Investigation of Irradiation Damage of SiC Single Crystal

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Abstract. A SiC single crystal was irradiated with 1.248 MeV Ar⁶⁺ ions at a fluence of 5×10¹⁴ cm⁻². X-ray diffractometry and Raman spectroscopy were employed to investigate the irradiation damage. The simulation results suggested that the damage peak was at the depth of about 700 nm, and the corresponding value was about 0.35 dpa. The XRD peak at about 35.503° was detected. It should originate from the irradiation-induced amorphous SiC. For Raman measurement, the 199, 265, 435, 540, and 659 cm⁻¹ peaks were recorded and assigned to Si-Si vibrations. The 1415 cm⁻¹ peak was attributed to C-C vibration. The asymmetric broadening of 786 and 963 cm⁻¹ peaks are observed. The tails at the frequency ranges of 690-777 and 816-925 cm⁻¹ were caused by the phonon confinement effect resulting from the irradiation-induced damage.

1. Introduction
Due to the excellent radiation resistance, SiC is considered as a promising candidate material for use in nuclear reactors [1]. The SiC-based component serve in harsh environments and is irradiated by energetic particles. Particle bombardment leads to the generation of lattice defects, change the microstructure, and deteriorate the performance. Therefore, it is very important to understand the irradiation-induced modification and then assess the application safety. In the present work, we will investigate the effect of Ar⁶⁺ ion irradiation on SiC single crystal and reveal the characteristic of irradiation behavior.

2. Experimental
A commercial 6H-SiC single crystal was supplied by the TankeBlue Semiconductor Co., Ltd. Ion irradiation experiment was performed at the 320 kV Multi-discipline Research Platform for Highly Charged Ions of the Institute of Modern Physics in Lanzhou. The SiC was irradiated with 1.248 MeV Ar⁶⁺ at a fluence of 5×10¹⁴ cm⁻² at room temperature (RT). Ar ion concentration and damage level profiles were calculated with SRIM 2013. Threshold displacement energies of C and Si atoms were 20 and 35 eV, respectively. A specific gravity of SiC single crystal is 3.21 g/cm³. After the irradiation, SiC were investigated by X-ray diffractometry and Raman spectroscopy. A D/max-2500/pc X-ray diffractometer was used with the 0-20 scanning mode to record the x-ray diffraction (XRD) patterns and A Renishaw inVia Raman microscope was used with 532 nm laser excitation to record Raman spectra in the backscattering configuration. All of measurements were carried out at RT.
3. Results and discussion

![Fig. 1](image1.png)

**Fig. 1** Depth profiles of Ar concentration and damage level of as-irradiated SiC.

Fig. 1 shows the calculated depth profile of Ar concentration and damage level of SiC irradiated at a fluence of $5 \times 10^{14}$ cm$^{-2}$. The values of Ar concentration and damage level varied significantly with the depth. The Ar atoms were mainly deposited in the range of 400-970 nm. The Ar concentration peak was at the depth of approximately 790 nm, and the corresponding value was $2.3 \times 10^{19}$ cm$^{-3}$. Damage region was in the depth range of 0-750 nm. The damage peak was at the depth of approximately 700 nm, and the corresponding value was approximately 0.35 displacement per atom (dpa). The depth value of damage peak is smaller than that of Ar concentration peak.

![Fig. 2](image2.png)

**Fig. 2** (0006) diffraction peaks of virgin and irradiated SiC samples.

Fig. 2 shows the (0006) diffraction peaks of virgin and irradiated SiC samples. For the virgin SiC, the (0006) diffraction peak position is centered at 35.663°, and the corresponding FWHM (full width at half maximum) value is 0.056°, as shown in Fig. 2(a). After the irradiation, the (0006) peak is decreased to 35.590° and its FWHM value become to be 0.062°. Moreover, an additional peak at 35.503° appear, as shown in Fig. 2(b). In the present study, damage level of as-irradiated sample is relatively low due to the small ion fluence. According to the experimental data, the irradiation at the
fluence of $5 \times 10^{14}$ cm$^{-2}$ cannot lead to an obvious increase of FWHM value, but it can decrease significantly the peak position. The (0006) peak FWHM and position shown different trends. This suggests that the effects of irradiation defects on peak parameters were different. The weak peak at 35.503$^\circ$ should originate from the irradiation-induced amorphous SiC. The high-energy ion bombardment can cause the transformation of crystal to amorphous states in cascade collision zone.

The lattice vibrational modes of 6H-SiC are classified as $6(A_1 + B_1 + E_1 + E_2)$. In the present measurement configuration, the vibrational modes of $A_1$ and $E_1$ symmetry can be recorded. The Fig. 3(a) present the Raman spectrum of virgin SiC. This spectrum gives four well-defined Raman peaks. The weak peak at approximately 146 cm$^{-1}$ correspond to acoustic phonon peak, and the strong peaks at approximately 764, 786, and 963 cm$^{-1}$ correspond to optical phonon peaks [2]. Raman spectra for irradiated SiC are different from those for virgin SiC due to the presence of damage.

![Raman spectra of virgin (a) and irradiated (b) SiC in the frequency range of 100-1000 cm$^{-1}$](image)

Ar ion bombardment led to the appearance of lattice damage. The intrinsic Raman peaks are almost absent, while five additional peaks at 199, 265, 435, 540, and 659 cm$^{-1}$ are present, as shown in Fig. 3(b). The 764, 786, and 963 cm$^{-1}$ peaks become very weak. It is sure that the five peaks are induced by the irradiation and correspond to local vibrational modes. Based on previous results of the Si, the 199, 265, 435, and 540 cm$^{-1}$ Raman peaks should be assigned to the Si-Si vibrations [2,3]. The homonuclear Si-Si bonds are produced by ion irradiation. The 659 cm$^{-1}$ peak is not detected in perfect SiC crystals. It appears in a damaged SiC and correspond to the Si-C vibration. In addition, the asymmetric broadening at the low frequency sides of the 786 and 963 cm$^{-1}$ peaks are observed. Two obvious tails locate at the frequency ranges of 690-777 and 816-925 cm$^{-1}$, respectively, which are indicated by the red rectangles in Fig. 3(b). The presence of tails at low frequency sides originate from the phonon confinement effect resulting from the irradiation-induced damage.

The irradiation also changes the second-order scattering. Fig. 4 shows the Raman spectra of virgin and irradiated SiC in the frequency range of 1000-2000 cm$^{-1}$. The figure presents the effect of ion irradiation on second-order Raman scattering. In Fig. 4(a), the intrinsic peaks at 1514, 1618, and 1712 cm$^{-1}$ were recorded. They originated from second-order Raman scattering. When the SiC is irradiated, the Raman spectrum change significantly. The three peaks disappear completely and only a new peak at approximately 1415 cm$^{-1}$ was recorded, as shown in Fig. 4(b). The C(sp$^3$)-C(sp$^3$) vibration for diamond gives a peak at about 1332 cm$^{-1}$, and C(sp$^2$)-C(sp$^2$) stretching vibration for graphite gives a peak at about 1585 cm$^{-1}$ [4-6]. Therefore, the 1415 cm$^{-1}$ peak should originate the mixed C(sp$^3$)-C(sp$^3$) vibration.
Fig. 4 Raman spectra of virgin (a) and irradiated (b) SiC in the frequency range of 1000-2000 cm\(^{-1}\).

4. Conclusions
The ion-irradiated SiC single crystal was investigated by using X-ray diffractometry and Raman spectroscopy. The damage peak was at about 700 nm, and the corresponding value was about 0.35 dpa. The XRD peak at about 35.503° appeared after irradiation and originates from the amorphous SiC. The Raman peaks related to Si-Si and C-C vibrations were detected. The phonon confinement effect resulting from the irradiation-induced damage led to asymmetric broadening of 786 and 963 cm\(^{-1}\) peaks.

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