Investigation of Radiation Defects in Silicon under Proton and Heavy Ion Irradiation


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MAIN AIM:

• Investigation of track microstructure in Si irradiated by high-energy heavy ions. Such information can be useful for study of Si degradation under swift heavy ion irradiation.

• NOTATION

• L – track length
• $r_0$ – radius of A-region
• $r_1$ – radius of B-region
• $p$ – pressure on the boundary between A- and B-regions
• $E$ – Young’s modulus
• $\sigma$ – Poisson coefficient
• $\gamma$ – numerical dimensionless parameter
TRACK MODEL

Considered track model involves two regions:
1. Kernel track region – A-region
2. Elastically compressed region – B-region
Main assumptions:

- tracks are perpendicular to the irradiated surface,
- tracks don’t overlap,
- atomic displacements in the B-region have only radial component,
- atomic lattice in the A-region has only displacement along the track axes,
- tracks have the same length $L$ and their influence on the crystal structure at $z>L$ can be neglected,
- the boundary between A and B-regions $\rho_0(z)$ can be determined from the condition, that the residual pressure $p$, acting from A to B is constant and proportional to the energy loss by projectile ion at the depth $p \sim \rho_0^{-2} d\varepsilon/dz \sim \varepsilon^{1/2}$.
The boundary between A and B-regions

- $\rho_0(z)$ can be approximated by the equation
  \[ \rho_0^2(z) = r_0^2 f(z/L) \left(1 - \frac{z}{L}\right), \]

The atomic displacement fields in the A and B-regions have the following forms:

- For the A-region:
  \[ u_z = \gamma c (\rho_0 - \rho^2/\rho_0) \]
  \[ u_r(\rho, z) = c \frac{\rho_0^2(z)}{\rho} \]

- For the B-region:
  \[ c = p \frac{(1+\sigma)}{E}, \]

$\sigma$ is the Poisson coefficient and $E$ is the Young’s modulus.
DIFFUSE SCATTERING

Intensity of DS: \[ I(q) = I_0 N |F(q)|^2 \]

\[ I_0 \] - the intensity of incident X-ray beam

\[ N \] - the number of tracks

\( F(q) \) – amplitude of diffuse X-scattering

\[ F(q) = \int d^3r (bu) \exp(iqr). \]

\[ q = k - k_0 - b \] is the transmitted momentum

\[ k_0 \] – wave vector of incident X-ray beam \( (k_0 = 2\pi/\lambda) \)

\[ k \] - wave vector of scattered X-ray beam

\[ b \] – reciprocal lattice vector \( (b = 2\pi/d) \)

\[ \lambda \] – wave length of incident X-ray

\[ u \] - displacement
Triple crystal measurements

Fig. 1. The triple crystal scheme for asymmetric diffraction experiment, where M – monochromator, A – analyzer, O – sample, D – detector.
Fig. 2. Crystal rocking curve obtained using triple crystal measurements in irradiated Si material by Bi\(^+\) ions with the energy E=710 MeV at irradiation dose 10\(^{12}\) cm\(^{-2}\).
Asymmetric Scattering Scheme in the (x,z) plane

ψ – angle between l surface (111) and reflected planes (331)
Δθ= θ - θ_B determines the angular position of the crystal-analyzer
θ_B – Bragg’s angle

\[ q_x = k_0 \sin(\theta_B - \psi)[(1+\beta)\alpha - \Delta\theta], \]
\[ q_z = k_0 \left[ \cos(\theta_B - \psi) \Delta\theta - 2\alpha \sin\theta_B \sin\psi \right] \]
\( \alpha \) - angular deviation of crystal from the exact Bragg's position

\( \beta = \sin(\theta_B + \psi)/\sin(\theta_B - \psi) \) - asymmetry coefficient for the chosen scattering scheme

\( q_0 \) - the aperture parameter

- After averaging over the momentum \( q_y \), transmitted perpendicularly to the scattering plane \((x,z)\), can be obtain the \((\alpha, \Delta \theta)\)-dependence of the DS intensity, which is measured due to the triple-crystal technique

\[
I(\alpha; \Delta \theta) = I_0 N |F(q)|^2
\]

\[
F(q) = F_A + F_B, \quad F_B \sim q_x
\]
X-RAY SCATTERING MEASUREMENTS AND CALCULATIONS

- Experimental curves were obtained from Si(111) samples, irradiated by Bi ions at energy $E_0 = 710$ MeV and doses $D_1 = 10^{10}$ cm$^{-2}$ (sample 4) and $D_2 = 10^{11}$ cm$^{-2}$ (sample 3).
- The penetration depth of Bi ions in Si is $R_p \sim 100 \mu$m.
- X-ray measurements were performed at $\alpha > 40^\circ$ in order to extract DS from coherent scattering.
- The measurements are performed by using of CuK$_\alpha$ radiation with wave length $\lambda = 1.54$ Å near the (331) Bragg's reflection of Si-(111) crystal.
- In this case the asymmetric scattering scheme is characterized by $\theta_B = 38.2^\circ$, $\psi = 22.0^\circ$ and the asymmetry coefficient $\beta = 3.11$.
- Calculated curves are listed for $\alpha = 41^\circ$ and $51^\circ$. 
Sample 4
Dose = $10^{10}$ cm$^{-2}$
Alfa = 51"
Sample 4
Dose $= 10^{10} \text{cm}^{-2}$
$\alpha = 41''$

Angular dependence of X-ray scattering intensity
Angular dependence of X-ray scattering intensity

Sample 3
Dose = $10^{11}$ cm$^{-2}$
Alfa = 51"
Sample 3

Dose = $10^{11} \text{ cm}^{-2}$

$\alpha = 41^\circ$

Angular dependence of X-ray scattering intensity
Transmission Electron Microscopy in Si Irradiated by heavy ions.

Fig. 9 TEM results in Si after swift heavy ion irradiation by Bi\(^+\)ions with the energy of 710 MeV at different doses:

a) \(-10^{10}\text{cm}^{-2}\), b) \(-10^{11}\text{cm}^{-2}\), c) \(-10^{12}\text{cm}^{-2}\), d) \(-2\times10^{12}\text{ cm}^{-2}\)
TEM Results

- The sizes of tracks are located in the interval 10-25 nm with the average size near 10 nm.
- The small tracks have the elliptical shape and big one has the circus shape. The big tracks have complicated diffraction contrast showing that they have more difficult microstructure.
- The density of tracks is increased with irradiation fluence. The density of observed tracks per unit surface are equal $N_1=10^9\text{cm}^{-2}$ for $\Phi_1=10^{10}\text{cm}^{-2}$, $N_2=10^{10}\text{cm}^{-2}$ for $\Phi_2=10^{11}\text{cm}^{-2}$, $N_3=10^{11}\text{cm}^{-2}$ for $\Phi_3=10^{12}\text{cm}^{-2}$, $N_4=2\times10^{11}\text{cm}^{-2}$ for $\Phi_4=2\times10^{12}\text{cm}^{-2}$ respectively.
Investigation of interstitial oxygen contain in Si after fast proton and heavy ion irradiations using optical absorption method

- Two plates of mono-crystal Si of type (Standard FZ Si) with the orientation <111> and sizes ~ (10×10×0.31) mm³
- The oxygen atoms have been entered in the Si samples using the thermal treatment in the oxygen atmosphere at the temperature $T = 1150 \, ^\circ C$ during 48 hours.
- The average concentration of oxygen is equal ~ $2 \cdot 10^{17} \, \text{cm}^{-3}$.
- One sample has been irradiated by protons with the energy 35 MeV.
- The second sample has been previously irradiated by fast heavy ions of Kr with the energy $E = 200 \, \text{MeV}$ up to dose $\Phi_{Kr} \sim 5 \cdot 10^{15} \, \text{cm}^{-2}$ and then by fast protons 35 MeV.
- Optical absorption at room temperature have been measured in the area of infrared spectra (1400 - 400 cm$^{-1}$).
Fig. 10. Change of interstitial oxygen concentration after $p^+$ (32 MeV) irradiation of Standard FZ Si with and without preliminary $Kr^+$ (200 MeV, $5 \times 10^{15}$ cm$^{-2}$) irradiation.
Fig. 11. Divacancy absorption band (~1.8 µm) in Kr⁺ irradiated sample.
Main Results:

• Under these irradiation conditions only one strip has observed with the wavelength 1100 cm$^{-1}$ connected with the absorption on the interstitial oxygen atoms.

• The amplitude of this strip has increased under the increasing of proton irradiation dose approximately on the value $\sim (15 - 17)\%$ (see Fig. 10).

• The saturation of absorption for proton-irradiated samples has been observed.

• The sample previously irradiated by fast heavy ions Kr$^+$ together with the oxygen strip the divacancy strip of absorption with the wavelength ($V_2 \sim 1.8$ $\mu$m) has observed too (see Fig. 11).

• The obtained here experimental results under proton and heavy ion irradiation show that oxygen atoms can accumulate in the matrix due to the radiation induced resolution of oxygen-point defect clusters.
Conclusions:

- It was shown, that X-ray diffuse scattering (DS) measurements are very sensitive to the determination of track formation and main parameters of tracks: size, length of tracks and residual pressure near track.
- The obtained TEM results of microstructure change on irradiated Si samples allow estimating the density and sizes of tracks. The sizes of tracks are located in the interval 10-25 nm with the average size near 10 nm.
- The density of tracks is increased with dose of irradiation.
- The investigations of oxygen contain in Si samples after irradiation by fast protons with the energy 32 MeV and heavy ion irradiations by Kr⁺ ion with the energy 200 MeV have been performed using optical absorption method.
- Under proton irradiation only one strip on optical absorption has observed with the wavelength 1100 cm⁻¹ connected with the optical absorption on the interstitial oxygen atoms.
- The Si samples previously irradiated by fast heavy ions Kr⁺ with the energy 200 MeV and follow by fast protons with the energy 32 MeV show, that together with the oxygen strip the divacancy strip of optical absorption has been observed too with the wave length (V₂ ~ 1.8 µm)