## 3.3 MAGNESIUM PRECIPITATION AND DIFUSSION IN $Mg^+$ ION IMPLANTED SILICON CARBIDE —

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This extended abstract reports on some of the major results in a paper recently published in the *Journal of Nuclear Materials* [1].

### Abstract

As a candidate material for fusion reactor applications, silicon carbide (SiC) undergoes transmutation reactions under high-energy neutron irradiation with magnesium as the major metallic transmutant; the others include aluminum, beryllium and phosphorus in addition to helium and hydrogen gaseous species. Calculations by Sawan *et al*. [2] predict that at a dose of ~100 dpa (displacements per atom), there is ~0.5 at.% Mg generated in SiC. The impact of these transmutants on SiC structural stability is currently unknown. This study uses ion implantation to introduce Mg into SiC. Multiaxial ion-channeling analysis of the as-produced damage state indicates a lower dechanneling yield observed along the <100> axis. The microstructure of the annealed sample was examined using high-resolution scanning transmission electron microscopy. The results show a high concentration of likely non-faulted tetrahedral voids and possible stacking fault tetrahedra near the damage peak. In addition to lattice distortion, dislocations and intrinsic and extrinsic stacking faults are also observed. Magnesium in 3C–SiC prefers to substitute for Si and it forms precipitates of cubic $Mg_2Si$ and tetragonal $MgC_2$. The diffusion coefficient of Mg in 3C–SiC single crystal at 1573 K has been determined to be $3.8 \pm 0.4 \times 10^{-19}$ $m^2/s$.

### Highlights

Figure 1a shows the inverse fast Fourier transformation (IFFT) of a high-angle annular dark field (HAADF) STEM image for 3C-SiC implanted at 673 K to $9.6\times10^{16}$ ions/$cm^2$ and annealed at 1573 K for 12 h in Ar. The dark triangles are likely to be tetrahedral voids with 4 non-faulted sides on {111} planes and 6 dislocation-free edges along <110> directions. Similar spatially oriented non-faulted tetrahedral voids have been observed [3] in neutron irradiated 3C-SiC at 1733 K. In addition, the brighter triangles in Figure 1a resemble those observed for energetically favored stacking fault tetrahedra (SFTs) in low stacking fault energy face centered cubic (fcc) metals and alloys. Figure 1b is the fast Fourier transformation (FFT) of Figure 1a, which shows 6 dark spots besides the expected pattern of brighter spots from 3C-SiC. The 6 spots belong to two separate groups of patterns that are labeled with circles and squares and their d-spacing values are determined to be 0.3623 and 0.5070 nm, respectively. The best d-spacing matches suggest that the circled spots are from cubic $Mg_2Si$ with (111) d-spacing of 0.36685 nm and the squared spots from tetragonal $MgC_2$ with (001) d-spacing of 0.502 nm. Comparison with the known electron diffraction patterns of fcc crystals suggests that $Mg_2Si$ is (110)-oriented, or $Mg_2Si$ (110)//3C-SiC(110). Figure 1b shows only 2 diffraction spots from $MgC_2$ {001}. In principle, the $MgC_2$ orientation can be <100> or <hk0> with h and k being equal to or greater than 1. Because strong {110} diffractions from <100>-oriented $MgC_2$ are not visible off the center line and high indices are not probable, the $MgC_2$

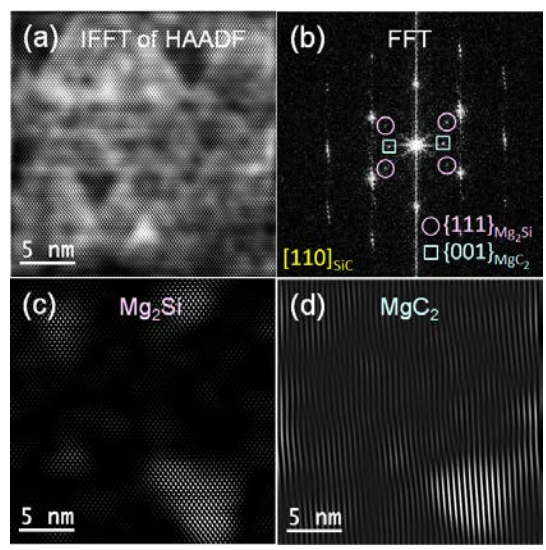


**Figure 1.** (a) IFFT of HAADF STEM micrograph for cross-sectional view of 3C-SiC irradiated with 200 keV $Mg^+$ to $9.6\times10^{16}$ ions/$cm^2$ at 673 K and post annealed at 1573 K for 12 hours in Ar. (b) FFT of the micrograph in (a). (c) and (d) IFFT of precipitates $Mg_2Si$ and $MgC_2$, respectively [1].

[1] PNNL is operated for the U.S. Department of Energy by Battelle Memorial Institute under Contract DE-AC06-76RLO 1830.

orientation is likely to be <110>, or $MgC_2$ (110)//3C-SiC(110). Determination of the complete orientation relationships of $Mg_2Si$ and $MgC_2$ with 3C-SiC requires further studies. Based on the PDF-4+ database, the minimum lattice mismatch for the lowest possible indices suggests $Mg_2Si$ $(1\ \bar{1}0)$ //3C-SiC(001) and $MgC_2(1\ \bar{1}2)$//3C-SiC(001) with mismatches of 2.9% and 3.3%, respectively. Figures 1c and 1d show the images from IFFT operations for the precipitates filtered from specific spots in the FFT pattern (Figure 1b). The bright areas show where the precipitates are in the microstructure. The two large second-phase precipitates (~5 nm in size) are overlapping in the images and are likely located at different depths in the TEM specimen.

Figure 2 shows an Arrhenius plot for the relative peak width square of the ToF-SIMS Mg depth profiles in 3C-SiC implanted with 200 keV $Mg^+$ ions to $9.6\times10^{16}$ ions/cm$^2$ at 673 K and isothermally annealed at 1573 K for a cumulative time of 180 and 720 min in Ar, respectively. Mg diffusion is observed at 180 min, below which it is not noticeable. There is significant Mg diffusion into the bulk at 720 min. For a Gaussian distribution $C(x,t) = K[\pi Dt]^{-1/2}\exp(-x^2/4Dt)$ in the dilute limit, the solution to Fick's equation leads to

$$[W(t)]^2 = 4Dt\ln 2 + [W(0)]^2,$$

where $W(t)$ is the FWHM of the peak at time $t$. The diffusion coefficient $D$ can be determined through a linear fit to the data in the Arrhenius plot. While experimental profiles are not exactly Gaussian, the Mg peaks are assumed to consist of two independent Gaussian portions for the convenience of data analysis. The side towards the surface has implantation damage and the other side towards the bulk is largely a pristine crystal. Linear fits to the data lead to the diffusion coefficients of Mg in 3C-SiC at 1573 K:

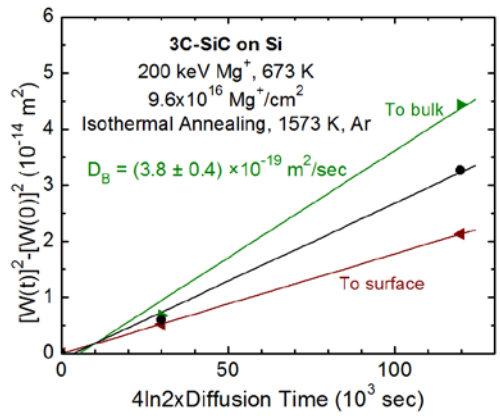


**Figure 2.** Arrhenius plot for the isothermal annealing data at 1573 K. Two separate diffusion regions (towards the surface and bulk) are considered, along with the FWHM broadening in black [1].

$D_S = (1.8 \pm 0.1) \times10^{-19}$ m$^2$/sec (towards surface),
$D_B = (3.8 \pm 0.4) \times10^{-19}$ m$^2$/sec (towards bulk), and
$D_A = (2.8 \pm 0.2) \times10^{-19}$ m$^2$/sec (average).

$D_S$ and $D_B$ are obtained through doubling the half FWHM on the corresponding side of the peak, while $D_A$ is obtained from the FWHM of the peak. They have the same order of magnitude, but $D_B$ may be most representative for Mg diffusion in unirradiated 3C-SiC bulk.

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**References**

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