Neutron irradiation effects in SiC

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**Abstract**

SiC is a wide band gap semiconductor material with potential applications in harsh environmental conditions. In this work we investigate the effects of neutron irradiation on the properties of two SiC polytypes. Changes to the optical properties were analyzed using a range of techniques including visible transmission, infra-red reflectance, Raman spectroscopy and photoluminescence.

**1. Introduction**

It is well known that SiC is a wide band gap semiconductor material with excellent potential for electro-optical applications and devices in harsh environmental conditions such as high temperatures and environments subjected to high levels of irradiation. In this paper we investigate the effects of neutron irradiation on the properties of two different polytypes, 4H(hexagonal) and poly-crystalline 3C(cubic), of SiC. Changes to the optical properties were analyzed using a range of techniques including infra-red reflectance, visible transmission, Raman spectroscopy and photoluminescence (PL).

**2. Experimental details**

Neutron irradiation was performed by placing samples in an experimental nuclear reactor (SAFARI-1) for time periods of 33 s (series A), 167 s (series B) and 333 s (series C). At the irradiation position the total neutron flux was $2.34 \times 10^{14}$ nc m$^{-2}$ s$^{-1}$. Of this 13% ($3.0 \times 10^{13}$ nc m$^{-2}$ s$^{-1}$) were fast neutrons ($E > 0.82$ MeV) and 56% were thermal neutrons ($E < 0.625$ eV). Assuming that it is mainly fast neutrons which are responsible for lattice damage the effective irradiation fluences are $10^{15}$ nc m$^{-2}$ (series A), $5 \times 10^{15}$ nc m$^{-2}$ (series B) and $10^{16}$ nc m$^{-2}$ (series C).

The equilibrium temperature at the irradiation site is estimated to be around 300 °C. Consequently a limited degree of annealing can be expected during the longer irradiation periods.

**3. Results and discussion**

**3.1. Visible transmission**

Series B and C both showed a clearly measurable effect of irradiation for all methods of investigation. Analogous to the well known darkening [1,2], related to the partial amorphization of SiC after ion-implantation, we also see a marked drop in visible transmission for series B and C (see Fig. 1). The relative change in transmission ($\Delta T/T$) can be related to the induced change in absorption coefficient by:

$$\Delta x = -\frac{1}{d} \ln \left(1 - \frac{\Delta T}{T}\right).$$

with $d$ the sample thickness. For both crystal types, series B exhibits a $\Delta x$ value smoothly increasing from around $4$ cm$^{-1}$ at $14,000$ cm$^{-1}$ to about $7$ cm$^{-1}$ in the blue at $21,000$ cm$^{-1}$. For series C the radiation induced absorption coefficient is roughly doubled. Amorphous
SiC has an absorption coefficient of about \(0.6 \times 10^6\) cm\(^{-1}\) at 14,000 cm\(^{-1}\) rising to around \(1 \times 10^6\) cm\(^{-1}\) at 21,000 cm\(^{-1}\). One can therefore make an order of magnitude estimate of the radiation-induced amorphous fraction in the visible spectrum \([2]\) as \(D_A \approx a\) of about \(7 \times 10^6\) for series B and twice that for series C. Hence, even an irradiation fluence of \(10^{16}\) cm\(^{-2}\) produces almost negligible amorphization.

### 3.2. Infra-red reflectance and Raman spectroscopy

Both the 4H and 3C samples show an unambiguous drop in the reststrahlung peak (700–950 cm\(^{-1}\)) for series C (see Fig. 2(a) and (b)) and to a lesser extent also for series B. The effect can be quantified by comparing measurements with modeled values for the complex dielectric function of SiC \([3]\):

\[
\varepsilon(\omega) = \varepsilon_\infty \left( \frac{\omega_{\text{LO}}^2 - \omega^2 + i \omega \Gamma_{\text{LO}}}{\omega_{\text{LO}}^2 - \omega^2 + i \omega \Gamma_{\text{LO}}} \right)
\]

where \(\omega_{\text{LO}}, \omega_{\text{TO}}\) and \(\omega_p\) are phonon and plasmon frequencies respectively and \(\Gamma_p\) is the plasmon damping constant. Reflectance can then be calculated by substitution of the complex index of refraction, \((n - ik)^2 = \varepsilon\), into the Fresnel equations \([4]\). The drop in the reflectance maximum is mainly due to an increase in the values of the damping constants \(\Gamma_{\text{LO}}\) and \(\Gamma_{\text{TO}}\) due to lattice damage. As can be seen in Fig. 2(a) the virgin 4H sample can be quite accurately modeled by using damping constant values close to that of a perfect crystal (\(\Gamma_{\text{LO}} = \Gamma_{\text{TO}} = 5\) cm\(^{-1}\)) while series C requires a \(\Gamma_{\text{TO}}\) value of 10 cm\(^{-1}\) to match the measured curve. The 4H sample is (unintentionally) n-doped giving a free carrier density of \(3.6 \times 10^{18}\) cm\(^{-3}\).
giving a plasmon frequency of $\omega_p = 365 \text{ cm}^{-1}$. After neutron irradiation the reflection minimum shifts to a slightly lower value ($\Delta \omega = 2.5 \text{ cm}^{-1}$) which corresponds to a free carrier density of $3.4 \times 10^{18} \text{ cm}^{-3}$. The lowered carrier density is presumably the result of traps related to the formation of lattice defects.

The 3C samples (Fig. 2(b)) show a similar behavior where $\Gamma_{TD}$ increases from 14 cm\(^{-1}\) for the virgin sample to 20 cm\(^{-1}\) for the series C sample.

Raman spectroscopy (see Fig. 3) confirms the observations for the 4H samples where the LO-phonon line, which is known to couple to plasmon oscillations, shifts to a lower frequency when the free carrier concentration drops. In this case a shift of about 3 cm\(^{-1}\) is observed for the series C sample.

### 3.3. Photoluminescence

For all the investigations mentioned above (IR reflectance, visible transmission and Raman spectroscopy) series A exhibits almost no radiation damage. Only PL (see Fig. 4), which is known to be very sensitive to lattice damage, shows a substantial drop in signal for series A as well. This is presumably due to the formation of damage-induced deep levels allowing electron–hole recombination, usually with very little or no visible luminescence.

In 4H the PL spectra consist of a fairly weak excitonic region containing a series of fairly sharp well defined lines around 380 nm [5] followed by broader peaks due to donor–acceptor pairs and a very broad continuum extending well into the visible region. As can be seen in Fig. 4 all three series of neutron irradiated samples follow this scheme with the whole spectrum systematically dropping with increased irradiation fluence. Series B is an interesting exception where two relatively strong additional broad luminescence bands appeared at around 410 nm and 430 nm.

In 3C (not shown) a single fairly weak excitonic line at around 510 nm is observed without a broad continuum and with only a few weakly resolved other spectral features. For series A the excitonic line is almost completely gone and the samples subjected to higher irradiation fluences produced no detectable luminescence at all.

### 4. Conclusions

The effects of neutron irradiation on two different SiC polytypes have been investigated. Due to the absence of Coulomb interaction very large fluences are required to obtain effects which are noticeable with the usual optical characterization techniques. However at a fluence of $10^{16} \text{ cm}^{-2}$ unambiguous evidence of a deterioration of the crystal quality is seen.

Transmission measurements in the visible range clearly indicate that there is a small but measureable amount of amorphization present after irradiation. The infra-red reflectance and Raman spectroscopy show that the long-range order in the SiC crystals has been disrupted and that some of the dopant species have been deactivated, presumably to the formation of point defects acting as traps for free carriers.

### References