Centroid shift of $\gamma$ rays from positron annihilation in the depletion region of metal-oxide-semiconductor structures

I. C. Leung, Y. Kong, K. G. Lynn, and B. Nielsen
Brookhaven National Laboratory, Upton, New York 11973

Z. A. Weinberg and G. W. Rubloff
IBM Research Division, T. J. Watson Research Center, Yorktown Heights, New York 10598

(Received 4 June 1990; accepted for publication 6 November 1990)

Using metal-oxide-semiconductor (MOS) structures, the shift of centroid (peak) of $\gamma$-ray energy distributions emitted from positron annihilation has been measured as a function of incident positron energy. The Doppler centroid shift was found to be consistent with the positron motion in the MOS depletion region. The results are described by a one-dimensional positron diffusion model, and provide information on “effective” positron diffusion length under applied field.

Variable energy positron beams have recently been used for the study of SiO$_2$/Si structures and have provided unique new information because of their sensitivity to defects and ability to depth profile. These measurements make use of positron annihilation induced $\gamma$ rays. In the center of mass frame, the energy of each annihilation gamma ray is 511 keV. In the lab frame, the energy of one $\gamma$ ray is shifted up by a term linear in $v/c$, while the other is shifted down by an equal amount. If the distribution of velocities is isotropic, then the detector is equally likely to measure upshifted and downshifted energies. The 511 keV peak is Doppler broadened, but its center is not affected. If, however, an electric field creates a directional motion of the positron or electron, then the detector can be positioned to preferentially detect either upshifted or downshifted $\gamma$ rays. In this case, the centroid of the 511 keV peak will be shifted.

In this letter, we will describe a new technique based on the centroid shift measurements of the $\gamma$-ray spectra produced by positron annihilation in a metal-oxide-semiconductor (MOS) structure. The measurement is carried out on two samples. One had an $n$-type Czochralski-grown Si(100) substrate, upon which 500 Å of wet oxide was grown and 500 Å of Al overlayer evaporated without a post-metal anneal. The substrate doping density was $\sim 2-6 \times 10^{14}$ cm$^{-3}$. The second sample had a $p$-type Si substrate upon which 500 Å oxide was grown and 500 Å of Al was evaporated. The substrate doping density was $\sim 3-7 \times 10^{12}$ cm$^{-3}$. During the measurement the substrate is always grounded and the Al overlayer is forward or reverse biased at 10 V for the $n$-type sample and 6 V for the $p$-type sample. Variable energy positrons are implanted into the samples, with implantation depth approximated by

$$X_i = AE^{1.6}/\rho,$$

where $A = 375$ Å gm/(cm$^3$ keV$^{1.6}$), $\rho$ is the density of the material (gm/cm$^3$), $E$ is the incident beam energy in keV, and $x_i$ is in Å.

The corresponding annihilation $\gamma$-ray spectrum is then analyzed to obtain the relative centroid shift caused by positive or negative bias conditions. The positron beam facility used in the experiment is described elsewhere. It should be noted that the $\gamma$-ray Ge detector is facing in the direction of the applied electric field on the MOS sample and hence provides an optimal measure of the centroid shift.

As a positron enters the sample, it is rapidly thermalized, then travels with a velocity which depends on its thermal energy and the effects of the electric field in the depletion region ($\sim 10^6$ cm/s). The width of the 511 keV peak ($\sim 1$ keV) is almost entirely due to the relatively large electron velocities. If the positron drift velocity changes under bias by $v$, it will shift the centroid of the $\gamma$ ray of mean energy $E$ by an amount of $\Delta E/E = v/2c$. This relative centroid shift is of the order of $2 \times 10^{-5}$, or about 10 eV energy shift for a 511 keV annihilation line.

In the present setup a Be$^7$ radioactive source (which emits 477 keV $\gamma$ rays) is used as a reference. The centroid position from the positron annihilation $\gamma$ rays ($\sim 511$ keV) with respect to the Be$^7$ 477 keV peak is determined by calculating the first moment of the $\gamma$-ray energy distribution from a pulse height analyzer. To avoid systematic centroid drifts during the measurements, we alternately measured the relative centroid shifts at the positive and negative bias conditions ($10^6$ counts for each bias) at a given incident positron energy. The positron incident energy is varied to obtain the depth-dependent centroid shifts for both samples. Since the accumulation of majority carriers at the Si surface does not affect the positron diffusion behavior in the bulk Si, the measured centroid shifts are only associated with the centroid shifts caused by the field depletion region.

Figure 1 shows the measured centroid shifts for an $n$-type sample as a function of positron incident energy in the range of 5–40 keV. Figure 2 shows the results for a $p$-type sample in the range of 5–30 keV. The positrons that contribute to the measured centroid shift are those that annihilate when under the effect of the applied electric field. Those positrons which annihilate in the field-free region will have zero contribution to the measured centroid shift. In addition, if the positron is in a certain immobile state such as a trapped state or positronium, a measurement of the centroid shift will see no difference under different bias conditions as long as the state is immobile. The insensitivity of the centroid shift measurement towards the “immobile” state indicates that this technique is used in...
Another case of potential interest is when positrons are accelerated by the electric field so that they may become heated (epithermal) if the electric field is large enough. If this occurs near the SiO₂/Si interface region, one may observe the heating effects from the centroid shift measurements. However, this would require appropriate interpretation of the data and may require simultaneous determination of other experimental parameters.

In this work we have not considered positron heating effects and have assumed that the positrons which are annihilated beyond the electric field region will have zero contribution to the measured shift. The initial increase of the centroid shift in Figs. 1 and 2 with incident energy can be understood as due to the increase in the fraction of positrons that annihilate while in the electric field region. With further increases in the positron incident energy, more positrons will be implanted beyond the electric field region. Thus the fraction of the positrons that are annihilating in the depletion region decreases, resulting in a smaller centroid shift.

For the n-type substrate a depletion region is formed for a bias of -10 V with the electric field inside the bulk Si directed towards the SiO₂/Si interface, and the effective diffusion length of the positrons towards the interface will be larger than for the field-free situation. The +10 V bias corresponds to the accumulation case and the bulk positron diffusion behavior is not affected. For the p-type substrate (Fig. 2) the opposite is true. The depletion region is formed when the sample is positively biased, and the electric field is directed away from the SiO₂/Si interface. The effective positron diffusion coefficient towards the interface is smaller than for the field-free case. The negative bias situation for this sample will have little effect on the positron bulk diffusion behavior because of the accumulation of majority carriers. The accumulation and depletion conditions reached under the applied bias are confirmed by comparing with the capacitance voltage (C-V) curves of both samples. The effects of electric field enhanced diffusion and larger depletion layer length are clearly seen from Figs. 1 and 2, where the n-type sample has a maximum centroid shift which occurs at a much larger incident energy (~18 keV) than the p-type sample (~8 keV). We have used an effective diffusion length, \( L_{\text{eff}} \), to describe the positron mobility towards the interface and have approximated the electric field in the depletion region as a constant. A derivative Gaussian distribution is represented for the positron implantation profile:

\[
P(x) = \frac{1}{x_1} \exp\left[-\left(\frac{x}{x_1}\right)^2\right],
\]

where \( x_1 \) is defined in Eq. (1) except that the energy \( E \) is with respect to the incident energy (~3 keV) of the positron towards the interface. We emphasize here that the exact shape of the stopping profile does not affect the estimations below. In fact, we have employed an exponential stopping profile and found the fitted results to be of the same order of magnitude. The depletion region has a width \( x_d \), therefore the fraction of positrons that annihilate in the electric field region and contribute to the measured signal is

\[
F = \int_0^{x_d} \left[1 - \exp\left(-\frac{x}{L_{\text{eff}}}\right)\right] P(x) \, dx,
\]

which can be evaluated to get

\[
F = \frac{1}{L_{\text{eff}}} \exp\left(\frac{x_1}{2L_{\text{eff}}}\right) \left[\text{erf}\left(\frac{x_d}{x_1} + \frac{x_1}{2L_{\text{eff}}}\right) - \text{erf}\left(\frac{x_1}{2L_{\text{eff}}}\right)\right] - \left[1 - \exp\left(-\frac{x_d}{L_{\text{eff}}}\right)\right] \exp\left[-\left(\frac{x_d}{x_1}\right)^2\right].
\]
The centroid shift is associated with the effective diffusion length of the positrons. A short diffusion length will correspond to a sharp rise to the maximum centroid shifts, but when the diffusion length becomes comparable to the depletion layer length, the slope of the centroid shift as a function of incident positron energy begins to saturate. For a fixed positron diffusion length, a longer depletion layer means the peak position will be shifted towards the higher energy side, and more positrons will annihilate in the depletion zone and contribute to the signal. The height of the peak increases with increasing depletion layer length. However, the slope of the initial increase is only slightly affected. Figure 3 shows that the centroid shift measurements are sensitive to the positron diffusion behavior in the electric field as well as to the MOS geometry including the depletion layer width.

The fraction in Eq. (4) has to be multiplied by the corresponding centroid shift, which will be determined by the positron drift velocity. The parameters $X_{ph}$ left, and positron drift velocity are free to change when fitting the data as shown in Figs. 1 and 2 for $n$- and $p$-type samples. For the $n$-type substrate, the fitted effective diffusion length is $5600 \pm 50$ Å, while the depletion layer length is $16000 \pm 2000$ Å. For our sample, since the doping density is known, we can calculate the depletion layer width from:

$$W = \frac{\sqrt{4 \varepsilon \kappa T_c} \ln \left( N_A/n_i \right)}{q N_A},$$

where $\varepsilon$ is the dielectric constant, $n_i$ the intrinsic carrier density, and $N_A$ the doping concentration of Si. We obtain $W = 12000 \pm 18000$ Å in agreement with our fitted value for the $n$-type sample. For the $p$-type sample, the fitted effective positron diffusion is $(3 \pm 1) \times 10^5$ Å. The depletion layer width is $(6\pm 1) \times 10^5$ Å, which also agrees with the calculated depletion layer width $\sim (4-7) \times 10^5$ Å from Eq. (5). The average electric field present in the depletion zone can be estimated from the fitted effective diffusion length assuming that the field-free diffusion length is $L_0 \sim 2400$ Å, which corresponds to a diffusion coefficient of $D \sim 2.7 \text{cm}^2/\text{s}$. Using a positron mobility in Si of $\mu \sim 70 \text{cm}^2/\text{V s}$, the effective diffusion length under an electric field $E$ is given by:

$$(1/L_{eff}) = (\mu E^2/4D_+) + (1/L_0^2) = \mu E/2D_+,$$

where the $\pm$ sign depends on whether the $E$-field is directing towards or away from the interface. From Eq. (6) one obtains the electric field strength for the $n$-type sample as $\sim 3 \times 10^7 \text{V/cm}$ and for the $p$-type sample as $\sim 1 \times 10^7 \text{V/cm}$. The average electric field is larger in the $p$-type sample than in the $n$-type sample because of the larger doping concentration ($N_A$) in the $p$-type sample, which gives a shorter depletion width as well as a larger surface band bending.

It is worth noting that the electric field in the depletion region is given by the linear relation $E = E_0(1 - x/x_d)$, which results in a higher electric field close to the interface. This electric field gradient, along with the fact that the average electric field in the $p$-type sample is greater than that in the $n$-type sample is possibly the reason that the maximum centroid shift of the $p$-type sample is a little larger than the maximum centroid shift of the $n$-type sample.

In summary, we have measured the centroid shift of positron annihilation induced $\gamma$ rays in the presence of an electric field in $n$- and $p$-type substrate MOS samples. The results can be well represented by a positron diffusion model. Using the same procedure it will be possible to obtain information on the SiO$_2$/Si interface trapping properties, positron heating effects, and the electric field configuration. The results not only provide a better understanding of the physics of positron interactions with matter, but will also be important in characterizing device quality. The optimum bias condition for the maximum positron charge collection at the interface is easily deduced from the results. This enables one to make positrons more sensitive to the interface region.

Work performed at Brookhaven was supported by US DOE contract No. DE-AC02-76CH00016.

---