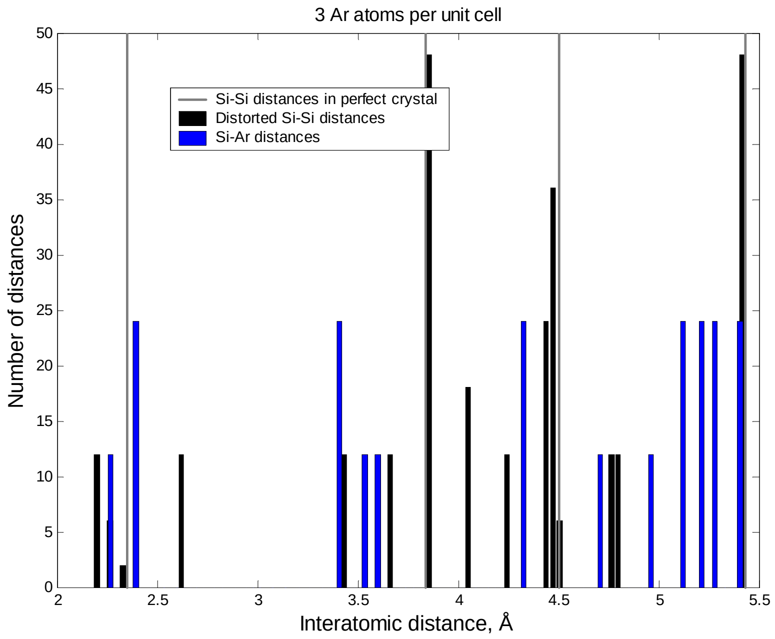

Figure 1: Interactomic distances in Si after high dose irradiation by Ar. The gray dashed lines presents interatomic distances of a perfect Si crystal. Blue and black color correspond to the Si-Ar and modified Si-Si distances, respectively.

In order to understand crystal modification due to Ar beam irradiation we have performed a geometry optimization of a Si crystal structure with different amount of embedded Ar atoms. The calculation have been performed using WIEN2k program package, which exploits full potential linearized augmented plane wave (LAPW) method for density functional calculations in crystals. We supposed that Ar atoms implanted into the structure of the Si crystal are randomly distributed within the positions of structural voids of the unperturbed crystal. The presence of Ar atoms there leads to a displacements of neighbouring Si atoms from their original positions and change the average interatomic distances in different coordination spheres. The later effect is visible via the measurement of the scattered X-ray intensity. To get a qualitative estimation the perturbed Si structure was calculated using a different amount of implanted Ar atoms. Low irradiation dose ($\sim 10^{16} cm^{-2}$) corresponds to approximately from one-eight to one-fourth Ar atom per Si unit cell and high irradiation ($>10^{17} cm^{-2}$) dose corresponded to 3-4 Ar atoms per Si unit cell.

In the present experiment we investigated the possibility to use forbidden reflections for studying crystalline and non crystalline regions of an ion beam irradiated Si crystal. Using a focused beam at 9.5keV without mirrors (at ID1) provides a beam size below 10x10µm² and allows us to carry out a two wave length experiment (due to the used Si(111) monochromator 9.5 keV and 28.5 keV). This enabled us to scan through the damaged sample area measuring out-off plane diffraction and to detect signals at the forbidden 002 and 006 Bragg diffraction that can be attributed to the strongly damaged crystalline structure after ion-implantation. The Bragg peak positions of the 002 and 006 differ significantly, which was already visible in the non-implanted sample area. The appearance of 006 may be caused by doping or residual strain of the virgin silicon and vanishes after attenuating the third harmonics of the beam by mirrors. However, because the absorption length at 28.5 keV is factor 10 larger than at 9.5 keV, the narrow 006 results mainly from the deeper, slightly damaged region of the crystal, while the larger width of the 002 originates mainly from the heavily damaged silicon near the surface. Then the shift of the Bragg difference angles measures a lattice mismatch between the both regions. It was shown that the difference in Bragg position of both peaks is changing with the spatial position within the ion beam damaged sample area. This experiment demonstrates the capability of using fcc-forbidden reflections for strain measurements. Moreover, the use of forbidden reflections has the advantage of self-control of the information depth. They will appear only in regions where the Si fcc structure is destroyed due to the ion impact.

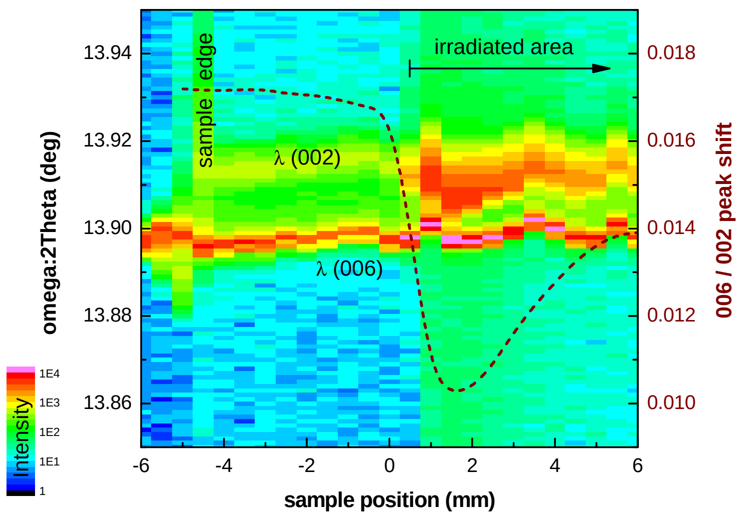

Figure 2: ω:2Θ scans across an irradiated (dose of 7 $10^{17} cm^{-2}$, (right) and non-irradiated (left) region of the Si sample. The strong intense lines refer to the Si(002) and Si (006) forbidden reflections. The right Y-axis describes the shift of the Bragg difference angle between the (006) and (002) reflection; the X-axis corresponds to the sample position.

Fig.2 shows intensity of forbidden reflection depending on spatial position on the sample. One can see strong increase of the (002) Bragg reflection intensity on the right-hand site of the figure 2 which correspond to the irradiated area of the sample. Additionally, there is a strong broadening of (002) reflection that reveals the existence of a strongly distorted sample with modified Si positions according to WIEN2k.

References

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