

Photovoltaics Characterization: An Overview

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PHOTOVOLTAICS CHARACTERIZATION: AN OVERVIEW

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Abstract. In order to move to a next generation of characterization methods, the requirements must be fully understood and documented. Presented herein are the required functionalities for the next generation of characterization methods. This paper is not meant to be exhaustive, but instead presents new developing characterization methods. The basic characterization requirements are outlined in the introduction. It is expected that in the future, phenomena will be understood on the atomic scale and applied to large-scale arrays for a complete understanding of the various affects that determine the real cell efficiency. There is a need for a fundamental understanding from atomic and nanoscale characterizations of impurities, native defects, extended defects and interfaces to provide the necessary understanding of these types of PV cells. This information from fundamental probes should be used for input to the performance characterization of the developing technologies, which include high-flux operation, multijunction and lower band-gap systems. These methods will allow new materials to come to realization at a much faster rate than was possible in previous years.

INTRODUCTION

Materials characterization plays a pivotal role in photovoltaic (PV) research and is essential in realizing the breadth of new technologies on the horizon. A number of techniques from atoms to arrays are currently available to determine the structure and properties of PV materials, devices, and systems. However, a clear understanding of the relationship between the underlying materials' characteristics and device performance is still lacking. Efforts and techniques should be devoted to the identification of a set of physical parameters, which can be quantitatively correlated with actual solar cell performance using nondestructive and in-situ characterization techniques. Special electrooptical characterization methods, such as minority-carrier parameter determinations and chemical defect resolutions are needed for the next generation of industrial tools. Figures of merit, namely, minority-carrier lifetime, interfacial recombination velocity, and especially room temperature efficiency, still need to be improved. A serious modeling effort is a necessary component to achieve the final solution. This will require a combined and collaborative effort on the part of industry, national labs, and universities working hand-in-hand to develop the necessary understanding from point defects and impurity complexes to arrays of solar energy panels.

To understand compensation by native defects and/or unintentional impurities, and, in the case of polycrystalline material, grain boundary defects and impurities, leads to understanding of real cell efficiencies. The final solution can be achieved only with a combination of new characterization methods to input the necessary details and industry to use the understanding to make cost-effective solutions for the next generation of PV devices for the United States and the world.

The determination of the device parameters of solar cells and modules is essential to the establishment and tracking of the progress in this arena. When performed under standard conditions, this also provides the mechanism to objectively compare various PV technologies. Finally, since the "device" is the proof of any PV material system, the determination and demonstration of device performance is important for establishing credibility, and providing guidance for further development. The accurate, rapid, and precise determination of efficiency and related device parameters has become an essential part of solar cell research, development, and manufacturing.

A significant need for a centralized, independent laboratory facility has proved to be a requirement for the credible evaluation of photovoltaic devices. Constant inputs are needed for new and unique front-end research methods to provide industry with the necessary input for evaluation, but an understanding of the process is also important. The centralization of the standard measurement capability has also helped to disseminate standard test methods and reporting conditions within the photovoltaic community. It has led to international intercomparisons to make sure that efficiencies measured in one part of the world track those in other locations. Almost all of these central and standard performance-evaluation laboratories can trace their standards and references to common sources. However, new measurement techniques need to be generated in order to understand and improve cell efficiencies.

General Needs for Characterization

In the near term (next 5-10 years), a number of areas of performance evaluation are already in development or identified, as needed to meet anticipated needs. The ability to determine and compare the operational characteristics of solar cells and modules has progressed significantly over the past 15 years, especially with the adoption of international standards for measuring and reporting efficiencies and the initiation of certification procedures and laboratories under the PV (Photovoltaic) GaP program. With the guidance of the PV Program's Five-Year Plan and the recent PV Industry Roadmap, coupled with the experience of those working in this field, several needs are identifiable:

Precision and Accuracy. Measurement uncertainty analysis has been applied to every step of the standard cell and module evaluation processes. Work continues to refine the techniques to provide customers with the best possible evaluation of parameters. The *best* current methods at the standards laboratories have accuracies (or uncertainties in the efficiency with respect to standard conditions) of $\pm 1\%$ for single-junction cells, $\pm 5\%$ for concentrator cells, and $\pm 3\%$ for modules. For multijunction devices, these range from $\pm 3\%$ for 1-sun cells to about $\pm 5\%$ for modules. The single-junction, 1-sun cell uncertainties are acceptable. The need for concentrator and module technology development requires refinement in those techniques in order to provide better comparisons and evaluation of progress with these technologies.

Standards. New and novel device technologies require rating methodologies. Examples include bifacial cells and holographic concentrators. Many alternatives to the standard "accepted" reporting techniques must be evaluated for their utility and accuracy. In general, standards activities require almost constant attention to ensure equity for evolving technologies. For example, qualification tests developed and accepted for crystalline Si modules might not be appropriate for thin-film technologies.

Standard test and reporting conditions must be checked periodically, as the range of devices in the photovoltaic portfolio expands. On the module side, the development and implementation of other rating schemes (power, energy, etc.). Alternatives to efficiency are required as more appropriate for this component area.

Concentrators. With some renewed interest in these technologies (with some added focus in the High-Performance Photovoltaics Initiative for the coming 10-year period), the current state-of-the-art is not prepared to meet the needs for many of these device evaluations. Issues relating to linearity must be resolved to adequately and fairly evaluate these technologies. Methods for determining efficiencies in the 30%-35% range are currently lacking from precision, time-to-perform (responsiveness), reproducibility, and controllability aspects. Much time has been devoted to the development and refinement of the measurement of these concentrator cells as with AM1.5 technologies. There exists a whole range of concentrators in the 20–50 concentrator range that use a substantial portion of diffuse radiation. This has not been standardized, and procedures to compare the performance at such levels (with diffuse and direct components) have not been established. To provide reproducible determinations for these concentrators is critical. Finally, there is a very significant need in the area of concentrator measurements to determine the quantum efficiencies of devices *under the concentrated light conditions*.

This is a non-trivial problem, which is exacerbated at higher concentrations and for multiple-junction concentrator technologies.

New technologies. New device types, such as thermophotovoltaics, dye-sensitized and electrochemical cells, quantum-dots/porous, material/organic semiconductors, and a host of other next-generation technologies not yet reported, need attention for performance determinations. Spectral effects, response times, and illumination response are critical, and methods for ensuring these must be considered and adequately addressed. Criteria for these device technologies might have been substantially different, and imposition of "current" test and measurement formalities could be erroneous.

Artifacts. Sensitivities and measurement artifacts are always concerns for the measurement scientist. For new device types, these must be probed and identified before standard measurements are adopted. For these and existing technologies (e.g., Cu(In,Ga)(S,Se)₂, CdTe, a-Si:H), stabilization criteria must be established. Changes with light exposure are certainly concerns; whether a device diminishes in performance upon exposure or whether it improves! Area is a known problem for research (<1 cm² areas) devices in which collection from outside the "defined" area is significant, area definition is complicated by ragged or less defined edges, and probe contacts have reliability and shading problems. Area is currently the most common source of error for research devices. For larger area device measurements, accuracy is still a concern. Pulsed-light simulators used for modules in both development and in manufacturing environments may have problems with uniformity and accurate spectral determinations. Capacitive and other transient effects in the module can hinder measurement accuracy. Large-area continuous simulators are now in operation that can alleviate some of these problems and permit the application of spectral correction methods used in cell-efficiency measurements. Module ratings and measurement methodologies (e.g., power vs. efficiency, temperature, etc.) must also be addressed to better meet the needs of the industry and the client.

In-situ and smart diagnostics. Characterization will become more integrated into the research equipment and into the manufacturing environment. To realize thin-film technologies with greater than 20% efficiencies and multiple-junction thin-film technologies with greater than 25%, for example, it will be required to evaluate the surfaces of materials as they grow in order to exactly engineer their properties. In the manufacturing facility, the lines will become more automated, and materials and device performance will have to be evaluated during processing to ensure yields and manufacturing cost effectiveness. Non-contact evaluation methods will become critical. Performance evaluation and other techniques will have to be developed to meet these manufacturing criteria.

For long-term needs (10 years and out), performance measurements and characterization have much in common with other technology requirements—they have to be responsive to technology directions and development. The coming PV Industry Roadmap should serve as a useful document in guiding planning for characterization efforts, much like the Semiconductor Roadmap provided the electronics industry equipment manufacturers and other stakeholders with a strategy for equipment development and supporting technology requirements. For the next generation of photovoltaics, those technologies that will be R&D interests after 2010 and commercialized from 2015 through 2025, measurements

and characterization technologies have to position themselves to be flexible and responsive to the needs. Many of the techniques that need to be used to address the needs of the technologies in this longer period of time will be developed in response to other requirements in the related electronics industries. Others will have to be adapted or specifically developed for these next-generation PV technologies. For performance, some areas will likely include (2006 and beyond):

- Very high concentration devices, with operating environments exceeding 1000 suns and perhaps approaching 5000 suns.
- Multi-junction approaches, with 4-10 junctions possible. This will require techniques that not only evaluate performance parameters for these extremely complex solar cells, but also provide techniques and standards for devices having efficiencies exceeding 50%.
- Low-bandgap cells, determining parameters for devices down to 0.2 eV. The multi-cell problems addressed in the previous bullet apply. Thermophotovoltaics for terrestrial applications might require extending to these low band-gap regimes. Accompanying the problems of low band-gap evaluations will be the system performance determinations that are critical to such technologies.
- Area performance measurements will require both larger areas (for product evaluation, with simulators and techniques capable of perhaps 20 m² for some large-area technologies.) On the other end of spatial resolution, nanoscale-type performance measurement systems will be needed for research optimization of ultra-small area devices and for determination of localized efficiencies on device surfaces to optimize processing and growth parameters. Such tools will become important for maximizing device operation, linking performance events on the nanoscale to eventual macroscale operations. Nanotechnology will be part of PV, both for device development and for characterization efforts.
- Reliability and durability criteria, both for qualifying these new cell technologies and for ascertaining their operating-lifetime probabilities. This would include efforts at service lifetime predictions and development of acceptable accelerated lifetime tests and procedures.
- Systems, including balance of system components, cannot be neglected. As this PV technology becomes more commonly deployed (especially for the US markets), the system reliability is a major concern. This will call attention to the balance of system components (inverters, charge controllers, batteries). Certainly, their reliability is essential, and will require characterization support to establish parameters. Moreover, storage (next-generation batteries and non-conventional approaches) will become a greater part of the R&D activity.
- Resource assessment and metrology will become increasingly important. First, the measurement of the illumination sources for simulators will become more complex. With the more complicated designs for cells and spectral matching specifications for devices, the exact and rapid determination of the source power density, spectral distribution, and uniformity will become more critical for standards and other laboratories. Secondly, for the proper deployment and design of systems (especially that

generation that we do not even yet know), the solar resource determination will become essential. This will mandate the mapping of wide areas of the globe for this solar commodity (e.g., satellite and remote sensing) and having mobile and inexpensive equipment for monitoring these resource parameters "on location". The design of systems will become more locality sensitive, especially with a growing and different portfolio of PV technologies.

The communications revolution will become a partner with performance and all characterization techniques in the 21st century. No longer will the ability "to witness", transfer data, or control systems be confined by the locality. Many laboratories have already embarked on techniques to provide immediate transfer of data. The future will focus on these areas, and control of instrumentation will not require operators in remote locations. As the business of manufacturing becomes global, the cost of remote operations will be minimized by "remote viewing" via a much expanded and dedicated Internet capability to control and measure outside the more distant facility.

It is realized that the more standard techniques of characterization will provide a baseline for PV characterization in a large number of cases. These include SIMS, TEM, Raman, STM, STS, SAXS etc. All of these methods are developments of the research community and many are used for needed characterization of the PV industry. One needs to provide a balance between the fundamental community and those in the private sector. Below are a few examples of new techniques that have been developed in the last few years and applied to the PV studies. It is not meant to be exhaustive but as a useful view into the need for this area of research. One needs to always try and couple the characterization techniques with the various growers to ensure a constant feedback on the various results.

Examples of New Innovative Techniques

The development of NSOM [1,2] has not only extended optical microscopy beyond the diffraction limit, but has also allowed spectroscopic properties to be measured with submicron resolution. Such resolution is sufficient to provide optical characterization of *extended* defects and grain boundaries in polycrystalline solar cells. The technique works with a proximal probe: a single mode optical fiber drawn to a fine tip and coated with an opaque metal. The resolution is governed by the size of the aperture formed at the apex of the fiber tip, and it can be an order of magnitude less than the diffraction-limited resolution, as illustrated in Fig. 1.

Spatial and Time-Resolved PL and PLE

Near-field and far-field optics can be used simultaneously, allowing localized photoluminescence (PL) or photoluminescence excitation (PLE) experiments to be carried out (using illumination-mode NSOM or collection-mode NSOM). Using the scanning confocal microscopy technique (here, both the exciting and PL light go through a microscope objective that is used in place of the NSOM tip) one can achieve a spatial resolution of 0.5 μm under special circumstances with the sample at 5K. For higher spatial resolution (0.1 μm), the NSOM tip can be used to illuminate the sample, while the far-field lens is used to collect the PL. In this mode, a measure of carrier diffusion to localized traps (e.g., at grain boundaries) may be inferred by examining NSOM images.

By collecting the PL in far-field, submicron measurements of PLE can be obtained giving additional data on alloy composition and band tailing effects. Alternatively, exciting in far field, PL spectra may be recorded with submicron resolution, and both grain interiors and grain boundaries can be locally probed. The PL can be spectrally resolved, for determining alloy composition and identifying impurities, or time-resolved, for identifying areas of rapid recombination. In ternary alloys, the technique can be used to map the variations in exciton emission wavelength due to compositional fluctuations (Fig. II). For the first time, these measurements can focus directly upon the suspect regions, rather than studying the macroscopic spatially averaged properties of polycrystalline films.

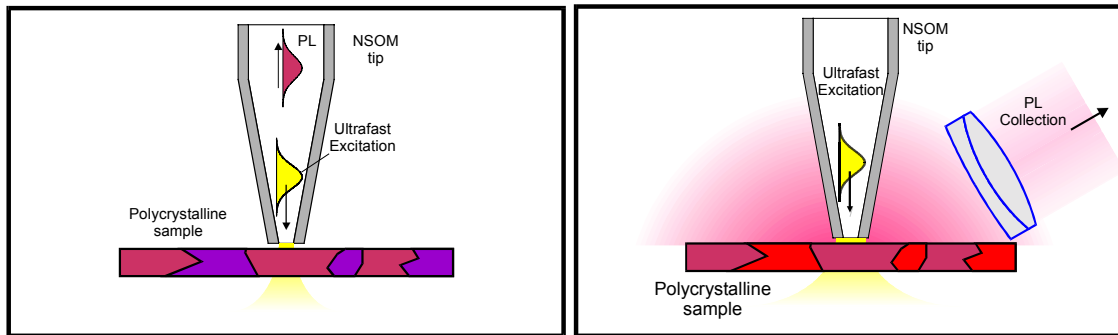


Figure I: (Left) Schematic of the near-field scanning optical microscopy (NSOM) technique showing near-field excitation and collection of light. (Right) Here, the excitation is through the fiber tip whereas the PL is collected by the far-field lens.

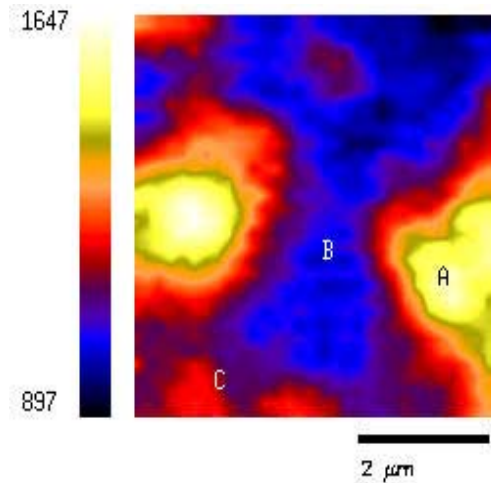


Figure II: Spatially resolved PL of polycrystalline CdTe cell taken at 5K. Points labeled A-C are locations where corresponding spectra showed peak shifts due to variations in sulfur content resulting from interdiffusion and alloying of sulfur with the CdTe (the sulfur diffuses across the heterojunction formed with CdS in a CdTe/CdS solar cell).

A femtosecond laser system is ideal for time-resolved spectroscopy of PV materials. Tunability is achieved through parametric amplification of a visible-light continuum to provide the necessary broadband probe, with a multichannel CCD detector for parallel measurements of a large spectral region around a semiconductor band edge. The system provides femtosecond pulses through most of the visible and near-infrared spectrum. The femtosecond laser can be coupled into the cryogenic NSOM to enable time-resolved studies to be carried out at submicron spatial resolution (see refs. [3-5]).

Spatially-Resolved Photo-Current Using NSOM

The highly localized optical excitation provided by NSOM can be used to obtain high-resolution images of solar cell efficiency by mapping the collected photocurrent, as the probe is scanned [6]. This is the analogue of electron-beam-induced current in the scanning electron microscope, a well-established technique for mapping electrical properties. However, it has the advantage that one can select the excitation wavelength, and so obtain maps for any desired part of the solar spectrum—again, with sufficient resolution to distinguish single defects within grains or single grain boundaries. Alternatively, with the probe stationary over a specific defect, localized photocurrent spectroscopy can be performed by varying the wavelength of the optical excitation to provide the full absorption spectrum of an individual defect or a grain boundary [7]. Again, the combination of spatial and spectral resolution provided by NSOM provides detailed insight into local cell properties. It demonstrates directly which regions of the cell are less efficient, while the spectral capability provides a diagnostic capability for identifying impurities.

Transient Differential Absorption

By combining the ultrafast time resolution of the laser system with the submicron spatial resolution of the NSOM, one can observe carrier populations at individual crystal grains using the transient differential absorption technique. This is a valuable spectroscopic technique that can reveal the occupation of electron states much more directly than does PL. The femtosecond laser system must be specifically chosen for this type of measurement for materials with bandgaps in the 400nm-1.5 μ m range. Here, the white-light continuum is capable of measuring absorption at the entire near-band-edge region simultaneously. This spectral range corresponds to an important energy scale for carrier processes in disordered materials. Of particular interest will be time-resolved vibrational spectroscopic techniques that can probe local vibrational modes associated with the defect centers.

Simple transmission data with submicron spatial resolution is valuable for identifying regions of sulfur diffusion, however, the true potential of this technique is to measure differential absorption. In measuring the *change* in absorption caused by an intense earlier pulse, the spectral population of photoexcited carriers created by that pulse are observed. The dynamics of this population is time-resolved because of the sampling nature of the experiment, and it is limited only by the 150-fs pulsewidth of the laser. Low-spatial resolution measurements of this type in CdS [8] have been performed. If one can introduce a limited white-light continuum into the NSOM tip and then collect this light after transmission through a specially prepared sample, a spatial and energy map of

carrier occupation can be obtained. Since such maps can be obtained at different times in the carrier evolution, information regarding carrier transport in a complex polycrystalline sample can also be obtained.

X-ray Scattering, Fluorescence, and Absorption Methods

Realizing the tremendous financial commitment invested in synchrotron sources over the past two decades by DOE, one should take advantage of this investment. X-rays from synchrotron radiation provide convenient tools for characterizing microstructures, interfaces, impurities, atomic-density profiles, and defects in PV materials. For the purpose of investigating these microscopic short-range structures, the conventional x-ray diffraction method is not useful. Recent progress in short-range probing techniques, such as grazing incidence x-ray scattering (GIXS), angular dependence of x-ray fluorescence (ADXRF), and x-ray absorption fine structures (XAFS) has made it possible to obtain *element-specific* information about various types of PV materials, especially the thin-film junctions that are widely recognized to be extremely important for the development of next-generation PV devices.

The angular dependence of x-ray scattering and fluorescence is especially useful tools for investigating the interface morphology of multilayer materials [9-21]. Measurements of GIXS and ADXRF can afford a *nondestructive* approach to obtain important microstructural information about the *buried* interfaces, such as the layer thickness, interfacial roughness, and correlation lengths of height fluctuations. Through a control of the x-ray probing depth and field distribution by varying the wavelength and incidence angle, the depth profile of a selected atomic species in the layer structure can be obtained. X-ray fluorescence and anomalous scattering also allow an element-specific method to probe the impurity location and intermixing of constituent atoms in the interfacial region. Theoretical analysis of x-ray propagation in layer structures, as well as methods used for obtaining interfacial roughness and correlation lengths can be found in [15] and references cited herein. It should be emphasized that the usual determination of rms roughness is insufficient to characterize a random interface; two rough surfaces with totally different rates of height fluctuations along the surface could have the same value of rms roughness. It must at least be complemented by specifying the correlation lengths in order to properly define an actual rough interface.

XAFS generally refers to extended x-ray absorption fine structure (EXAFS) and near-edge x-ray absorption fine structure (NEXAFS or XANES). These spectra can be used to obtain valuable atomic-scale information on the local structure and chemical states of a specific atomic species in multicomponent materials, such as interatomic distance, coordination number, and local disorder. Detailed descriptions of the XAFS techniques can be found in several review articles [22-23].

Positron Annihilation Spectroscopy

Of greater significance are atomic-sized defects, which degrade the electronic properties of *a*-Si. The dominant type is an amphoteric Si dangling bond, labeled *D* that can trap up to 2 electrons, which determine its charge. In intrinsic *a*-Si:H the uncharged variety prevails. The negatively charged state, D^- -- occupied by 2 electrons -- is most common in *n*-doped *a*-Si:H.

Recently, new results from positron beams have also helped answer fundamental questions regarding amorphous Si. Direct experimental confirmation and theoretical modeling was obtained with positron (antimatter to electron) annihilation spectroscopy (PAS). Positrons are attracted and trapped by negatively charged defects in materials, and eventually annihilate with an electron sitting in or near the trap. With a sophisticated coincidence detection system, the Doppler broadening of the annihilation radiation is used to “*fingerprint*” the chemical element type of atoms next to the defects. In combination with a theoretical model phosphorous was identified for the first time by comparing P-implanted and P-doped samples to samples without phosphorous.

The background of figure III depicts a two-dimensional raw data set from the P implanted sample. The comparison (i.e., ratio) of the data and data of the P-doped sample to the reference samples is shown in the overlay. A broad component due to conduction band electrons was taken out of the spectrum. The phosphorous “*fingerprint*” appears as a line at 1.3 atomic units. This directly correlates with the theoretical model of positron trapping and annihilating at the P decorated dangling bond site *D . The basic atomic structure of a-Si and the positron wave function around a dangling-bond Si in the center where the wave function is enhanced by 10% are shown in figure IV.

Now that the charge-trapping site has been identified, research can focus on the reduction of the P content in solar cells and the number of dangling bond sites. With the positron technique, the P content can be monitored for the first time.

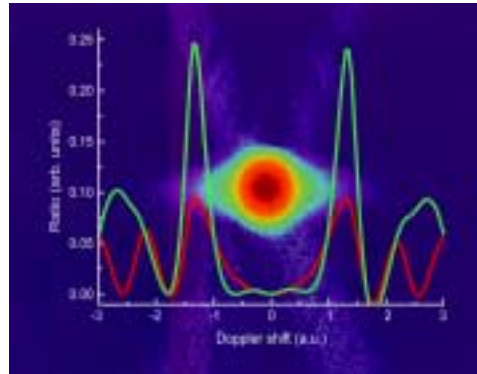


Figure III

Figure III Background: A 2-dimensional positron annihilation spectrum of P-implanted *a*-Si. The two annihilation quanta are registered in coincidence and their difference in energy (Doppler shift) is plotted versus their sum energy. Accumulated counts in each bin are color coded with blue corresponding to 1 and red to 10^5 counts. Foreground: The Doppler broadening information extracted from the raw 2D data in ratio to the Doppler data from a phosphor-free sample. The P-implanted sample data are in green and the P-doped data are in red. The P-“*fingerprint*” appears at 1.3 atomic units. The data are symmetric about 0 momentum. A broad component due to conduction band electrons was subtracted.

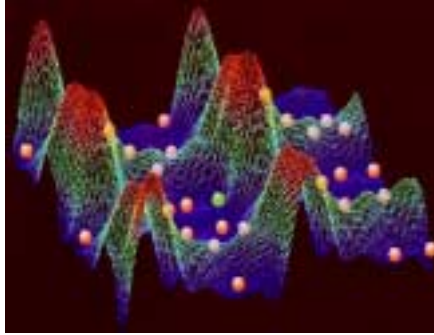


Figure IV

Figure IV: A 3D representation of an atomic model of a -Si (red spheres). Drawn is a section through a $4 \times 4 \times 2$ super cell where a Si atom with a dangling bond is located in the center (in green). Drawn round the atoms is the positron wave function (high probability in dark red). The most likely place for the positron is near the dangling bond Si.

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