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The study of sub-surface and interface characteristics of semiconductor heterostructures by slow positron implantation spectroscopy

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Abstract. Experiments are described in which the controlled implantation of mono-energetic positrons is used to gain information non-destructively on epilayer and interface defects in semiconductor heterostructures. The implantation, and hence annihilation, profile is changed by varying the incident positron energy from 1 to 35 keV. Characteristics of the positron state at the annihilation site are reflected in the width of the measure Doppler-broadened annihilation line. The fractions of positrons annihilating from each state are deduced by solving the steady-state diffusion equation. The application of the technique is illustrated by application to a series of SiO_2–Si samples.

1. Introduction

The last decade has seen spectacular advances in semiconductor technology, especially in the construction of heterostructures whose composition is controlled to produce devices with specific physical or electrical properties for a vast range of applications. The successful exploitation of these layered structures depends strongly on an understanding of the fundamental characteristics of the layers and the interfaces between them. During the past few years the potential of the slow positron beam in this area has been demonstrated [1–4]; the positron is especially sensitive to open-volume defects and its mobility is affected by electric fields due to active impurities which may be trapped at an interface. The measured annihilation parameter, discussed below, depends sensitively on the presence of both defects and impurities. An excellent recent review of slow positron spectroscopies of condensed matter is that of Schultz and Lynn [5].

The propensity of positrons implanted and thermalised in materials for trapping at open-volume defects is well known [6]. The exploitation of slow positron beams in the study of sub-surface defect phenomena is a natural extension of traditional bulk studies employing β decay positrons. Indeed, the first demonstration of the sensitivity of positrons implanted into a sample with mean energy of a few keV to the presence of thermally generated vacancies near the surface [7] came only a year after the first true positron surface experiments were performed at Bell Laboratories [8].

There are two experimental techniques employed in near-surface positron studies. Firstly, the fraction of implanted positrons diffusing back to the sample surface is determined by measuring the number of ortho-positronium (o-Ps) atoms formed there and ejected into the vacuum to decay via 3γ emission. In the second technique the mean

shape parameter S, related to the width of the Doppler-broadened annihilation line, is measured as a function of positron implantation energy, again with a Ge detector. The magnitude of S depends essentially on the electron momentum density at the annihilation sites. For example, if a significant fraction of the positrons is trapped in vacancies then the absence of core electrons reduces the mean electron momentum and the S-parameter increases. The Ps fraction technique, although highly sensitive to surface conditions, has been successfully applied to the determination of open-volume defect distributions within ≈ 10 nm of the surface of homogeneous systems [9]. However, for defect profiling in the 10^2–10^3 nm depth range, particularly in layered systems, the S parameter technique is favoured, and is therefore chosen for the measurements discussed below.

For a multilayered system the measured S parameter may be written as

$$S = \sum F_j S_j \tag{1}$$

where F_j are the fractions of positrons annihilating from each state j (i.e. at the surface, within layers and at interfaces). Significant contributions from surface and interface states clearly require diffusion to and trapping at them. The surface contribution $F_s S_s$ is better defined here if those positrons which reach the surface are trapped and are annihilated there (rather than be ejected into the vacuum as free positrons or Ps); hence the surface does not require thorough surface cleaning and preparation, and strict ultrahigh-vacuum conditions need not be maintained.

Vehanen *et al* [10] performed the first multilayer S parameter measurements on an Al_2O_3–ZnS–Al_2O_3–glass structure, in which positron diffusion lengths were very small. They demonstrated that the positions of interfaces at depths up to $\sim 10^3$ nm could be well determined by the method, which also enabled them to test the approximate validity of the simple implantation profile.

$$P(x) = [2x/(x_0^2)] \exp[-(x/x_0)^2] \tag{2}$$

with $x_0 = 1.13\bar{x}$; the mean implantation depth $\bar{x} \approx (40/\rho)E^{1.6}$ nm (E = positron implantation energy in keV).

Pioneering work in the area of layered semiconductor structures has been performed by Schultz *et al* [2], who demonstrated the sensitivity of the positron technique to the presence of defects and electric fields associated with impurities at the Si–Si(100) interface.

2. Experimental method

The experiments described below were performed on the University of East Anglia magnetic-transport positron beam system, details of which may be found elsewhere [11, 12]. Beams of $\sim 5 \times 10^4$ positrons s^{-1} and 8 mm diameter are delivered to the target in vacua lower than 10^{-6} Pa, at mean energies between 1 and 20 keV and with a spread of approximately 1.5 eV. The samples are mounted on a post with (x, y, z, θ) movement; the beam position is checked before each measurement by viewing the sample/sample holder shadow on a microchannel plate-phosphor screen assembly at the end of the beam line. Annihilation photons from the target are recorded by a Ge detector, whose output pulses are amplified and stored by a multichannel-analyser system. Typically, one million photopeak counts are accumulated in runs at each incident positron energy.

The S parameter of the Doppler-broadened annihilation line is defined as the ratio of the total number of counts in a chosen central region of the photo-peak to the total peak counts. The integration limits are chosen so that $S \sim 0.5$.

3. Data analysis

The fraction F_j in equation (1) are determined by solving the steady-state diffusion equation for the distribution of positrons in a sample, $p(x)$ [13]. In the absence of internal electric fields this may be written

$$D_+ \, \mathrm{d}^2 p(x)/\mathrm{d}x^2 - [\lambda + n(x)\nu]p(x) + P(x) = 0 \tag{3}$$

where D_+ is the positron diffusion constant, λ is the bulk annihilation rate, ν is the specific trapping rate and $n(x)$ is the atomic concentration of defects. $P(x)$ is the positron implantation profile, describing the initial distribution of positrons at thermalisation.

The fraction of implanted positrons diffusing to and annihilating at a sample surface is

$$F_s = D_+(\mathrm{d}p(x)/\mathrm{d}x)|_{x=0}. \tag{4}$$

For a semi-infinite medium with a constant density of defects (n) a Green function approach maybe used to solve equation (3) to yield

$$F^s = \int_0^\infty P(x) \exp(-x/L) \, \mathrm{d}x \tag{5}$$

where the characteristic positron diffusion length L is given by

$$L = [D_+/(\lambda + n\nu)]^{1/2}. \tag{6}$$

4. Results for SiO_2–Si

The SiO_2–Si system provides a relatively simple structure in which to investigate the sensitivity of implanted positrons to different sub-surface environments. It is assumed that the diffusion length for positrons in the oxide layer is very small, so that diffusion through the epilayer to the exit surface and to the interface is negligible. It is consequently possible to make a direct measurement of S for the oxide. Positrons are able to diffuse to the interface from the substrate, but at high incident energies the measured S tends to the bulk Si value.

Nielsen *et al* [1] and Uedono *et al* [3] have studied the SiO_2–Si interface. Their respective results are markedly different, even given the different oxide thicknesses; this is undoubtedly due to dissimilar sample qualities. Nielsen *et al* observed a pronounced decrease in S in the vicinity of the energy equivalent to a mean implantation depth $\bar{x} \approx d$, the interface depth. They interpreted their result as evidence that positrons are diffusing to and annihilating from an interface state whose low characteristic S-value is attributed to impurities rather than defects—the latter leading to a higher, not lower, S-value.

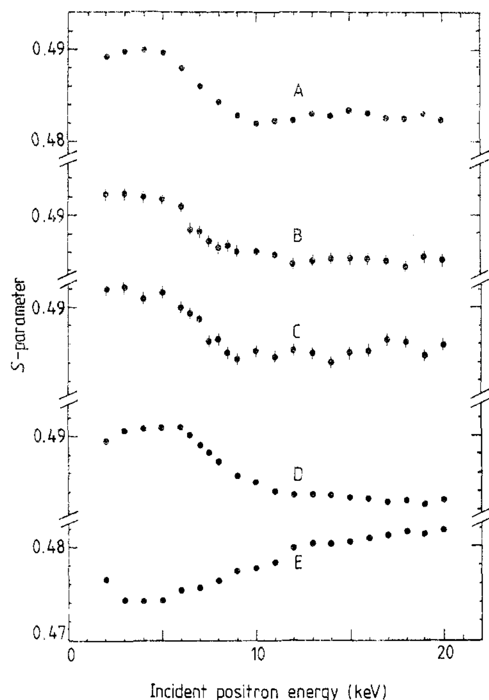

Figure 1. Mean S-parameter against incident positron energy for five SiO_2–Si samples. Samples A, B and C are thermally grown, with B and C under steam and dry conditions respectively. Sample E is an as-grown LTO sample, and D is an LTO sample after annealing (see text). Interface depths d for A–E are 500, 492, 465, 659 and 686 nm respectively; substrates in A–C are p(100)Si and for D and E are n(100)Si.

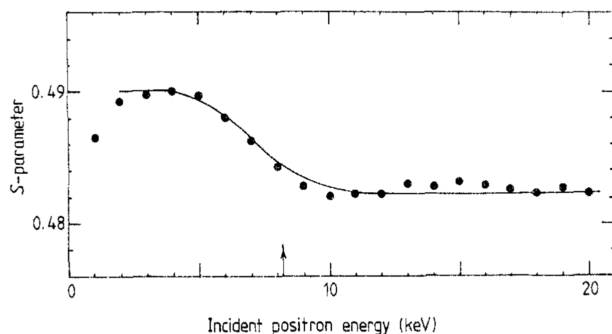

Figure 2. Results for sample A showing the fit obtained using equations (1)–(10). The arrow indicates the energy corresponding to a mean implantation depth $\bar{x}$ = the interface depth d (500 nm).

Results for a series of SiO_2–Si samples are summarised in figure 1. An almost universal result is obtained for most of the oxide samples. In contrast to the norm, the sample prepared by low-temperature oxidation (LTO) is markedly different, with $S(\text{oxide})/S(\text{substrate}) = 0.98$, compared with a typical value of 1.015 for the other samples; however, after annealing at 1300 °C for five hours the LTO results are again similar to those for the other samples. Clearly, none of the samples exhibits a dip in S in the vicinity of 8 keV, the energy corresponding to $d \simeq 500$ nm, similar to that observed by Nielsen *et al*. It is of interest to note, however, that in the current measurements the Ge detector is placed to the side of the sample, whereas Nielsen *et al* used a detector which viewed the target from behind; the two detectors thus sample different positron–electron momentum components.

Figure 2 illustrates the results of applying the fitting procedure described by equations (1)–(6) to one of the typical sets of data from figure 1. This essentially follows the

approach of Nielsen *et al* [1]. The assumptions are made that L for the oxide layer is very small, that the effects of any internal electric fields are negligible, and that all positrons diffusing to the interface from the substrate side are trapped there with 100% efficiency and are annihilated with an S parameter characteristic of the interface state. Equation (1) is then simplified to

$$S = F_o S_o + F_i S_i + F_b S_b \tag{7}$$

where the subscripts o, i and b refer to the oxide overlayer, the interface and the bulk (substrate) respectively. The surface fraction F_s is essentially zero for E above about 2 keV. For the interface at depth d the fraction F_o is simply given by

$$F_o = \int_0^d P(x)\,dx. \tag{8}$$

F_i is evaluated as was F_s in equation (5) by changing the origin from 0 to d: i.e.

$$F_i = \int_d^\infty P(x) \exp[-(x-d)/L]\,dx. \tag{9}$$

Then

$$F_b = \int_d^\infty P(x)\{1 - \exp[-(x-d)/L]\}\,dx. \tag{10}$$

F values are evaluated for each incident positron energy and S values chose to give the best fit to the experimental data. For figure 2, $S_o = 0.4980$, $S_i = 0.473$ and $S_b = 0.483$.

5. Discussion and conclusions

Apart from the absence of a pronounced feature at 8 keV associated with a very low interface S parameter, and the apparent universality of results for a number of different oxide samples, the most interesting feature of the results presented is the large difference between the as-prepared and annealed low-temperature (LTO) samples. Unambiguous interpretation of this observation awaits further research; among possible explanations is that hydrogen, known to be present at the interface, is also trapped in the epilayer during low-temperature growth, and diffuses from the oxide on annealing. This scenario requires that the presence of hydrogen effectively increases the mean momentum of electrons in the oxide layer available for annihilation, with the consequent depression of S_o.

The representative fit shown in figure 2 demonstrates that an S_i somewhat lower than S_b has to be assigned to the interface state to fit the relatively abrupt transition from oxide to substrate S-parameter. The higher S-parameter in the oxides suggest that the positrons are sensing larger open volumes in the overlayers.

In order to gain a full understanding of results such as those shown in figure 1, many more high-precision studies will be needed on samples manufactured under strictly controlled conditions. The large number of fitting parameters means that in more complex structures different assumptions may lead to equally acceptable fits to experimental data; ambiguities will be reduced, however, when a bank of information on positron diffusion through well characterised samples has been amassed, and when the effects of internal fields have been systematically studied. Further, more accurate

expressions for the implantation profile $P(x)$ must be developed, especially for inhomogeneous structures. To these ends, experimental and theoretical research in this area is continuing in our laboratories.

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