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1991 J. Phys.: Condens. Matter 3 3205

(http://iopscience.iop.org/0953-8984/3/18/015)

J. Phys.: Condens. Matter 3 (1991) 3205–3209. Printed in the UK

LETTER TO THE EDITOR

The determination of interface characteristics for SiO_2 on Si with slow positrons

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Received 7 March 1991

Abstract. A low-energy positron beam apparatus has been employed to study a device-quality silicon dioxide layer grown on silicon (100). The Doppler broadening of the annihilation photons, related to positron energies, showed features corresponding to annihilations at the surface, oxide layer, interface and Si substrate. Analysis of the data using the diffusion model resulted in a measurement of the oxide depth, the electric field in the Si and hence the charge at the interface.

The development of monochromatic low-energy positron beams (Schultz and Lynn 1988) has enabled the use of positrons to probe defects at or near the surface of a solid. Essentially, energetic positrons from a radioactive source or a LINAC are slowed down to a few eV by a moderator and are then transported as a beam to a target. By varying their energy, it is possible to control the depth to which positrons will penetrate the material, with the stopping depth distribution being given by the Makhovian profile

$$P(z, E) = (\mathrm{d}/\mathrm{d}z) \exp(-z^2/z_0^2).$$

Here $z_0 = \alpha E^{1.6}/\rho$, with $\alpha = 4.5\ \mu\mathrm{g\ cm^{-2}}$ and ρ, the material density, in $\mathrm{g\ cm^{-3}}$ (Vehanen *et al* 1985). The final distribution of thermal positrons (n) is then given by solutions of the time-dependent positron diffusion equation

$$(\mathrm{d}^2/\mathrm{d}z^2)n(z) - v_\mathrm{d}(\mathrm{d}/\mathrm{d}z)n(z) - (\lambda/D+)n(z) + P = 0$$

where $D+$ is the diffusion coefficient, λ is the annihilation rate and $v_\mathrm{d} = \mu_+\mathscr{E}$ is the positron drift velocity (μ_+ is the positron mobility and $\mathscr{E}$ is the electric field strength) (Van-veen *et al* 1990). Experiments with such beams have been able to provide information on the depth distributions of vacancy-type defects in ion-sputtered metals (Bentzon *et al* 1987) and ion-implanted metals (Britton *et al* 1988, Smith *et al* 1990) and the depth profiles of multilayer structures (Vehanen *et al* 1987).

The SiO_2–Si interface is a highly important technological structure and has been the subject of extensive study (Sze 1985). Two recent studies of this structure with low-energy positron beams (Nielsen *et al* 1989, Baker and Coleman 1989) have shown it is possible to obtain the depth of the oxide layer and some information on the nature of interfacial defects. However, no account was taken of internal electric fields in their analyses. Often the SiO_2–Si interface will have some trapped charge that will be due to its structure and chemical composition. The resulting potential at the interface is given by

$$V_i = Q_i/C_{ox} = Q_i/\varepsilon_o\varepsilon_{ox}x$$

where Q_i is the net charge at the interface, C_{ox} is the capacitance of the oxide layer, x is the layer thickness and ε_{ox} is the relative permittivity of the oxide (=3.9). In a carefully grown SiO_2 layer Q_i/q (q is the charge of an electron) will often be as low as $10^{10}\,cm^{-2}$ for (100) oriented Si (Sze 1985). Although the charge density is low, it will induce an electric field distribution in the semiconductor near the interface which will affect the motion of positrons. The field in this depletion region at $z' = z - x$ is defined by

$$\mathscr{E}(z') = dV/dz = (W - z')qN_d/\varepsilon_o\varepsilon_{si}$$

where N_d is the donor concentration, ε_{si} is the relative permittivity for silicon (=11.9) and W is the width of the depletion region. The effect of electric fields on the motion in Si has recently been the subject of a study by Makinen *et al* 1990); they were able to demonstrate that a field of the order of $10^4\,V\,cm^{-1}$ would give rise to a positron drift length of 2–3 μm and, by solving the positron diffusion equation, obtained a positron mobility of $120 \pm 10\,cm^2\,V^{-1}\,s^{-1}$ at 300 K.

The purpose of the work described here was to use a low-energy positron beam to provide an accurate depth profile of a thin oxide layer grown on silicon and to determine the electric field in the semiconductor and hence the charge at the interface.

The sample under investigation was cut from a Wacker (100) n-type silicon (P-diffusion doped with a carrier concentration of $8 \times 10^{14}\,cm^{-3}$) 5 cm wafer with a device-quality thermally grown oxide layer of nominal thickness 1000 Å.

Experiments were performed on the *Xenophon* low-energy positron beam at Royal Holloway (Britton *et al* 1985). The incident energy of the positrons was controlled in the range 0–12 keV by electrodes defining a lens with the target at a negative bias. Photons arising from positrons annihilating in the sample were recorded using a germanium detector placed immediately behind the target. The lineshape parameter S would then be calculated for each spectrum, with S being defined as the ratio of the contents of the central region of the 511 keV photopeak to the total contents of the peak.

Figure 1 shows the lineshape parameter plotted as a function of positron energy, with features relating to annihilations at the SiO_2 surface ($E \sim 250$ eV), the oxide layer ($E \sim$ keV), the SiO_2/Si interface ($E \sim 3$ keV) and in the bulk Si ($E \sim 12$ keV).

In figure 1 the lineshape parameter at a given energy will consist of contributions from annihilations at each state, such that

$$S(E) = J_sS_s + J_oS_o + J_iS_i + J_bS_b$$

where S_s, S_o, S_i and S_b are the lineshape parameters corresponding to 100% annihilations in the surface, oxide, interface and the bulk of the sample, respectively. J_s, J_o, J_i and J_b are the probabilities of annihilating at each state and are derived from solutions of the time-independent positron diffusion equation above.

The general solution including electric field effects is (Van-Veen *et al* 1990)

$$n = A\exp(\gamma^- z) + B\exp(\gamma^+ z) + P\lambda/D^+$$

with

$$\gamma^\pm = -[v_d \pm (v_d^2 + 4\lambda/D^+)^{1/2}]/2.$$

In the silicon dioxide μ_+ and D^+ are not known, hence for the epilayer we have used a field-free solution

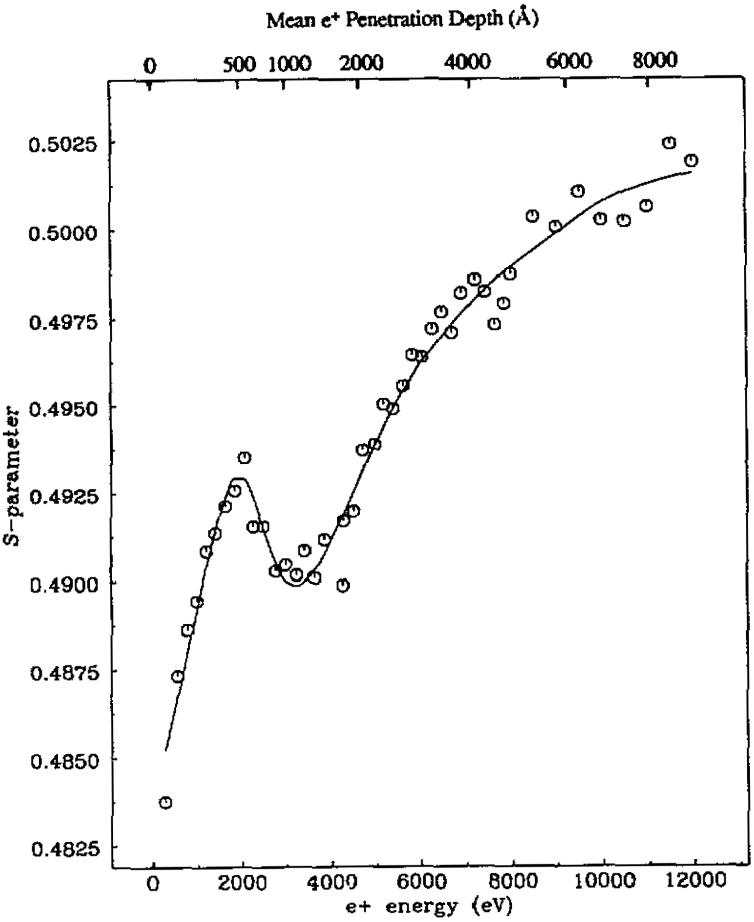

Figure 1. The S parameter data plotted as a function of incident positron energy for silicon with a thermally grown SiO_2 overlayer. The full curve is the fit of a model accounting for positron states at the surface, oxide and interface and in bulk Si. The oxide layer depth was found to be 1125 ± 20 Å. The mean penetration depth was calculated using $z = 400\,E^{1.6}/\rho$.

$$n = A\exp(-z/L_\mathrm{o}) + B\exp(+z/L_\mathrm{o}) + P/L_\mathrm{o}^2$$

where L_o is an effective diffusion length in the oxide. Assuming that all positrons arriving at the surface or interface will become trapped, the fractions J_s, J_o, J_i and J_b will be given by

$$J_\mathrm{s} = (1-\beta)\int_0^x P(z,E)\exp(-z/L_\mathrm{o})$$

$$J_\mathrm{o} = \int_0^x P(z,E) - (1-\beta)\int_0^x P(z,E)\exp(-z/L_\mathrm{o}) - \beta\int_0^x P(z,E)\exp(z/L_\mathrm{o})$$

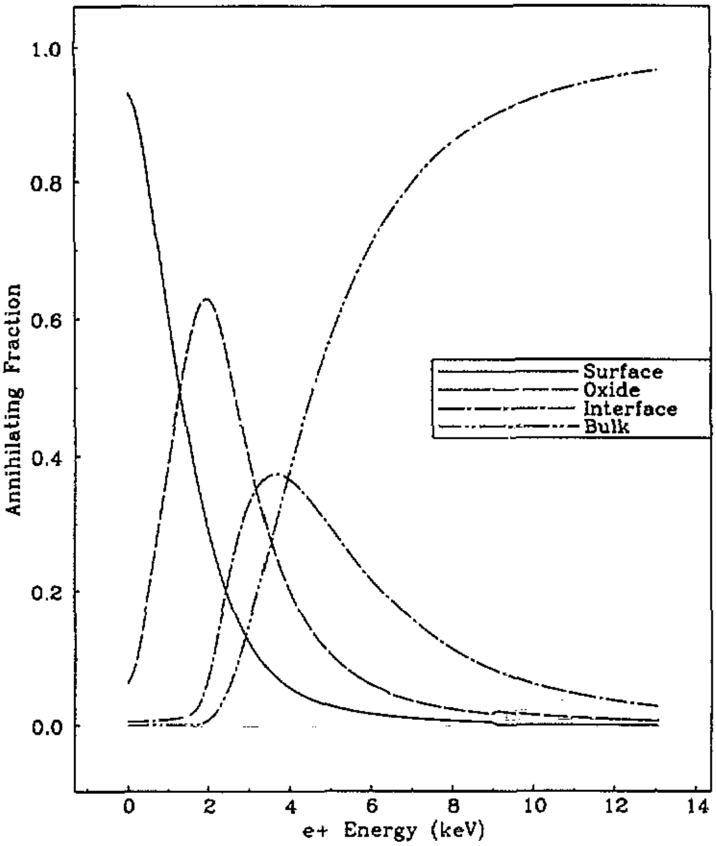

Figure 2. The calculated fractions of positrons annihilating at the surface, oxide, interface and Si substrate plotted against positron energy.

$$J_i = \beta \int_0^x P(z, E) \exp(z/L_o) + \int_x^\infty P(z, E) \exp(\gamma^-(z - x))\,\mathrm{d}z$$

$$J_b = \int_x^\infty P(z, E)(1 - \exp(\gamma^-(z - x)))$$

with parameter β defined as

$$\beta = [1 - \exp(-x/L_o)]/[\exp(x/L_o) - \exp(-x/L_o)].$$

Since the electric field is not constant, it was necessary to split the region between x and $x + W$ into a series of layers with a field strength $\mathscr{E}(z')$ and to calculate the fraction of positrons diffusing through and annihilating in each layer.

An initial fit of the model to the data ignoring the electric fields, i.e. with no positron-drift terms, produced an oxide layer depth of 990 ± 30 Å, which is in good agreement with the nominal value. The diffusion lengths in the oxide and the bulk silicon were found to be 380 ± 60 Å and 1030 ± 50 Å respectively, with $S_s = 0.4833$, $S_o = 0.4994$,

$S_i = 0.4765$ and $S_b = 0.5023$. The fractions of positrons annihilating at each state as a function of positron energy are shown in figure 2. We note that in this case the resulting diffusion length in the silicon is much shorter than the expected value of 2150 Å measured by Schultz *et al* (1988) in the absence of internal fields. Our observation agrees well with that of Nielsen *et al* (1989) from their study of SiO_2 on Si.

The fitting procedure was repeated allowing for electric fields and, hence, including the positron-drift terms, this yielded a layer depth of 1125 ± 20 Å, again in good agreement with the nominal value but slightly higher than the previous result. The width of the depletion region (W) was found to be 1650 ± 40 Å. This gave a value for the density of interface charges Q_i/q of $0.32 \times 10^{10}\,\mathrm{cm}^{-2}$ (±5.4%).

In conclusion, by applying the positron-diffusion model to low-energy positron beam results for a sample of Si with an overlayer of SiO_2 we have been able to determine the interface depth, the width of the depletion region and the charge at the interface.

The difference in the result for the layer depth (990 ± 30 Å excluding electric fields and 1125 ± 20 Å including fields) highlights the importance of accounting for electric fields in the analysis of positron-beam measurements in semiconductors. Where no electric field is included, it is assumed that the positron drift is constant throughout the Si. Thus, the fraction diffusing to the interface will depend on a single diffusion length. This is clearly incorrect, since the field and hence the positron drift will vary with depth. It was possible to include drift terms in the case studied here since there is an abrupt interface and the electric field is clearly defined. However, in ion-implanted samples the analysis may well be more difficult due to the non-uniform nature of the regions.

Acknowledgement

We wish to thank Professor A K Jonscher for useful discussions and the Science and Engineering Research Council for funding.

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