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Positron re-emission microscopy of perfect and O^+-implanted SiC

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Abstract. Positron re-emission microscopy in reflection geometry has been used to obtain images of 6H-SiC implanted with 50 keV O^+ ions (at 1×10^{13} cm^{-2}) through a micromesh mask. Positrons were re-emitted from areas exposed to the implantation at an average intensity 85(5)% of that characteristic of unimplanted regions, as a result of trapping by the vacancy-type defects created below the surface of the SiC. This result is consistent with a model which assumes that the positrons are thermalized prior to re-emission, a model which is also supported by microscope performance simulations. By comparison with vacancy creation simulation by the code TRIM the microscope contrast also provides evidence that post-implantation vacancy migration and coalescence leads to a reduction of almost 95% in open-volume defect concentration in the subsurface region.

1. Introduction

Positron re-emission microscopy provides a very sensitive way of imaging near-surface vacancy-type defects in materials that re-emit positrons [1, 2]. In this study images have been recorded of an SiC surface implanted with 50 keV O^+ ions through a mask consisting of a nickel micromesh (10 μm bars spaced at 50 μm). SiC was chosen for two reasons: (a) it is known to re-emit low-energy positrons with high efficiency without the need for surface cleaning or annealing [3], and (b) there has been some discussion as to whether the positrons re-emitted from SiC are truly thermalized and ejected by the negative work function of the surface, or whether the high band-gap of $\sim$3 eV prevents significant thermalization of positrons whilst allowing copious re-emission of positrons at epithermal energies. Positron microscopy offers a new look at the question of re-emission from SiC because epithermal positrons are not expected to form good quality images; additionally, the contrast seen between implanted and unimplanted regions can be compared with that predicted by simulations of thermal positron trapping at vacancy-type defects.

2. Experimental system

The positron microscope at the University of East Anglia is based on reflection geometry, not unlike the prototype constructed at the University of Michigan [4]. This geometry allows thick samples to be studied. The microscope is described in detail in [5] and [6]; in summary, positrons from a 1.5 GBq ^{22}Na source are moderated and focused by a two-stage brightness-enhancement unit so that the majority of those reaching the sample fall within an ellipse 70 μm by 180 μm. In this experiment the positrons hit the sample with an energy of 1.1 keV. An immersion-type objective lens then forms an image on a position-sensitive detector array that is coupled to a PC framestore. This single-lens system gives a fixed magnification of $\times 80$. The system is designed so that when feasible a projector lens can be added allowing magnification of between $\times 800$ and $\times 2000$.

Significant changes have been made to the microscope since [6]. An enclosure fabricated from double-skin mumetal, which excludes magnetic fields, was added to reduce image blurring due to field changes; this is the main limit on resolution. To augment this shielding active damping of the fields outside the enclosure via three large Helmholtz coils is planned. The design of the immersion objective lens has been slightly changed after simulations suggested a design capable of better resolution; at present the best resolution achievable is less than 4 μm FWHM. Other minor practical improvements have improved flux at the sample to over 2000 e^+ s^{-1} and briefly, directly after heating remoderator and sample surfaces, to $\sim$6000 e^+ s^{-1}.

The 6H-SiC sample was implanted with 50 keV O^+ ions at a dose of 1×10^{13} ions cm^{-2} at the University of Surrey Ion Beam Centre.

3. Theoretical considerations

In order to calculate the relative intensities of re-emitted positrons for defected and virgin material to compare with experimentally determined values we first assume that implanted positrons are thermalized inside SiC. The fraction F_S of positrons implanted with energy E which diffuse back to the surface is given [7] by

$$F_S = \int_0^\infty P(E, z) \exp(-z/L)\, \mathrm{d}z \tag{1}$$

where $P(E, z)$ is the positron implantation profile, assumed here to be the Gaussian derivative $(2z/z_0^2)\exp[-(z/z_0^2)]$ with $z_0 = AE^n/\rho$ [8, 9]. We shall use $A = 4.0$ μg cm^{-2}, $n = 1.61$ and $\rho = 3.217$ g cm^{-3}. L is the effective positron diffusion length; for virgin SiC, $L = L_0 = 70$ nm [3]; in general $L = L_0[\lambda/(\lambda + \nu C)]^{1/2}$ [7], where λ is the positron annihilation rate in undefected SiC $= 7.14 \times 10^9$ s^{-1} [10], ν is the specific rate for positron trapping by vacancies, taken as 3×10^{14} s^{-1} [10], and C is the concentration of vacancy-type defects per atom. The ratio F_d/F_v of F_S values for defected and undefected (virgin) SiC, derived from (1) for incident positron energy $E = 1.1$ keV, is plotted against C in figure 1.

An estimate of C for the sample studied may be found using the Monte Carlo simulation code TRIM [11], which gives the depth distribution of vacancy concentration per implanted ion (prior to any defect migration or combination). Comparing this distribution to the positron implantation profile $P(E, z)$ an estimate is obtained of the mean defect concentration in the region in which the distributions overlap. Results for 50 keV O^+ ions and 1.1 keV positrons (for 10^{13} ions cm^{-2} and a SiC atomic number density of 9.6×10^{22} cm^{-3}) are shown in figure 2. In this example the average C is calculated to be 2.3×10^{-3} per atom immediately after implantation.

4. Results

The image of the implanted SiC sample shown in figure 3 was taken (after removal of the micromesh mask) over a period of three days. The incident positron energy was 1.1 keV. The collection rate of 0.59 h^{-1} per pixel indicates efficient positron re-emission from the SiC, in contrast to epithermal emitters such as Si, which typically give signal rates an order of magnitude lower than this.

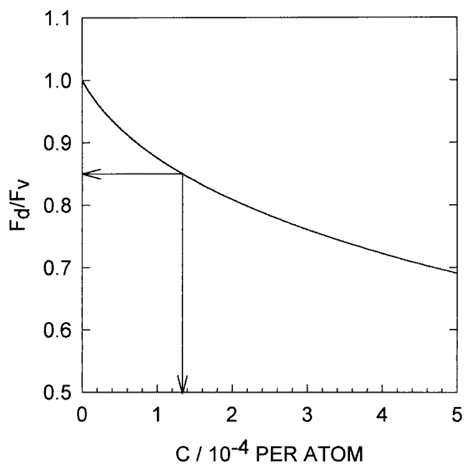

Figure 1. The ratio of the fractions of positrons re-emitted from defected and undefected SiC as a function of defect concentration. The horizontal arrow indicates the mean ratio observed experimentally.

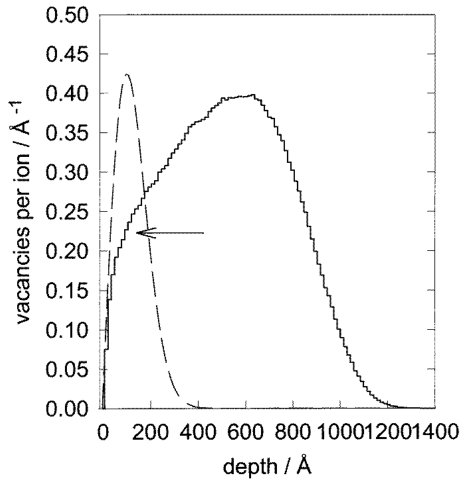

Figure 2. Solid line: vacancy concentration depth profile calculated by TRIM for implantation of 50 keV O^+ ions into SiC. Broken line: implantation profile of 1.1 keV positrons in SiC (see text). The arrow indicates the mean vacancy concentration in the region of positron implantation.

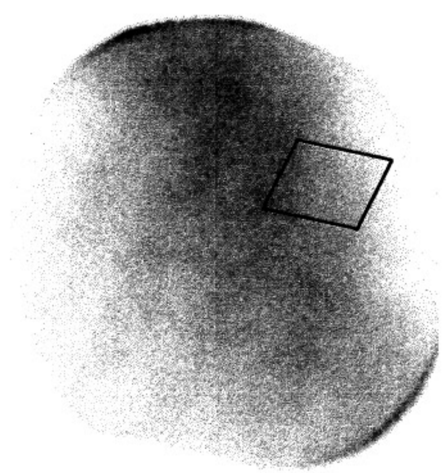

Figure 3. Raw positron microscope image of SiC implanted with 50 keV O^+ ions through a Ni micromesh (lines 10 μm, spacing 40 μm). Incident positron energy 1.1 keV; resolution $\sim$10 μm. Darker grey corresponds to higher re-emitted intensity. Direct visual discrimination is hampered by the 15% mean intensity variation between regions protected by the micromesh and those implanted with O^+ ions; one square of the mesh pattern is drawn on the image to aid the eye.

Denser lines can clearly be seen in the image, corresponding to the areas shielded behind the mask. They are somewhat clearer in one axis than the other, which is a characteristic of most of the images from the microscope and is due to its geometry.

The sharpness of the image is a good indication that the positrons seen are predominantly emitted in a small forward cone by the negative work function of SiC (~ -2 eV [3, 12, 13]). The particle optics simulation code Simion demonstrates that epithermal positrons cannot be sharply imaged with this system at present. For example, epithermal positrons with a $\sim$2 eV energy spread leaving the centre of the viewed area of the sample in a cone of 45° half-angle have a point spread function whose FWHM is approximately 25 that of thermalized positrons ejected in a 10° half-angle cone by the negative work function of SiC. The resulting 100 μm smearing associated with epithermal positron 'images' would make them uninterpretable in the present system.

Examining the image of the SiC sample by taking average intensities over several small areas inside and outside the damaged areas and taking the average of each, the emission ratio was found to be $85 \pm 5\%$. By reference to figure 1 one sees that this ratio corresponds to a defect concentration C of 1.35×10^{-4} per atom, which is only 6% of the value suggested by TRIM (figure 2). This suggests that almost 95% of vacancies produced below the surface during implantation of the O^+ ions migrate to sinks or coalesce into divacancies.

5. Conclusions

The data collection rate and sharpness of the image of the undefected regions of the SiC sample in this experiment provide evidence that positron re-emission from SiC is via thermalization and subsequent work-function ejection. This conclusion is substantiated by the observation of trapping by vacancy-type defects created below the surface of the sample by ion implantation with a probability in line with that expected of thermalized positrons. Comparison with TRIM calculations suggests that almost 95% of vacancies formed by the implanted ions recombine, migrate to sinks or coalesce into larger open-volume defects (likely to be predominantly divacancies).

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