Study of Crystalline Disorder Induced by Ion Irradiation in Si (100) Substrates

Abstract

Present work investigated the 100 MeV ion irradiation induced effects in Si wafer using X-ray diffraction (XRD) and Raman spectroscopy. XRD shows that orientation of the peak does not influence by the fluence of ion irradiation, however, irradiation promotes crystalline disorder. A significant reduction of band intensity is observed for the band appearing at 615 cm^{-1}. Other minor bands appearing in the Raman spectra also diminishes with irradiation. This confirms the results obtained from X-ray diffraction study.

Keywords: Si Substrate, Orientation, Crystalline disorder

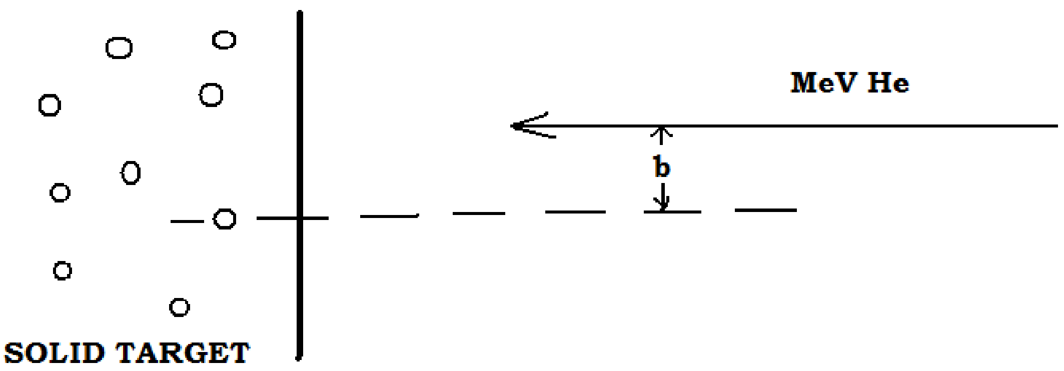
1. Introduction

Ions incident on a solid influence its properties and are used to tailor the properties in different ways (Table 1). The interaction of an energetic ion depends on its kinetic energy and the distance of closest approach.

Table 1: Effect of ions of various energies on the solid surface

S. N.	Ion energy	Effect on solid surface
1	10-100 eV/amu	Epitaxial layers
2	1 keV/amu	Sputtering process
3	100-300 keV/amu	Ion Implantation
4	~MeV/amu	Penetration through solid surface

This distance of closest approach is closely related to the impact parameter as shown in the Figure1.3.1. Since, the atomic spacing in a typical crystal is of the order of few angstroms, the largest impact parameter is also of the same order. At this distance the ion transfers small amount of energy, ≈10 eV, to the valence electrons. The cross section for this process is of the order of $\pi b^2 \approx 10^{-15}$ cm^2, and it is responsible for the gradual energy loss of the ion as it penetrates into the solid. At smaller impact parameters the interactions is with the inner electrons, with correspondingly larger energy transfers. For impact parameters comparable to the nuclear size larger energy transfers occur (≈100 keV); in billiard ball like collisions resulting in large angle of scattering of the indent ion (**Feldman *et al.*, 1982**). The fast ion while moving



Impact Parameter (b)		Energy Transfer
~ 1 Å	Inelastic excitation of valence electrons	S_e~ 10 eV
~ 10^{-1} Å	Inelastic excitation of L-shell electrons	S_e~ 100 eV
~10^{-2}Å	Inelastic excitation of K-shell electrons	S_e~ 1 KeV
~10^{-4}Å	Elastic scattering from Nuclei	S_n~ 100 KeV

Figure 1: Classification of the types of collision and their corresponding energy transfer in terms of impact parameter for the process. S_e refers to energy transfer to electron and S_n to energy transfer to the nuclei

through the target looses its energy in the medium. The energy loss per unit length is called stopping power and denoted as 'S'. The energy loss in the medium is generally governed by two processes (Figure 1.3.2)- (1) Inelastic scattering with the electrons in the target (electronic energy loss or EFL) represented by $(dE/dx)_e$ or S_e and (2) elastic collision with the nucleus of the target atoms (nuclear energy loss or NEL) represented by $(dE/dx)_n$ or S_n (**Ziegler *et al.*, 1985**).

In terms of ion velocity ν, elastic collisions are important if $\nu \ll \nu_o$, where ν_o is the orbital velocity of the electrons in the target. As the ion energy E increases, S_n diminishes as 1/E. Electronic interactions start to play a role when the ion velocity becomes comparable to the velocities of orbital electrons in the target materials. As a result, electronic energy loss S_e varies linearly in the velocity range $0.1\nu_o$ to $Z_1^{2/3}\ \nu_o$, Z_1 is the atomic number of target atoms (**Gras-Marti *et al.*, 1991**). Outside this range it has lower values. The variation of S_e and S_n as functions of ion energy E is shown in Figure 1.3.3. It is also pertinent to note that relativistic effects must be taken into account for ion energies above 10 MeV/amu.
A large number of atoms in a magnetic insulator target are set into motion by the electronic excitation in the wake of swift (K. E. ≥ 1 MeV) heavy ions (SHI) during an irradiation experiment.

The atomic mobility set in the bulk leads to some well known effects, such as anisotropic growth, change in electrical, magnetic and optical properties. Although this area is now more than three decades old, there is no general consensus about the physical processes responsible for the observed effects. The advent of nanoscience also added complexity to the system. It is well established that these effects result from the atomic motion induced by electronic energy loss S_e of the incident ions in the target material. But the mechanism involved in this process is under discussion without any general agreement so far. There is still a need of a theory that could explain all these effects within a single framework in the bulk as well as nanomaterials. This is mainly due to the limited experimental data available on this subject. It is therefore required to carry out more experiments, which would become the part of worldwide activities in developing a general theory.

The present investigation was started with a motivation to study SHI irradiation induced effects in Si substrate, and to understand the involved physical process.

2. Experimental Details

In order to facilitate both side irradiations a target ladder was especially designed and fabricated at IUAC, New Delhi (Dhyani et al., 2024). The main parts of the ladder are made of good quality stainless steel and oxygen free copper. The copper block holding the samples could be maintained at low temperature by pouring liquid nitrogen through the stainless steel tube attached to it. Salient features of the target ladder include motorized vertical movement which could be controlled from remote and the possibility of rotation through 90°, in order to bring the samples in front of the beam exposure. All the irradiation experiments have been performed in the high vacuum chamber (HVC) at the Material Science Beam Line at IUAC, New Delhi The ion beam used in this beam time was 100 MeV O^{7+}. This particular ion and species were selected after a number of calculations for different ions with SRIM computer code.

3. Results and Discussion

3.1 X-ray Diffraction Study

Fig. 1 shows the XRD patterns of pristine and irradiated counterpart of Si(100) wafer. All patterns clearly shows the presence of (001) peak of Si showing that wafer maintains it's single crystalline nature after irradiation.

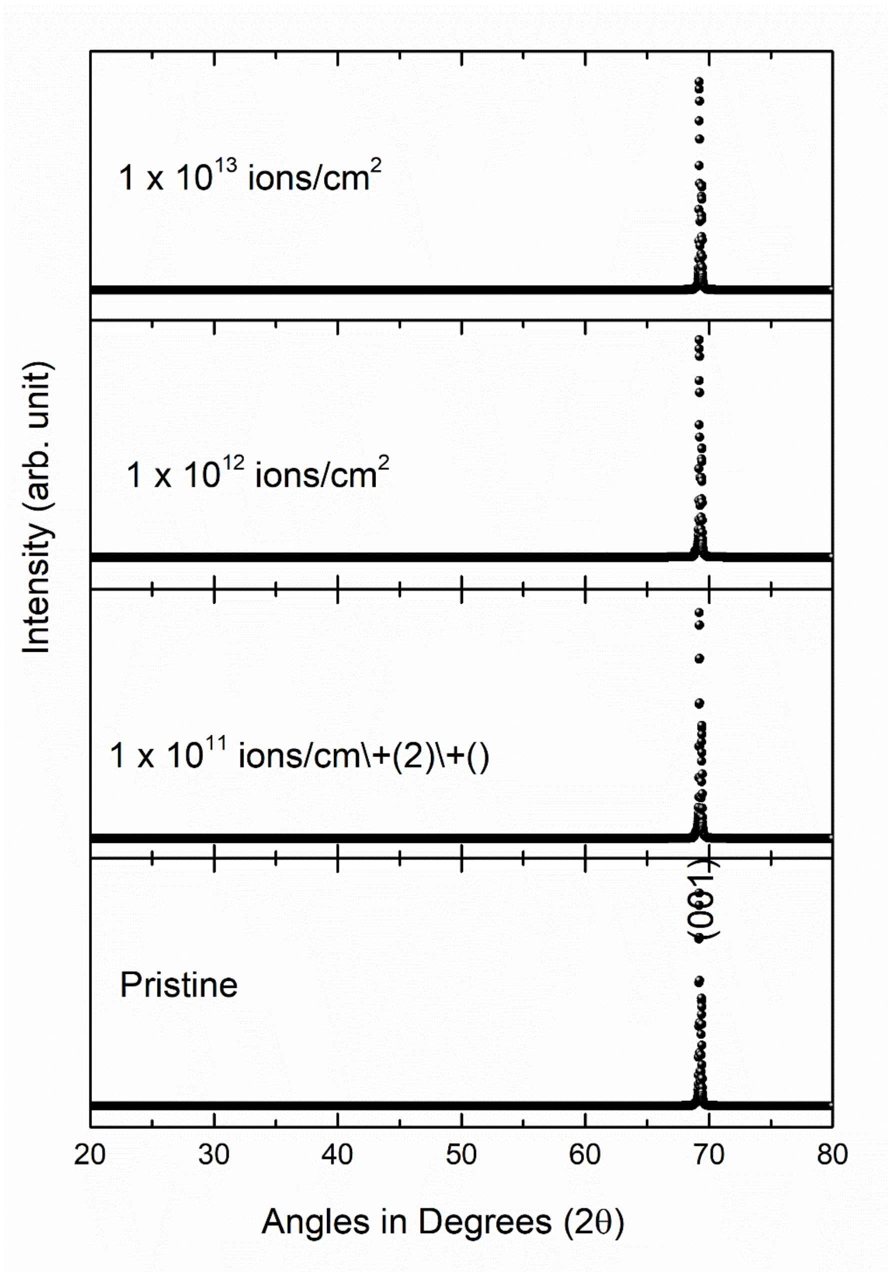


Fig. 2: X-ray diffraction patterns of Si(100) irradiated with 100 MeV O^{7+} ions at different fluences.

To further, investigate this effect, peak position, intensity and peak-width was estimated by fitting peaks using Lorentzian function as shown in Fig. 2. Variation of intensity with fluence of irradiation is shown in Fig. 3. Decrease in peak intensity is associated with crystalline disorder induced by heavy ion irradiation (Pfeifer et al., 2024). Full-width at half-maximum and peak position of this peak for all the samples is given in Table 1.

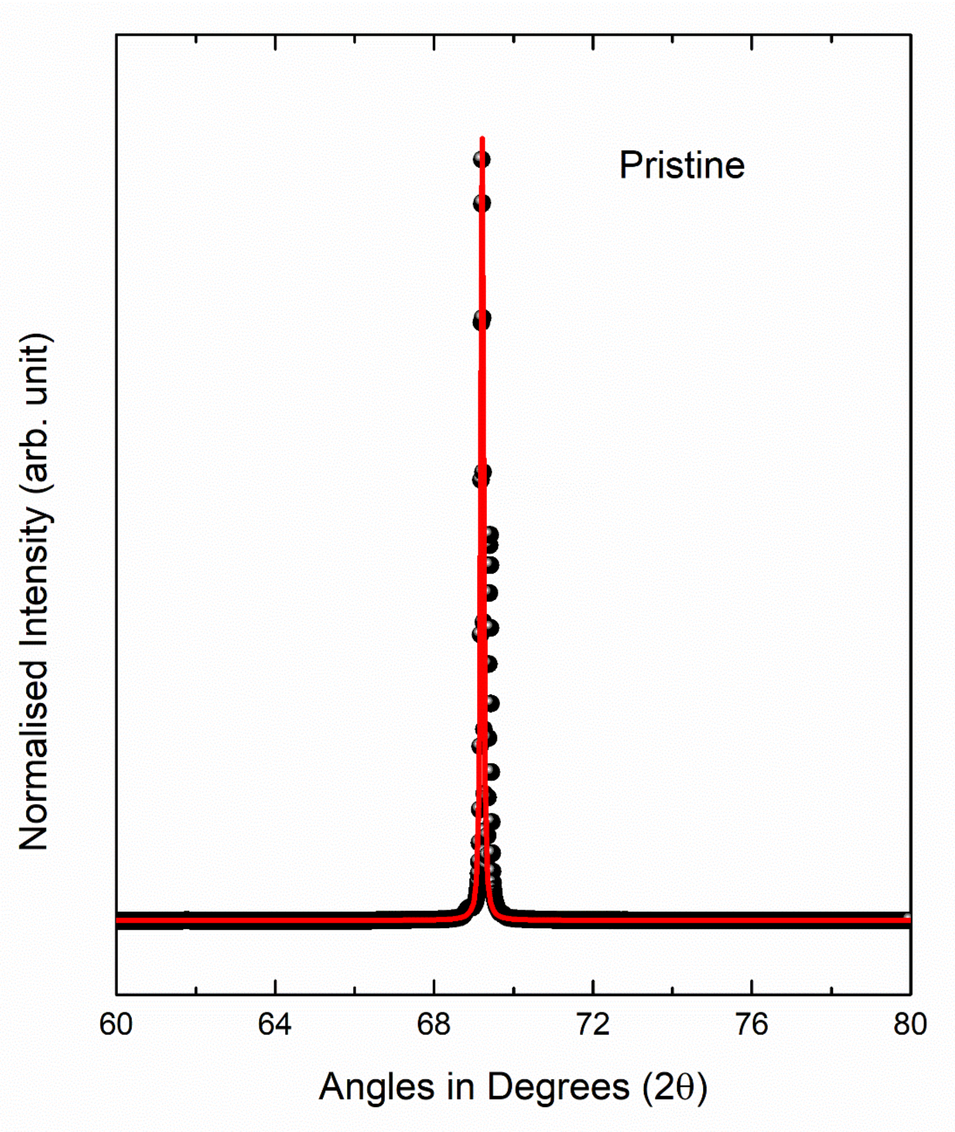


Fig. 3: (001) Peak fitted by Lorentzian function.

Lattice parameters of pristine and irradiated counterpart was estimated from peak position (2θ) using the following relation.

$$a = \frac{\lambda sin\theta}{2}$$

These parameters are shown in Table 1.

Table 1: Peak parameters and lattice parameters of pristine and irradiated Si

Fluence (ions/cm^2)	FWHM (degrees)	2θ (degrees)	Lattice parameter (Å)
0	0.065	69.21	
1×10^{11}	0.070	69.23	
1×10^{12}	0.067	69.23	
1×10^{13}	0.062	69.22	

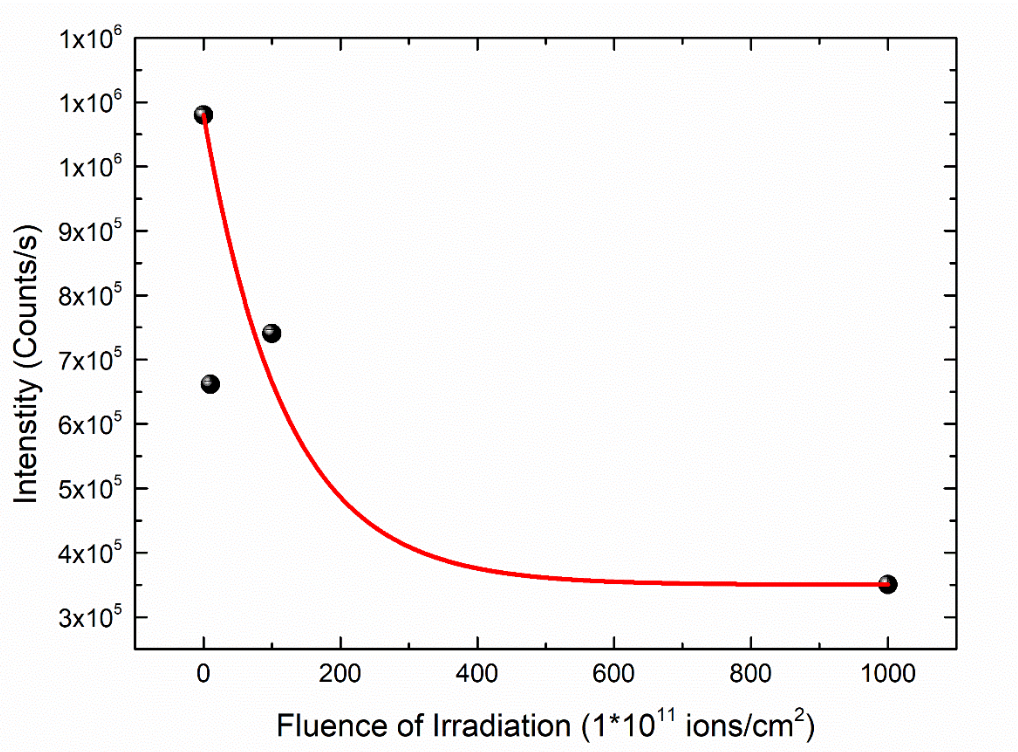


Fig. 3: Variation of peak intensity with fluence of irradiation

3.2 Raman Spectroscopic Study

As significant changes are observed in the peak Intensity of pristine and irradiated counterpart (fluence 1×10^{13} ions/cm^2), hence, Raman spectra of these two wafers are measured. Both spectra exhibit a major band around 615 cm^{-1} (Kadlečíková et al. 2022). This band is characteristics of Si showing that there is no phase change, which is relevant with the results obtained from XRD study. A visual inspection shows the huge reduction in the intensity after irradiation reflecting crystalline disorder. Table 2 shows the various parameters of Raman bands in both the samples. Raman images for irradiated counterparts are shown in Fig. 5. A uniform colour shows that crystalline phase remain same in the irradiated sample.

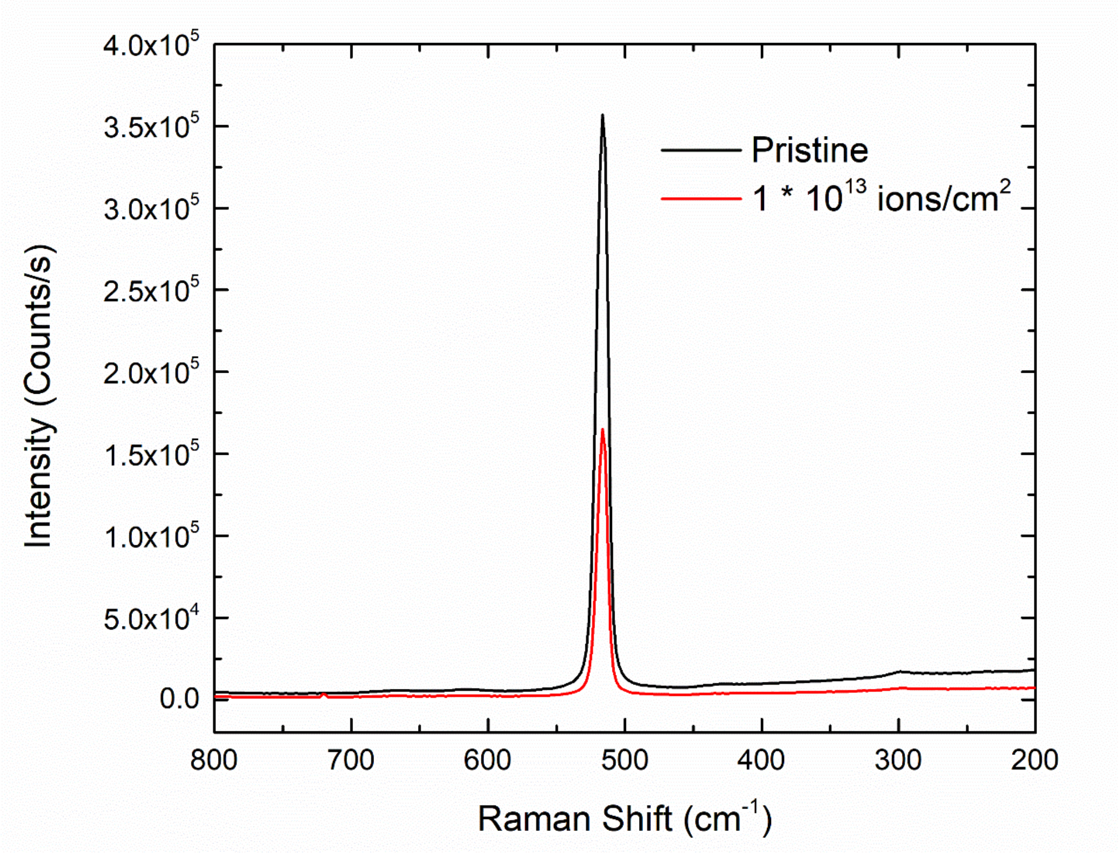


Fig. 4: Raman Spectra of Pristine and irradiated Counterpart Showing the most intense Raman peak of Si(100)

Table 2: Parameters of most intense Raman Peaks

Parameters	Pristine	Irradiated
Band position (cm^{-1})	516±1	516.5±0.5
Band width (cm^{-1})	10.0±0.1	8.9±0.1
Area of the Bands (arb. unit)	(3.74±0.05) $\times 10^6$	(1.5±0.2) $\times 10^6$

Fig. 5: Raman Image for irradiated Si

Further attention is given to minor bands observed in the Raman Spectra of these samples and spectra highlighting these minor bands are shown in Fig. 6. Parameters for these bands are shown in Table 3. It is clear that minor bands diminishes after irradiation.

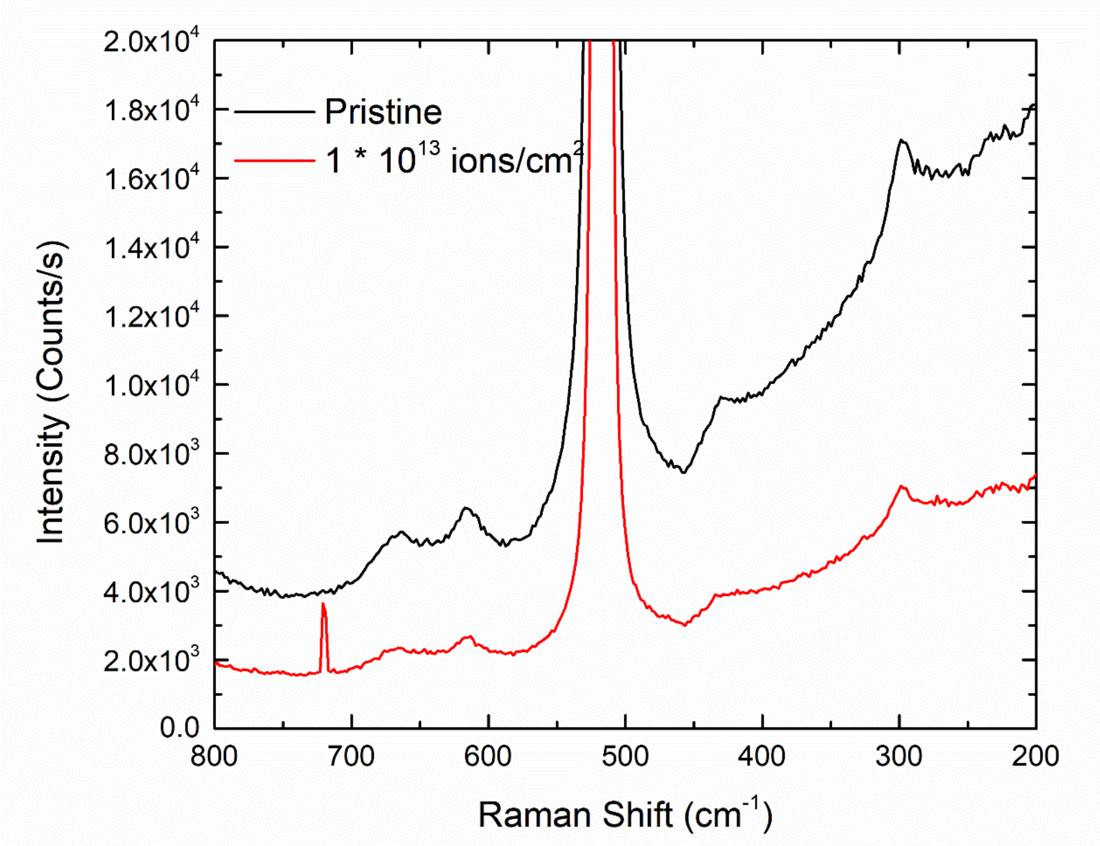


Fig. 6: Raman Spectra of Pristine and irradiated Counterpart Showing minor Raman peaks of Si(100)

Table 3: Band position (cm^{-1}) of minor Bands in the Spectra

Band	Pristine	Irradiated
1	663±2	669±2
2	616±2	616±2
3	430±2	434±2
4	297±2	297±2

4.Conclusion

Thus following conclusion are made from this investigation

1. Si is not a radiation resistant material
2. Though there is no change of orientation but onset of crystalline order can be seen.
3. Raman spectra support the results obtained from XRD.

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