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Defect profiling in elemental and multilayer systems:
correlations of fitted defect concentrations with positron implantation profiles

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Abstract

The results of several positron annihilation (Doppler broadening) experiments have been analyzed using the BNL Monte Carlo implantation profiles and the program VEPFIT. The program VEPFIT has been modified so that scaled, parameterized multilayer profiles can also be used as the initial condition for the diffusion equation solution. We have looked at both elemental (e.g. amorphous silicon) and multilayer (e.g. Pd/Si) systems. Strong correlations between the input implantation profile parameters and the fitted values obtained for the diffusion lengths and overlayer thicknesses for the multilayer systems have been found. The effect of uncertainties in the mean depth on the value of the diffusion length and hence the defect concentrations will be discussed. The impact of reimplanting backscattered positrons on both the implantation profiles and the fitted diffusion lengths will also be presented.

Introduction

The analysis of positron (e^+) annihilation (Doppler broadening) experiments is carried out in two separate steps [1,2]. The first step is the modeling of positron implantation, i.e. the generation of a stopping or implantation profile. This involves the simulation of the energy-loss processes (electron, phonon-assisted) by which a positron (of initial energy 1-50 keV) loses its kinetic energy and comes into thermal equilibrium with the host sample. Positron implantation or thermalization takes a few picoseconds. These thermalized positrons then diffuse in the material until they annihilate in the perfect lattice, at a defect site or return to the surface. The positron lifetime depends on the annihilation site, and is typically a few hundred picoseconds. This is the second step in the analysis procedure, modeling the evolution of the time-averaged positron density. This is accomplished by solving a diffusion-annihilation equation with appropriate boundary conditions and the implantation profile as the source term. Several different Monte Carlo methods have been developed to study positron implantation [2,3 and references therein]. Positron diffusion-annihilation has been modelled in the programs VEPFIT [4] and POSTRAP [5].

For the present analysis the positron implantation profiles were generated using the BNL Monte Carlo code [2,3]. These profiles were scaled with the mean depth [2,10] and fitted to a functional form

$$P(u) = \left[A_{lm} \left(\frac{u}{C_{lm}} \right)^l + B_{lm} \right] \exp \left[- \left(\frac{u}{C_{lm}} \right)^m \right] \quad (1)$$

where $P(u) \equiv \langle z(E) \rangle p(z)$; $p(z)dz$ is the probability of the positron thermalization between z and $z + dz$; u is the depth z scaled by the mean depth $\langle z(E) \rangle$ for a positron of incident energy E . Here $l, m, A_{lm}, B_{lm}, C_{lm}$ are all fitting parameters, and the mean depth

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The coupling of the input implantation profile parameters with the fitted diffusion length was explored for a bulk Si system, as well as for Pd overlayers on Si. The connection between the interface boundary condition and the interpretation of the fitting results is also discussed.

Amorphous Si Results

The dependence of the S-parameter on incident positron energy for a sample of Si, before and after annealing, is shown in Fig 1. The solid lines represent the theoretical fit. S-parameter measurements were made before and after annealing to study defect recovery and defect evolution during processing [7]. The S-parameter data were fitted using the program VEPFIT with three different implantation profiles as input. The first profile was a Makhovian [$\ell=m-1$, $B_{\ell m}=0$ in Eq. (1)] with $m=2$, $A=3.264$, and $n=1.56$. These values of A and n were obtained by fitting the energy dependence of the Monte Carlo mean implantation depth. The second was the Monte Carlo profile [$\ell \neq m-1$, $B_{\ell m}=0$ in Eq. (1)] generated by the BNL Monte Carlo without reimplanting the backscattered positrons. The third was the BNL profile with all positrons reimplanted into the sample. The last two profiles were scaled and parameterized, and the fitting parameters are listed in Table 1. Profiles 2 and 3 are illustrated in Fig 2. The values of the diffusion length required to model the S-parameter data using the different implantation profiles are listed in Table 2. The values utilized for D^+ , v_t , τ_f were $2.9 \text{ cm}^2 \text{ sec}^{-1}$, $3 \times 10^{14} \text{ sec}^{-1}$ and 217 psec, respectively (see [8], pg. 36, and references therein).

The essential difference between the results obtained with profiles 1 and 2 is due to the shape of the profiles; the BNL profile, even without reimplanting backscattered positrons has a non-zero positron density near the surface, in contrast to the Makhovian profile. This results in a slightly lower value for the diffusion length when using the BNL profile. Implantation profile 3, with reimplanted positrons, has an even larger pile-up of positrons near the surface, resulting in an even smaller (by about 20%) value for the diffusion length. In most experiments it is not easy to determine if some fraction of the backscattered positrons is being reimplanted into the sample; so the two BNL implantation profiles model the two limiting cases. Since the defect concentration depends on the square of the diffusion length, this results in a 40% uncertainty in the defect concentration.

The increase in the diffusion length after annealing corresponds to a decrease in the defect concentration. The reduction in the value of the S-parameter for bulk Si denotes a reduction in the size of the open-volume defects generated in the Si.

The coupling of the fitted Si diffusion length (before annealing) with the assumed mean depth parameters was studied using VEPFIT with Makhovian profiles as input. The value of the shape parameter m was kept fixed at 2. For fixed values of A , n was varied from 1.0 to 2.0, and the value of χ^2 was plotted as a function of n (see Fig. 3(a)). There is a well-defined minimum in χ^2 as a function of n , which is what one would expect. Next, the value of n was kept fixed at the value corresponding to the minimum in χ^2 , and the variation in χ^2 with A was studied. This result is plotted in Fig. 3(b). Except for very small values of A , χ^2 was found to be virtually independent of the value of A . The value of the diffusion length required to fit the S-parameter data was found to be directly proportional to the assumed value of A , showing that a larger fitted value of the diffusion length was required to compensate for the deeper implantation of positrons prior to diffusion. These results lead to the conclusion that the S-parameter data can be used to extract information about diffusion lengths and defect concentrations only if the

Conclusion

Given a set of S-parameter data, a wide range of mathematical fits (of the same order of goodness) can be found. These fits are dependent on the parameters characterizing the implantation profiles, on the diffusion lengths, as well as on the interface or surface boundary conditions; and some of these parameters are strongly correlated. Consequently, incorrect profiles and/or interface boundary conditions can lead to erroneous physical interpretation. Thus reliable implantation profiles and a measured value of the overlayer thickness (in the case of bilayers like Pd/Si) are essential to obtain accurate measures of e^+ diffusion lengths and defect concentrations. Uncertainties in the degree to which the experimental conditions permit e^+ to be re-implanted result in errors in defect concentration of ~40% in single-element samples.

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REFERENCES

- [1] P. J. Schultz and K. G. Lynn, *Rev. Mod. Phys.* 60 (1988) 701.
- [2] V. J. Ghosh, K. G. Lynn, and D. O. Welch, in: 9th Positron Spectroscopy in Solids, *Proc. of the International School of Physics Enrico Fermi, Course CXXV*, July 1993, in press.
- [3] V. J. Ghosh and G. C. Aers, unpublished.
- [4] A van Veen, H. Schut, J. de Vries, R. A. Hakvoort, and M. J. Ijpma, in: *Positron Beams for Solids and Surfaces*, Eds. P. J. Schultz, G. Massoumi, and P. J. Simpson, (AIP, New York 1990) p. 162.
- [5] G. C. Aers., in: *Positron Beams for Solids and Surfaces*, Eds. P. J. Schultz, G. Massoumi, and P. J. Simpson, (AIP, New York 1990) p. 162.
- [6] G. C. Aers, SLOPOS 6.
- [7] Bent Nielsen, V. J. Ghosh, O. W. Holland, T. C. Leung, and K. G. Lynn , to be published.
- [8] R. Hakvoort, Applications of positron depth profiling, Ph.D. Thesis, Interfacultair Reactor Institut, Technische Universiteit Delft, December 1993.
- [9] G. J. van der Kolk, L. J. van Ijzendoorn, Bent Nielsen, V. J. Ghosh, and K. G. Lynn, to be published.
- [10] V. J. Ghosh, D. O. Welch, and K. G. Lynn, in: *Proc. 5th International Workshop on Slow Positron Beam Techniques for Solids and Surfaces*, Jackson Hole, WY, Aug. 1992, Ed. E. H. Ottewite, in press.
- [11] G. C. Aers, *Appl. Phys. Lett.* 64 (1994) 661.
- [12] G. C. Aers, *J. Appl. Phys.*, in press.

Table 2. Diffusion lengths and defect concentrations in amorphous Si obtained by fitting the experimental data using three different implantation profiles.

unannealed		S_s	S_{Si}	$L_{Si}(\text{\AA})$	C_t
	Profile				
I	Makhovian with $m=2$, $A=3.264$, $n=1.56$	0.938	1.04	57.28	2.95×10^{-2}
II	BNL profile without reimplanted positrons	0.934	1.04	55.37	3.15×10^{-2}
III	BNL profile with reimplanted positrons	0.934	1.04	45.79	4.61×10^{-2}
annealed at $T = 450^\circ\text{C}$		S_s	S_{Si}	$L_{Si}(\text{\AA})$	C_t
	Profile				
I	Makhovian with $m=2$, $A=3.264$, $n=1.56$	0.924	1.026	96.4	1.04×10^{-2}
II	BNL profile without reimplanted positrons	0.922	1.028	93.93	1.10×10^{-2}
III	BNL profile with reimplanted positrons	0.922	1.028	80.14	1.51×10^{-2}

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