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LETTER TO THE EDITOR

Measurement of positron mobility in silicon

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Abstract. Measurements of positron, e^+, mobility in Si using a positron-lifetime technique are reported and values of $100 \pm 18\, cm^2\, V^{-1}s^{-1}$ and $990 \pm 170\, cm^2\, V^{-1}s^{-1}$ are obtained at 295 and 104 K respectively. These are compared with results from previous studies using different experimental methods.

In many defect-free materials, e^+ exhibit transport behaviour similar to that of holes and electrons, although the e^+-lattice coupling is stronger, implying a higher effective mass, m_+^*, and consequently lower diffusion constants and mobilities than for the other charge carriers. For example, using a method involving the angular correlation of e^+ annihilation radiation, Shulman *et al* (1975) found in Ge $m_+^* = (1.23 \pm 0.17)\, m_e$ compared with $m_{hole}^* = 0.35\, m_e$, where m_e is the electron mass. Although electron and hole transport have been extensively studied, only a few published results exist for e^+. The motivation for most of the e^+ measurements has been to obtain a better understanding of their behaviour in solids, but it has been suggested by Jorch *et al* (1984) that, in elemental semiconductors such as Si and Ge, these studies benefit from a simpler band structure than those for holes and electrons and thus might enhance our understanding of mobility limiting processes in these materials. Using a Ge sample and a 0–5 keV variable-energy slow-positron beam, they monitored the fraction of incident e^+ that, after thermalisation in the crystal and diffusion back to the surface, was subsequently re-emitted as positronium. Knowledge of the energy dependence of the e^+ implantation profile enabled a fitting procedure to be carried out and the e^+ diffusion constant, D_+, to be deduced. It was possible to extend measurements to high temperatures (up to 1020 K), beyond the range attainable by current techniques for holes and electrons, and thus demonstrate the inadequacy of conventional carrier-phonon scattering theory that satisfactorily explains the low-temperature behaviour. Using the same technique, Nielsen *et al* (1985) found D_+ in silicon to be $2.7 \pm 0.3\, cm^2\, s^{-1}$ at 300 K. The positron mobility, μ_+, can be deduced from D_+ by means of Nernst–Einstein relation, $D_+ = \mu_+ kT/e$, where T is the positron temperature ($\simeq$ lattice temperature). Assuming the above value for Si, this gives $\mu_+\,(300\, K) = 104 \pm 12\, cm^2\, V^{-1}\, s^{-1}$.

Another way of determining mobilities is to measure the carrier drift velocity, v_c, under the influence of an electric field, E. In this case the low field ($<10^5\, V\, cm^{-1}$ for Si

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and Ge) carrier mobility, μ_c, is given by

$$v_c = \mu_c E. \tag{1}$$

At higher fields v_c ceases to be a linear function of E and, for $T \leqslant 300$ K, is given by the expression for acoustic-phonon-limited drift velocity derived by Shockley (1951), namely

$$v_c = 2^{1/2}\mu_c E\{1 + [1 + (3\pi/8)(\mu_c E/v_l)^2]^{1/2}\}^{-1/2} \tag{2}$$

where v_l is the longitudinal sound velocity. In the high-field limit, optical phonon-processes begin to dominate and carrier velocities saturate.

The temperature dependence of the carrier mobility can usually be described by a power law

$$\mu_c \propto T^{-n} \tag{3}$$

where n is a positive constant. If acoustic-phonon scattering is the dominant mode, n will be 1.5, whereas for the optical mode processes n will be larger, as observed in Si, for which values of 2.42 and 2.20 for electrons and holes respectively have been measured (Jacobini *et al* (1977)).

There have been two previously reported electric-field measurements of μ_+ in silicon. Mills and Pfeiffer (1977) employed an intrinsic Ge detector to measure the electric-field-assisted motion of e^+ by observing the Doppler shift of the annihilation γ-rays. They found $\mu_+ = 460 \pm 20$ cm^2 V^{-1} s^{-1} at 80 K and 173 ± 15 cm^2 V^{-1} s^{-1} at 184 K, suggesting a value of n, from (3), of 1.2 ± 0.1. This is lower than that expected from acoustic-phonon scattering and Mills and Pfeiffer (1977) speculate that this might be due to the effect of impurity scattering. A $T^{-1.2}$ extrapolation of their 184 K measurement gives μ_+ (300 K) $\simeq 100$ cm^2 V^{-1} s^{-1}, in good accord with the diffusion constant value reported by Nielsen *et al* (1985). The other measurement relies upon a determination of the small shift in the e^+ implantation profile due to the electric field drift prior to annihilation. Using this technique Brandt and Paulin (1977) measured a significantly higher value of 430 ± 100 cm^2 V^{-1} s^{-1} at 300 K. The reason for this discrepancy is unclear (Mills and Pfeiffer 1979).

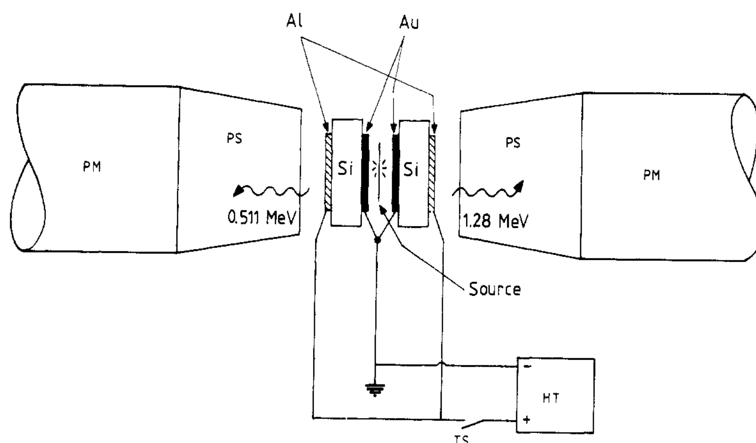

Figure 1. Schematic illustration of the source/sample arrangement. Source, ^{22}Na (between polyimide foil); Al, Al contacts ($\simeq$2000 Å); Au, Au contacts ($\simeq$ 2000 Å); PM, photomultiplier; PS, pilot U scintillator; HT, high tension supply; TS, timeswitch.

Beling *et al* (1987a) have reviewed the various experimental techniques available to measure μ_+ and D_+ and suggest how these measurements can elucidate the understanding of e^+ interactions with defect and impurity sites present in the crystal. They also demonstrated that a measurement of the fraction of e^+ drifting to an interface in a solid can be related to the positron mobility. This is the basis of the present study, stimulated by the possibility of developing a new type of efficient (field-assisted) moderator for the production of intense slow-positron beams (Beling *et al* 1987b, c). It was also hoped that an independent measurement of μ_+ at 104 and 295 K might resolve the experimental disagreement between the results of Brandt and Paulin (1977) and Mills and Pfeiffer (1977).

15 mm-diameter, 1 mm-thick discs of 10 kΩ cm n-type Si were cemented into printed circuit board mounts using epoxy resin and 2000 Å layers of Al and Au were evaporated on either side. Electrical connections were formed via the mounts to avoid damage to the metal-silicon contacts. A 10 μCi ^{22}Na source sandwiched between 8 μm polyimide foils was used and the sample source configuration is shown in figure 1. A conventional fast-timing system with a resolution of about 300 ps FWHM was employed to collect e^+ lifetime spectra, which contained about 1×10^6 events over a 24 h period. The effect of electronic drift was reduced by incorporating a twostep (field on/field off) switching cycle into the arrangement. With an electric field applied to the samples, data were collected in the first half of a multi-channel analyser memory. After about 800 s, the field was switched off and the data routed to the second half of the memory. After a further 800 s this cycle was repeated. The 'active' periods were separated by 90 s 'dead' periods to ensure that the field applied to the samples had stabilised.

Lifetime spectra were analysed by either centroid shift calculations or using the RESOLUTION program described by Kirkegaard *et al* (1981), which reduces the spectra into their separate lifetime components and gaussian resolution functions. Using the latter method, zero-field spectra were well fitted by three lifetime components of 224, 370 and about 2000 ps, with intensities of about 83%, 16% and 1% respectively. The first component is due to annihilations in bulk Si, the last two being associated with annihilations in the source. Electric field spectra showed a fourth component with a lifetime, τ_2, of 400 ± 30 ps. The variation in intensity of this component with electric field is shown in figure 2 for both temperatures investigated. Although the exact nature is uncertain it is expected that, owing to the amorphous nature of the interface, a significant concentration of large open-volume voids (vacancy agglomerates) is likely to occur and the measured lifetime is typical of those observed for voids in many metals and semiconductors. Assuming that the concentration of defects is high enough that the e^+ trapping is governed only by their drift to the interface, the situation can be treated, after subtraction of the source contribution, as a two-state system with annihilation rates λ_1, λ_2 and a transition rate, κ, from state 1 (bulk) to state 2 (interface). Following Beling *et al* (1987a), κ can be written as

$$\kappa = \alpha\mu_+ E \tag{4}$$

which leads to expressions for the intensity, I_2, of the interface component and an effective rate, λ_1', at which the e^+ disappear from the bulk Si:

$$I_2(E)/(1 - I_2(E)) = \mu_+ E\alpha/(\lambda_1 - \lambda_2) \tag{5}$$

and

$$\lambda_1' = \lambda_1 + \mu_+ E\alpha \tag{6}$$

where α is the ^{22}Na β^+ absorption coefficient in Si ($=79.05\ cm^{-1}$). By fitting a straight line to the data in figure 2(*a*) a value of $\mu_+(295\ K) = 131 \pm 31\ cm^2\ V^{-1}\ s^{-1}$ is obtained. The quoted error reflects the statistical error (about 8%) and an error (about 23%) arising from the uncertainty in τ_2.

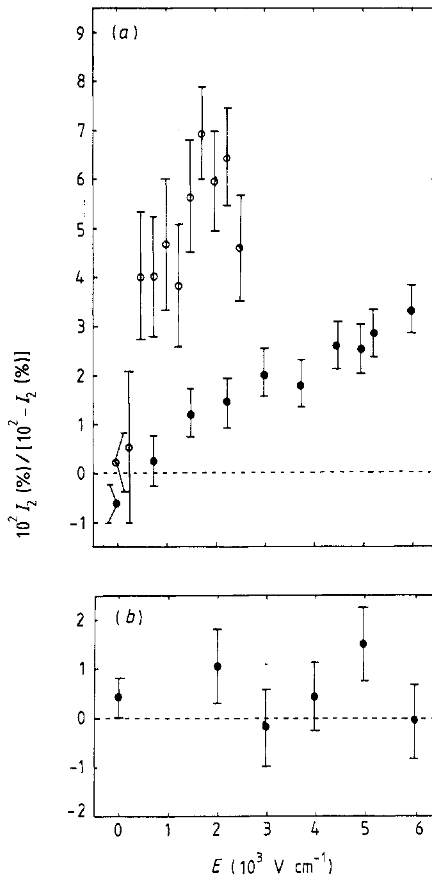

Figure 2. (*a*) Variation of the intensity of the interfacial lifetime component with the electric field, E, applied such that the e^- drift is towards the Au contact: ● (295 K); ○ (104 K). (*b*) As above but with the e^+ drift away from the contact. As expected there is no statistically significant change in the lifetime spectrum with E when the e^+ drift is in this direction.

Ideally, I_2 and λ_1 should be constrained via equations (5) and (6) to give the same value for μ_+. This is not possible using RESOLUTION, so the mobilities were also derived from the measured centroid shifts, $\Delta\bar{\tau}$, between pairs of field on/field off spectra. Assuming four-component spectra, the centroids of the field off and field on cases are respectively given by

$$\bar{\tau}_0 = I_{10}\tau_1 + I_{20}\tau_2 + I_{30}\tau_3 + I_{40}\tau_4 \tag{7}$$

and

$$\bar{\tau}_V = I_{1V}\tau_1' + I_{2V}\tau_2' + I_{3V}\tau_3' + I_{4V}\tau_4'. \tag{8}$$

In the present case, τ_2, I_3, τ_3, I_4 and τ_4 are unchanged by the presence of the electric field and, assuming that the interface intensity at zero field, $I_{20} = 0$, the centroid shift is given by

$$\Delta\bar{\tau} = \bar{\tau}_V - \bar{\tau}_0 = I_{1V}\tau_1' - I_{10}\tau_1' + I_{2V}\tau_2. \tag{9}$$

Making use of $I_{1V} + I_{2V} = I_{10} + I_{20}$ and substituting for $\tau_1' = \lambda_1'^{-1}$ from (6) gives the result

$$\begin{aligned}\Delta\bar{\tau} &= \Delta\bar{\tau}_0 + \alpha\tau_1(\tau_2 - \tau_1 I_{10})\mu_+ E/(1 + \alpha\tau_1\mu_+ E) \\ &\simeq \Delta\bar{\tau}_0 + \alpha\tau_1(\tau_2 - \tau_1 I_{10})\mu_+ E \end{aligned} \tag{10}$$

since $\alpha\tau_1\mu_+ E \ll 1$.

The centroid shift at zero field, $\Delta\bar{\tau}_0$, is included in the expression to allow for any significant shifts due to instrumental effects. A straight-line fit to the data gives a slope of 3.97 ($\pm$0.41) $\times 10^{-16}$ s cm V^{-1} and an intercept ($=\Delta\bar{\tau}_0$) of -0.044 ± 0.108 ps. This method gives a value for μ_+ of 100 ± 18 cm^2 V^{-1} s^{-1}, which is in reasonable agreement with that derived above from POSITRONFIT. Although more prone to the effects of electronic shift, centroid shift measurements show smaller statistical errors than those obtained from POSITRONFIT. A fit of the data to the expression (2) gave similar results for μ_+, showing that the low-field mobility is independent of applied field at 295 K. These results are in good accord with those of Nielsen *et al* (1985) and the $T^{-1.2}$ extrapolation of the data of Mills and Pfeiffer (1977).

To investigate the temperature variation of μ_+ a cryostat was constructed in which the samples are supported on a 'cold finger' arrangement in vacuo. With LN_2 in the cryostat, a steady temperature of 104 ± 4 K was maintained. The reduced solid angle subtended by the detectors at the source necessitated longer run times than those at 295 K, which resulted in larger errors due to the electronic drift. On cooling, an increase in leakage current through the sample was observed, which may be due to cracking of the epoxy mounts or stresses introduced into the samples by contraction. This made it impossible to extend measurements above about 250 V applied without significant Joule heating.

A fit of the centroid data to (2) gave μ_+ (104 K) $= 990 \pm 170$ cm^2 V^{-1} s^{-1} with a reduced chi squared, $\chi^2/\nu = 19.2/10$. A linear fit constrained through the origin gave μ_+ (104 K) $= 760 \pm 120$ cm^2 V^{-1} s^{-1} and $\chi^2/\nu = 28.0/10$. POSITRONFIT data gave similar values. This non-linear variation in v_c was also observed by Mills and Pfeiffer (1977), who similarly performed a fit to (2) to deduce their μ_+ (80 K) value. A $T^{-1.2}$ extrapolation of this measurement to 104 K gives 340 ± 15 cm^2 V^{-1} s^{-1}, which is significantly lower than our result. The present results imply a value of n, from (3), of 2.2 ± 0.5, a value higher than that expected from simple acoustic-phonon scattering theory. Although the possibility of a systematic error in μ_+ caused by the large uncertainty in τ_2 cannot be excluded, the good accord between the present results and those of others at 295 K is evidence against this. The discrepancy may be due to the effect of prethermalisation drift since, as suggested by Mills and Pfeiffer (1977), this effect will cause an overestimate of μ_+ derived from the e^+ displacement measurements. The thermalisation time, t_{th}, in solid media is strongly temperature-dependent. For example, calculations performed by Nieminen and Oliva (1980) in Al show an increase in t_{th} from 6.8 ps to 17 ps between 300 and 100 K. This variation may therefore explain some of the discrepancy between our data and that of Mills and Pfeiffer (1977) at 104 K though, since the agreement is good at 295 K, it is unlikely that such an effect can be big enough to be solely responsible.

In comparing Doppler and displacement measurements of μ_+ it is also important to note that the positron implantation profile may be field-dependent. Experiments performed by Heinrich (1978) in polyethylene show that discernable changes in the e^+ implantation profile occur at fields $\simeq 100$ kV cm^{-1}. These cannot be explained by the e^+ motion after thermalisation. However, in this material Doppler measurements of μ_+

published by Mills *et al* (1986) are in agreement with the displacement measurement of Mourino and Brandt (1979). Further experiments are therefore necessary to provide a clear picture of the e^+ motion in solid media under the influence of applied electric fields.

In conclusion it is noted that μ_+ has been determined in silicon using a technique based upon the drift of the e^+ to an interface and the measurement of e^+ lifetime spectra. Values reported using lifetime, Doppler and e^+ beam techniques are in good agreement at room temperature, though the present μ_+ (104 K) is much higher than that found in the only other low-temperature study. This suggests that further work is required. In this respect recent instrumental advances with fast timing circuits using efficient crystals as γ-ray detectors (e.g. de Vries *et al* 1989) suggest that important gains both in timing resolution and counting rates are feasible. These will lead to more precise determinations of μ_+ using the lifetime technique such that the possible influence of systematic errors can be investigated more fully. Finally it is noted that this experiment provides the first direct evidence that a significant fraction (about 7%) of the e^+ from a ^{22}Na source can be drifted to an interface by an electric field at 104 K. This result is of considerable consequence in demonstrating the practicability of field-assisted moderators for slow-positron beams.

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