Three-dimensional electron-positron momentum distribution of O$^{3+}$-irradiated 6H SiC using two positron spectroscopy techniques simultaneously

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Abstract. A three-dimensional (3D) positron annihilation spectroscopy system (3DPASS) capable of determining 3D electron-positron ($e^-e^+$) momentum densities from measurements of deviations from co-linearity and energies of photons from $e^-e^+$ annihilation events was employed to examine the effects of O-atom defects in 6H SiC. Three-dimensional momentum datasets were determined for 6H SiC irradiated with 24 MeV O$^{3+}$ ions. Angular correlation of annihilation radiation (ACAR) and coincidence Doppler-broadening of annihilation radiation (CDBAR) analyses are presented. In addition, a novel technique is illustrated for analyzing 3D momentum datasets in which the parallel momentum component, $p_{||}$ (obtained from the CDBAR measurement) is selected for annihilation events that possess a particular perpendicular momentum component, $p_\perp$ observed in the 2D ACAR spectrum.

1. Introduction

3DPASS measures three-dimensional electron-positron ($e^-e^+$) momentum distributions by simultaneously measuring correlated deviations from co-linearity and energies of coincident two-photon annihilation events. Data for deviation from co-linearity and for energy are typically collected individually using two common positron annihilation spectroscopy techniques, two-dimensional angular correlation of annihilation radiation (2D ACAR) and two-detector coincident Doppler broadening of annihilation radiation (CDBAR), respectively.[1] Our implementation of 3DPASS, described in [2,3], simultaneously collects a single dataset of correlated energies and positions for coincident annihilation photons using two solid-state double-sided strip detectors (DSSDs). 3DPASS analysis captures the 3D $e^-e^+$ momentum distribution enabling conservation of total momentum to be used to interpret results.

This research investigated the effect of oxygen-atom defects on the momentum distribution in 6H SiC. 3DPASS measurements were made on 6H SiC samples, undamaged and ion-irradiated by 24-MeV O$^{3+}$. 2D ACAR and DBAR spectra were extracted from 3DPASS datasets for 6H SiC single crystals that were implanted with oxygen ions. The 3DPASS datasets were further analyzed by extracting DBAR spectra.
corresponding to particular momentum features in the 2D ACAR spectra, enabling conservation of total momentum to be used to characterize the 3D momentum corresponding to a particular lattice direction.

2. Experiment

Two position-sensitive, high-purity germanium DSSDs coupled with high-speed digital electronics are the heart of our 3DPASS instrument [3]. The digital electronics contain four independent electronics boards, each with two 12-bit ADCs, 8 input channels, and two Alterra Cyclone FPGAs. Output data is stored in two data files: raw data and raw event logs. The raw data are energies recorded in ADC units at each 20 ns clock cycle from single triggers for recordable full-charge events on any of the 32-channels. The raw event log, which is processed to obtain 3DPASS spectra, only stores energy for events that achieve the trigger threshold based on that channel’s calibration. Event locations within pixels defined by the orthogonal intersection of front and rear DSSD strips are determined by interpolation based on the ratio of transient charge intensity on strips adjacent to the strip recording a full charge event. [3] Subpixel positions were determined within 0.22 mm standard error by analysis of transient charge intensities on strips adjacent to the strips collecting a full charge event giving angular resolution better than 0.5 mrad for our instrument configuration. DB lineshapes were extracted from the CDBAR energy spectra by selecting events within boundaries defined by equation (1), using $\Delta = 0.3$ keV:

$$E_1 + E_2 = 1022 \text{ keV} \pm \Delta$$  \hspace{1cm} (1)

where $E_1$ and $E_2$ are the energies of the annihilation photons detected coincidently in each of the DSSDs and $\Delta$ is the width of the diagonal DB stripe extracted from the CDBAR spectrum. An optimization analysis [2] showed that for our system, the value $\Delta = 0.3$ keV minimized fluctuations at the base of the DB spectrum and increased the number of events included in the DB spectrum without degrading the observed DBAR spectrum width. Using only a 106.5 $\mu$Ci $^{22}$Na source, 3DPASS datasets were measured for 6H SiC samples before and after irradiation by oxygen ions. 2D ACAR and CDBAR spectra, as well 3D momentum spectra, were reconstructed from the 3DPASS datasets.

Single-crystal 6H SiC samples procured from CREE Inc. were 254-μm thick research-grade, on-axis, N-type (0001) 6H SiC. O-ion implanted 6H SiC samples were prepared by irradiation with 24 MeV O$^{12+}$ ions at 20 particle-nanoamps at the Sandia National Laboratory’s Tandem Ion Beam Facility followed by sample annealing to 1000°C. During irradiation 1.25 x 10$^{14}$ O$^+$ ions were implanted at a depth of 10.8 μm, normal to the surface of several 6H SiC. The irradiated 6H SiC samples were dry-etched to ensure the depth of the thin O-ion implanted layer corresponded to the depth of the positron interaction within the 6H SiC samples which was calculated to be 105 mm using a GEANT4 simulation [4-5]. Positrons were directed into the sample on the side opposite to the face that was irradiated with the O ions to reduce the interaction of positrons with vacancy-type defects created during the thermalization of the oxygen ions.

3. Experimental Results

3DPASS datasets contain the three axial components of momentum of the annihilating $e^+e^-$ pair. In order to fully display the entire 3D momentum, four dimensions are required. Since this is difficult, a convenient approach is to display the momentum distribution for one component, either the component parallel or components in the plane perpendicular to the direction of propagation of the two annihilation photons, for momента selected in other directions. For example, we selected a momentum feature observed in the ACAR spectra and then displayed the DBAR spectra generated from the parallel component of the momentum of the photons that contributed specifically to that ACAR feature. Momentum anisotropies in the ACAR plane were selected for simplicity and also because the entire range of momentum in the ACAR application, limited to the region associated with mostly valence electrons (± 11 mrad or ± 11 x 10$^{-3}$ m$_c$ for both directions in the plane), was contained within the DBAR’s momentum range (40 m$_c$). This 3DPASS capability is demonstrated for 6H SiC samples: virgin and O-ion irradiated.

3DPASS datasets were analyzed to extract conventional 2D ACAR and DBAR spectra as shown in figure 1 for virgin 6H SiC and in figure 2 for O-ion irradiated 6H SiC. Subtle anisotropic momentum features, representing p$_i$ momenta, can be extracted from derivatives of the DB lineshape. Most CDBAR momentum features observed for virgin 6H SiC are observed in O-ion irradiated 6H SiC. The exception is the strong feature at 12.0 mm$_c$ which is absent in the O-ion irradiated 6H SiC. Weak momentum features in 6H SiC at about 4, 9, 11 and 15 mm$_c$ are strong in the O-ion irradiated samples, while the converse was
observed for features at 0.8 and 1.4 mm\(_{cc}\). All these momentum features are symmetrical about zero momentum except for the sharp, strong anomalies for O-ion irradiated SiC in which momentum is reduced, e.g. at -1.4 mm\(_{cc}\) in un-annealed, O-ion irradiated SiC. These unsymmetrical features in irradiated SiC we attribute to positron annihilation in the ion tracks produced by O-ion bombardment.

The 3D momentum distribution from the 3DPASS dataset for virgin, un-annealed 6H SiC was analyzed. Events encompassed in a square area surrounding each of the four quadrant anisotropies were extracted from the 2D ACAR spectrum (figure 1a). The data was extracted from the 3DPASS dataset uncorrected for DSSD charge collection strip efficiency, because it was essential that an event recorded in the ACAR spectrum correlated definitively with the same event in the DBAR spectrum; using efficiency corrected data would violate that restriction. The areas of the four quadrant momentum peaks contained a total of 13.4\% of the total counts recorded in the entire 2D ACAR spectrum for the virgin 6H SiC.

From the energy difference of the coincident events in the selected ACAR momentum peaks, the parallel component of the momentum distribution was calculated and plotted in the same manner as CDBAR spectra. The 3D momentum lineshape for the selected features was extracted just as was the DB lineshape, using \( \Delta = 0.3 \) keV for consistency. This 3D momentum lineshape represented the momentum component parallel to the propagation of annihilation photons for virgin, un-annealed 6H SiC for selected peaks in the ACAR spectrum. These peak events have similar momentum component in the plane perpendicular to annihilation photons propagation. The resulting 3D momentum lineshape for the virgin 6H SiC is shown in figure 1b which is dominated by \( p_\parallel \) peaks at \( \pm 8.1 \) mm\(_{cc}\) yielding a total, 3D momentum attributed to the anisotropy peaks of 11.4 mm\(_{cc}\).

![Figure 1](image)

**Figure 1.** (a) 2D ACAR spectrum for virgin 6H SiC (b) 3D momentum lineshape virgin 6H SiC illustrating \( p_\parallel \) component with \( p_\perp \) constrained by the momentum peaks contained in white boxes in 1a.

The two momentum peaks in the 3D momentum lineshape, indicated by the arrows, in the direction parallel to the annihilation photon’s propagation corresponded very well to the magnitude of the momentum of the four features that the perpendicular momentum component were constrained to and to the large peaks at \( \pm 2 \) keV observed in the DB lineshape as discussed in [2]. This indicated that a momentum of \( \pm 8.1 \) mm\(_{cc}\) existed in both momentum components, in the plane perpendicular and in the direction parallel to the propagation direction of the annihilation photons. The shoulder in the 3D momentum lineshape at approximately \( \pm 16 \) mm\(_{cc}\) did not correspond to any other previously observed feature. 3D momentum lineshapes for the anisotropies centered at (0,4.5 and 0, -4.5) and at (0,10.0) and (0, -10.0) were similarly analyzed, but there was no discernable features above the noise observed in the lineshape, due to the low number of events with momentum corresponding to those anisotropies.

The 3D correlated momentum distribution from the 3DPASS dataset for O-ion irradiated, un-annealed 6H SiC was analyzed. A square area, of the same size (in momentum space) as selected from 2D ACAR for virgin SiC, was extracted surrounding quadrant features in the O-ion irradiated, un-annealed 2D ACAR
spectrum. Events contained in the white boxes, shown in figure 2a, for the equivalent momentum peaks approximately centered in the spectrum quadrants were extracted from the 3DPASS dataset uncorrected for the DSSD charge collection strip efficiency. These four momentum peak areas contained 18.7% of the total counts. The resulting 3D momentum lineshape compared to the DB lineshape is shown in figure 2b.

![Figure 2](image)

Figure 2. (a) 2D ACAR spectrum for O-ion irradiated, un-annealed 6H SiC (b) 3D momentum lineshape for O-ion irradiated, un-annealed 6H SiC illustrating $p_\perp$ momentum

The two momentum peaks in the direction parallel to the annihilation photon’s propagation in the 3D momentum lineshape, indicated by the arrows in figure 2b, corresponded very well to the magnitude of the momentum of the two shoulder features at ±3 keV observed in the corresponding DB lineshape as discussed in [2]. This not only indicated a momentum of ±12 mm/c primarily existed in the component parallel to the direction parallel to the annihilation photons propagation, but also in the momentum in the plane perpendicular to the photon motion. The magnitude of the total momentum of the selected quadrant events was calculated to be 16.0 mm/c from the three dominant momentum components. This illustrates the potential utility of correlating projections of momentum magnitude in simultaneous 2D ACAR and CDBAR measurements which is not possible by analysis of the techniques when applied separately.

4. Conclusions
The large change in the ACAR momentum anisotropies show that the 6H SiC lattice structure at positron annihilation sites was significantly perturbed by the O-ion implantation due to the oxygen atom implantation in interstitial sites. Additionally, the manner in which the anisotropies changed suggests a slight realignment of the symmetry of positron annihilation sites. The change in the positron center of symmetry with O-ion implantation altered the directions of $e^-e^-$ momentum projections. The 3DPASS method is capable of directly measuring total momentum corresponding to observed ACAR anisotropies.

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References
[1] Krause-Rehberg R, Leipner H 1999 Positron Annihilation in Semiconductors (Berlin: Springer) 16-20
[2] Williams C, Burggraf L, Adamson P, Petrosky J submitted to Nuc. Instr. Meth. Phys. Res. A, 5/ 2010
[3] Williams C, Burggraf L, Adamson P, Petrosky J, Oxley M 2010 J. Phys Conf. Ser. 225 012058
[4] Agostinelli S et al. 2003 Nuc. Inst. Meth. Phys. Res. A 506 250-303
[5] Allison J et al. 2006 IEEE Trans. Nuc. Sci. Vol. 53 1 270-278