Simultaneous, coincident 2-D ACAR and DBAR using segmented HPGe detectors incorporating sub-pixel interpolation

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Abstract. A three-dimensional Positron Annihilation Spectrometry System (3D PASS) for determination of 3D electron-positron (e⁻−e⁺) momentum densities by measuring coincident annihilation photons was designed, constructed and characterized. 3D PASS collects a single data set including correlated photon energies and coincident photon positions which are typically collected separately by two-dimensional angular correlation of annihilation radiation (2D ACAR) and two-detector coincident Doppler broadening of annihilation radiation (CDBAR) spectrometry. 3D PASS is composed of two position-sensitive, high-purity germanium (HPGe) double-sided strip detectors (DSSD(s)) linked together by a 32-channel, 50 MHz digital electronics suite. The DSSDs data were analyzed to determine location of photon detection events using an interpolation method to achieve a spatial resolution less than the 5-mm width of the DSSDs’ charge collection strips. The interpolation method relies on measuring a figure-of-merit proportional to the area of the transient charges observed on both strips directly adjacent to the charge collection strip detecting the full charge deposited by the annihilation photon. This sub-pixel resolution, corresponding to the error associated with event location within a sub-pixel was measured for both DSSDs using the approach outlined in Williams et al [1] and was on the order of ± 0.20 mm (± one-standard deviation). As a result of the sub-pixel resolution, the distance between the DSSDs and material sample was reduced by a factor of five compared to what is typically required in 2D ACAR systems was necessary to achieve 0.5-mrad angular resolution. This reduction in the system’s footprint decreases attenuation of the annihilation photons in the air between the material sample and the DSSDs and increases the solid angle between the sample and the DSSDs, ultimately resulting in higher system detection efficiency. 3D PASS was characterized in the same manner comparable to state-of-the-art 2D ACAR and CDBAR spectrometers. 3D PASS spectra were collected and analyzed for single-crystal copper (Cu) and silicon carbide (6H SiC) and compared with the results in the literature.

1. Introduction
Several methods are currently used in the scientific community and industry to measure and characterize defects in semiconductor materials including electron paramagnetic resonance photoluminescence and positron annihilation spectroscopy (PAS). PAS relies on the measurement of...
radiation from the annihilation of an electron and a positron. PAS encompasses several experimental techniques; the most commonly used are positron annihilation lifetime spectroscopy, coincident Doppler broadening of annihilation radiation (CDBAR), and angular correlation of annihilation radiation (ACAR). These non-destructive PAS techniques have been gaining increasing popularity with technological improvements in detector performance and affordability of digital electronics.

The annihilation of an electron and a positron usually produces two oppositely directed 511-keV photons. Due to the conservation of energy and momentum, the two annihilation photons produced from the annihilation event are emitted exactly co-linearly in the center-of-mass frame-of-reference. In the laboratory frame, the emission angle deviates from 180° due to the momentum that the electron-positron (e⁻-e⁺) pair posses prior to their annihilation. CDBAR uses two high-energy resolution detectors to measure Doppler shifts of the coincident annihilation photon energies due to the distribution of e⁻-e⁺ momenta in the direction parallel to the photon emission. The CDBAR technique has been successfully demonstrated on metallic [2-3] and silicon carbide (SiC) [4] samples by several researchers. 2D ACAR, on the other hand, determines the e⁻-e⁺ pair’s momentum distribution in the 2D plane perpendicular to the photon emission direction using position-sensitive detection systems to measure the deviation of the emission angle from co-linearity between coincident annihilation photons. The 2D ACAR technique has been effectively demonstrated on metals [5-6] and SiC [7] by several researchers. Previously, ACAR and CDBAR techniques have been applied separately resulting in an incomplete description of the e⁻-e⁺ momentum distribution because momentum in the measurement plane was not correlated with momentum in the photon emission direction. Simultaneous momentum measurements can provide the complete, correlated 3D momentum distribution of the e⁻-e⁺ pair. This capability will be useful for future comparisons to theoretical models of e⁻-e⁺ wavefunctions, which can be used to predict PAS, as illustrated in Adamson et al [8].

While experimental PAS techniques can provide some information on the structure of the material interrogated, they have several measurement limitations. First, for CDBAR applications, the detection system should have high-quality energy resolution in order to reveal information about the material’s core electron environment, which is only marginally achieved by the resolution of the best HPGe semiconductor detector systems. Next, in order to adequately describe the momentum distribution, 2D ACAR measurements have required high activity sources and large distances between detectors and positron source. Typical 2D ACAR systems have used large footprints to achieve adequate angular resolution (~0.5 mrad), often having about 10 m distance between the sample and detectors depending on the pixellation of the detection system, resulting in inefficient detection. In order to record the large number of coincident events (>10⁶) necessary to achieve sub-milliradian (~0.5 mrad) angular resolution, sources having 100’s of mCi activity are typically used in order to collect a spectrum in a reasonable amount of time. Finally, the copious information produced by PAS measurements have not been effectively used due to the inability to efficiently collect, process and store the data. Although these problems continue to limit PAS effectiveness, we have reduced some impact of these limitations by applying two new engineering techniques to state-of-the-art PAS. On our way to making a single system to measure simultaneous, coincident 2D ACAR and CDBAR spectra in order to determine complete 3D e⁻-e⁺ momentum distributions, we have incorporated sub-pixel resolved DSSDs and multiplexed digital electronics on a common clock.

Pixelation created by double-sided orthogonal strip detectors (DSSDs) using planar HPGe crystals has been used for position-sensing gamma detection applications. By applying sub-pixel resolution, our first engineering improvement, in these high-resolution solid state detectors, we have reduced the 2D ACAR footprint and measurement time for a selected source activity. Many researchers [9-10] have shown that transient charge analysis in DSSDs can be used to significantly improve gamma image resolution for all but the external detector strips. Using the relative areas of transient (or induced) charge pulses on strips adjacent to the full-charge collection strips on DSSDs, location of charge deposition events across the width of strips produces sub-pixel spatial resolution much finer than the intrinsic pixilation of the orthogonal charge collection strips. Calibration of this sub-pixel interpolation method is described in detail by Williams et al [1]. Incorporation of transient charge
analysis allows considerable reduction of the distance between the sample and detectors without degrading angular resolution. This increases the solid angle between the sample and detector allowing more un-scattered annihilation photons to reach the DSSDs, increasing absolute efficiency. Our second engineering improvement incorporated multiplexed digital electronics using FPGA-logic on a common clock into the system design. These electronics permit characterization of charge deposition dynamics across many detector elements enabling us to ascertain coincident event locations and energies. Additionally, the electronics can be programmed to perform functions specific to our application, eliminating unnecessary data acquisition and storage.

These engineering techniques were applied to a new PAS technique designed to fully characterize 3D $\epsilon^{-}\epsilon^{+}$ momentum densities by measuring coincident photons from $\epsilon^{-}\epsilon^{+}$ annihilation events. The detection system is composed of two, position-sensitive, HPGe DSSDs coupled together with a digital electronics suite programmed specifically for measuring interpolated sub-pixel charge deposition event locations and energies. We demonstrated this 3D Positron Annihilation Spectroscopy System (3D PASS) by simultaneous measurement of 2D ACAR and CDBAR spectra for single-crystal Cu and 6H SiC.

2. Equipment
Two position-sensitive DSSDs and a digital electronics suite were the main components of our 3D PASS used for this research.

2.1. Detectors
The Ortec DSSD is the same HPGe detector described in Williams et al [1]. The second detector used for the 3D PASS is also a position-sensitive, planar HPGe DSSD. This HPGe DSSD, manufactured by PHDS Co, has a 9 cm diameter Ge crystal and an active depth of 11 mm, shown in Figure 1. The detector has 16 – 5 mm wide charge collection strips on each of the front and rear faces of the Ge crystal, orthogonal to each other. The charge collection strips on the front and back face of the crystal are metalized, amorphous germanium with a thickness of ~2 μm. Since the crystal is circular, only the 8 center strips on each face have a length of 8 cm. The strips beyond the center strips are shorter the further they are from the center of the crystal. Crystal volumes created by intersections of these 5-mm orthogonal strips create 220 intrinsic pixels. The rear strips, denoted as the AC side, are vertical, and are labelled 0 - 15 with 0 being the left-most strip and 15 the right. The front strips, denoted as the DC side, are horizontal and are labelled 16 - 31 with 16 being the top strip and 31 the bottom.

![Figure 1. Photo of PHDS DSSD sitting on its LN₂ dewar. Middle: Photo of PHDS DSSD’s Ge crystal with electrode masking. Right: PHDS detector’s electrode masking layout (not to scale).](image)

2.2. Digital Electronics
The Spec32 digital electronics system is a 32-channel, 50 MHz digitizer. The system contains four independent electronics boards, each with two, 12-bit ADCs, 8 input channels and two Alterra Cyclone FPGAs. Waveforms from the DSSDs’ preamplifiers are directly digitized and then processed through trapezoidal filters defined within the Spec32’s software, Imager. The FPGA forwards the
user-defined output data to the buffer and then over-writes the waveform data, saving valuable buffer memory and reducing the number of buffer spills. For our experiments, the FPGA’s were programmed to calculate the energy collected in the full-charge collecting strip and figure(s)-of-merit (FOM)’s proportional to the area of the transient charges in the strips directly adjacent. Because the Spec32 only accepts 32 inputs, all 10 of the Ortec (F1-F5 and R1-R5) and only 16 of the center-most strips of the PHDS (4-11 on the AC side and 20-27 on the DC side) DSSDs outputs were used.

Output data is stored in two data files: raw data and raw event logs. The raw data log stores energy data for each of the 32-channels, initiated by a single trigger of a recordable full-charge event on any channel. This type of file can be extremely large if there are a large number of event triggers. The raw event log stores energy data only for the channels that achieve the trigger threshold, based on that channel’s calibration. The FOMs for the transient charges in the strip to the left, denoted the predecessor (Pred) and the strip to the right, denoted the successor (Succ), as well as, the timestamp are also stored. Since the Spec32 is only a 12-bit system, the time stamp is reset every 256, 20 ns clock ticks, meaning multiple events must trigger within a 5.12 μsec window before the timestamp resets to know their relative event timing. No counter is available to list the time between timestamps.

2.3. Source/Sample Configuration
The positron source, 106.3 μCi $^{22}$Na, was positioned exactly orthogonal relative to the face of the detector. Two samples were measured: 1-cm$^2$ x 1.0-mm thick single-crystal Cu, growth orientation (100), procured from MTI Corp and 1-cm$^2$ x 0.268-mm thick research-grade, on-axis, N-type 6H SiC having growth orientation (0001), purchased from CREE Inc. The crystal face of each sample was turned 45° on a vertical axis orthogonal to the axis between the centers of the faces of the DSSDs in order to maximize positron interaction with the sample near the center point between DSSD faces. In order to reduce positron annihilation with air as positrons travelled from the source to the sample, the $^{22}$Na source and material sample were housed in a vacuum chamber, reduced to a pressure of 1 torr.

3. Experiment
Several independent experiments were conducted to determine the performance of the DSSDs in order to finalize the design of 3D PASS. First, in order to determine the distance the detectors must be placed from the sample, the sub-pixel resolution was determined. The interpolation method from Williams et al [1], shown in equation (1), was used to determine event locations.

\[
\text{Distance} = \left( \text{Strip #} - 1 + \frac{\text{FOM}_{\text{Pred}}}{\text{FOM}_{\text{Pred}} + \text{FOM}_{\text{Succ}}} \right) \times \text{strip width}
\]

This interpolation method employs a FOM proportional to the area of the transient charges observed on both strips directly adjacent to the full-charge collecting strip (Strip#), termed FOM$_{\text{Pred}}$ for predecessor and FOM$_{\text{Succ}}$ for successor strips to estimate sub-pixel location. Sub-pixel resolution, the standard deviation of the error associated with locating charge deposition events within a sub-pixel that met the energy and timing criteria for the interpolation method, was measured for both DSSDs using the same approach outlined in Williams et al [1]. To quantify the spatial resolution, the experimental sub-pixel count distribution from each DSSD was analyzed by a minimum-error least squares fit to a Gaussian point-spread function on a circular collimator aperture. The resulting sub-pixel resolution for the Ortec DSSD was ± 0.22 mm and was ± 0.19 mm for the PHDS DSSD.

Next, the energy resolutions for the DSSDs for full-energy peak (FEP) events, corresponding to complete charge-collection of the full-energy photoelectrons, were quantified. The resolution, of critical importance to CDBAR measurements, depends not only on the individual detector performance, but also on the noise in the Spec32 electronics. $^{22}$Na was not used to quantify detector resolution due to the inherent Doppler broadening of the annihilation photons. Photons at 514 keV from a 96.79 μCi $^{85}$Sr source were used to estimate the resolution of each DSSD at 511 keV. A 72-hour data set using the $^{85}$Sr source was measured using both DSSDs and the Spec32 electronics. The
centers of the detector faces were axially aligned and the $^{85}\text{Sr}$ source was located on the axis, centered between the detector faces at a detector/source distance of 12.0 in.

An in-house MATLAB code was used to process the raw event log from the Spec32. The code first discarded all recorded events outside of the energy range $514 \pm 30$ keV to isolate un-scattered $^{85}\text{Sr}$ gammas. Then, only coincident full-energy events between the front and rear strip in both DSSDs, in time (within 60 ns) and energy, were accepted and examined. The 514-keV FEPs were constructed for each intrinsic pixel in both DSSDs. The average FWHM for the intrinsic pixels in the ORTEC and PHDS DSSDs was calculated to be $1.76 \pm 0.24$ keV and $1.49 \pm 0.17$ keV, respectively. Additionally, these data sets were analyzed for potential correlation of the FOMs with FEP energy with the intent of using the FOMs to evaluate the sub-pixel response and possibly improve energy resolution. Each DSSD’s coincident events were plotted against their associated FOMs, both successor and predecessor, and fitted to linear, quadratic, and cubic functions. The resulting best fits, which were linear with slopes on the order of 0.04 keV, indicated no significant correlation between event energy and FOM values.

Based on the measured sub-pixel spatial resolution, the dimensions of sub-pixels for ACAR analysis were established as 1 mm$^2$ squares, corresponding to two standard deviations of resolution error associated with the interpolation method. To obtain an angular resolution of 0.5 mrad using a 1 mm$^2$ sub-pixel size, the face of the DSSDs were each placed 2.0 m from the center of the source/sample location, assuming a 1-mm$^2$ sample. Figure 2 displays the final 3D PASS configuration. The sub-pixel size was chosen 2.5 times larger than the spatial resolution, which compensates for some increase in the sample size used. Once this technique has been demonstrated and our positron beam has been built, our sample/source dimensions will not degrade the 0.5 mrad angular resolution.

With the footprint established, the 3D PASS was used to collect simultaneous momentum data sets, one for single-crystal Cu and one for single-crystal 6H SiC. Each data set was collected to accumulate $10^6$ coincident events that passed the energy and time criteria for the interpolation method. Then, 2D ACAR and CDBAR spectra were reconstructed from each data set of qualified coincident events. The 2D ACAR spectra were binned according to the angular resolution, in 0.5 mrad x 0.5 mrad bins, and the CDBAR spectra were binned into 0.1 keV intervals. Cu spectra were analyzed to evaluate and compare the 3D PASS performance to published results. Cu was chosen for calibration for two reasons: Cu has been extensively studied and because its 2D ACAR distributions perpendicular to the (100) is approximately symmetric.

4. Results

To evaluate the simultaneous 3D momentum capability, the 3D PASS data set for single-crystal Cu was collected and the 2D ACAR was reconstructed as shown in Figure 3. The 2D ACAR spectrum was populated by processing coincident annihilation events using the interpolation method (equation (1)) to determine event location. A benefit of using Cu to calibrate the ACAR spectrum is that the spectrum’s inherent symmetry can be used to precisely correct the source/sample misalignment shown in the contour plot of the Cu 2D ACAR spectrum. The system was 3.12 mm off in the X-direction and 2.51 mm off in the Y-direction, which was corrected by re-aligning the sample vacuum chamber, relative to the DSSD faces, also shown in Figure 3. The ACAR response of 3D PASS was evaluated...
using two alignment-corrected projections at X=0 and Y=0, slightly smoothed using a Savitsky-Golay 2nd order polynomial filter over a frame size of 5 data points. The smoothed projections, shown in Figure 4, compare closely to scaled ACAR data for single-crystal Cu collected by Senicki et al [2], measured using the 1D long-slit ACAR technique. The un-smoothed projections, however, exhibit notches at distinct angles in the raw Cu spectra. By applying the slight smoothing routine, these features are greatly reduced. The appearance of these features on the sides and the peak can be the result of either one or a combination of the following. First, our Cu sample was oriented 45° relative to the face of the DSSDs face, where Senicki et al’s was orthogonal. The slight anisotropy of Cu as discussed by Tanigawa et al [6] could contribute to the observed features. Second, Williams et al observed a decrease in efficiency in the charge collection strips the closer events occurred to the edge of the strips which could distort spectra depending on which sub-pixels detect the annihilation photons. Finally, many positrons from the 22Na source probably interacted and annihilated with the vacuum chamber materials, causing momentum data from those annihilations to alter the Cu momentum data.

Figure 3. Left: Cu 2D ACAR spectra with X and Y in mrad units and Z in count per bin. Right: Contour plot (at contour intervals of 10% of max counts) for the Cu 2D ACAR spectrum.

Figure 4. Left: Raw data for horizontal (X) and vertical (Y) projections. Right: Smoothed data compared to Senicki et al’s reconstructed data.

To investigate the CDBAR performance of 3D-PASS, the Doppler broadened (DB) lineshape was extracted from the Cu CDBAR spectra for coincident annihilation events. The resulting Cu DB lineshape, shown in Figure 5, compares favorably with Szpala et al’s [3] scaled annihilation lineshape in both the high and low momentum regions, except for the slightly larger background contribution on the low-energy side of the DB lineshape and the shoulder features on the sides of the lineshape. These shoulder features most likely are caused rotation of our sample and influenced by the slight anisotropy of Cu. Regardless of these slight features, the performance of 3D PASS for measuring simultaneous...
2D ACAR and CDBAR in a one measurement system compares well with published results for single-crystal Cu. Since performance of 3D PASS compared well with published results for Cu, the 6H SiC 2D ACAR and CDBAR were constructed in the same manner and are shown in Figure 6. Note the differences in the 2D ACAR spectra and CDBAR spectra when compared with the Cu data. It is evident from both spectra that the positrons interacted with higher momentum electrons in the 6H SiC than in the Cu sample. This is supported by the significant amount of interactions at larger angular deviations in the ACAR spectra and the larger shoulders on the DB lineshape slopes typically characteristic of interactions with higher momentum core electrons. This was expected by the anisotropies at higher momentum regions present in the 6H SiC 2D ACAR Kawasuso et al. [7] published. Although their spectra have many similarities to ours, we see a distortion particularly about the vertical axis due to our sample rotation. Because the sample orientations differed by 45°, our spectra was significantly transformed due to the high degree of anisotropy in the 6H SiC e⁻-e⁺ momentum density. The CDBAR, however, did compare well with Rempel et al’s [4] CDBAR results on similar 6H SiC samples. Their CDBAR lineshape was reconstructed from the data they presented and included in Figure 6 and was compared with the 3D PASS’ DB response for 6H SiC. Even though higher momentum interactions were expected in the SiC, the larger shoulders on the sides could be partly influenced by the source/sample orientation, low count statistics or less likely, the DSSD’s efficiencies.

![Graph showing differences in ACAR and CDBAR spectra for Cu and 6H SiC](image)

**Figure 5.** Left: CDBAR spectra for single-crystal Cu. Right: DB lineshape for Cu compared with Szpala et al’s lineshape reconstructed from their data. Shoulder features (arrows) suggest discrete momenta.

5. Conclusions and future work
The 3D PASS performance was verified by comparing experimental data with published 2D ACAR and CDBAR results for single-crystal Cu and 6H SiC. Further experimentation will be conducted to determine the origin of the ridge features on the peak and sides of the vertical and horizontal (X and Y = 0) projections for the ACAR spectrum and the slight increased background contribution in the DB lineshape. Currently, 3D PASS measurements of oxygen-atom inclusions in 6H SiC are underway. 3D PASS has been shown to be promising for simultaneously collecting the 3D e⁻-e⁺ momentum densities using a single measurement. In future work, we will use a pulsed slow positron beam source and moderator for synchronous 3D PASS measurements. This approach will allow positrons to be focused directly into a sample surface, minimizing contribution of extraneous annihilations while greatly increasing the number of coincident annihilation events for improved measurement efficiency. Additionally, the beam will allow surface annihilation measurements to be made using selected positron energies and varying sample orientations.

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![Diagram](image.png)

**Figure 6.** Upper left: 2D ACAR spectra for 6H SiC with contours at 10% of max counts (lighter indicates higher counts). Upper right: CDBAR spectra for 6H SiC. Bottom left: DB lineshape for 6H SiC extracted from CDBAR spectrum compared to Rempel and Szpala et al’s Cu DB spectra reconstructed from their data. Arrows indicate high angular momentum features observed in our spectrum that were not previously observed.

### References

[1] C. Williams, W. Baker, L. Burggraf, P. Adamson, and J. Petrosky, accepted by IEEE Trans Nuc. Sci. January 3, 2010.

[2] K. Lynn, J. MacDonald, R. Boie, L. Feldman, J. Gabbe, M. Robbins, E. Bonderup, and J. Golovchenko 1977 *Phys. Rev. Lett.* 38 pp 241-4.

[3] S. Szpala, P. Asoka-Kumar, B. Nielsen, J. Peng, S. Hayakawa, K. Lynn, H. Gossmann, 1996 *Phys. Rev. B* 54 pp 4722-31.

[4] A. Rempel, K. Blaurock, K Reichle, and H. Schaefer 2002 *Mat. Sci. Forums* 389-393 pp 485-8.

[5] S. Berko 1979 *Proc. 5th Int. Conf. on Positron Annihilation (Jpn:Jpn Institute of Metals)* pp 65-87.

[6] S. Taniigawa, K. Ito, S. Terakado, A. Morisue, S. Fujii, Y. Iwase 1985, *Proc. 7th Int. Conf. on Positron Annihilation (New Delhi:World Scientific)* pp 288-90.

[7] A. Kawasuso, T. Chiba, and T. Higuchi 2005 *Phys. Rev. B* 71, pp 193204.

[8] P. Adamson, X. Duan, L. Burggraf, M. Pak, C. Swalina, S. Hammes-Schiffer, 2008 *J. Phys. Chem. A.* 112 (6) pp. 1346-51.

[9] M. Amman and P. Luke 2000 *Nuc. Inst.Meth. Phys. Res. A* 452 (1) pp. 155-66.

[10] M. Burks, E. Jordan, E. Hull, L. Mihaiescu, and K. Vetter K, 2004 *IEEE Nuclear Science Symposium Conference Record* Italy pp. 1114-8.