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Measurement of positron mobility in Si at 30–300 K

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The temperature dependence of positron motion in silicon (Si:[P] $=4\times10^{14}$ cm^{-3}) is studied experimentally by measuring the drift length of positrons in the space-charge region of an Au-Si surface-barrier diode. At 300 K the positron mobility is 110 ± 15 cm^{2}V^{-1}s^{-1}, and it increases to 2800 ± 1000 cm^{2}V^{-1}s^{-1} at 30 K. Below 300 K the mobility varies with temperature in accordance with $T^{-3/2}$. This temperature dependence of carrier mobility is typical of scattering from longitudinal-acoustic phonons.

Positron diffusion in solids is most clearly seen in experiments involving positron motion to a surface. Several such experiments both in metals and semiconductors have been carried out recently, making use of the low-energy positron-beam technique.[1,2] In metals a consistent picture of positron diffusion emerges from theory and experiments showing that scattering from long-wavelength acoustic phonons limits the distance a positron travels within its lifetime.[3,4] In semiconductors the results of positron diffusion show unexpected differences between various experiments.[5–9] This scattering of data can, for the most part, be ascribed to the unknown electric field existing in the near-surface layer due to the surface charge.

We have studied positron motion under a controlled electric field in Si by investigating the drift of positrons to the Au-Si interface of a surface-barrier diode.[10] There the effect of an electric field in the space-charge region of a metal-semiconductor contact on positron motion was demonstrated. The experimental results can be explained in terms of the classical carrier transport models based on the drift-diffusion approximation. Within this approximation we found the positron mobility $\mu_+=120\pm20$ cm^{2}V^{-1}s^{-1} at 300 K in Si. The result is in good agreement with the diffusion constant $D_+=3.0\pm0.2$ cm^{2}s^{-1} measured in a high-purity Si sample in which the electric field can be neglected.

In this work, positron mobility is studied from 30 to 300 K using the same experimental technique. From 80 to 300 K the temperature dependence predicted for scattering from acoustic phonons gives a good description of the experimental results. This is found also at 30 K, although the experimental uncertainty is larger.

Because of the detailed description published earlier,[10] only an outline of the experimental technique is given below. In the experiment, positrons are implanted to silicon through a thin Au overlayer, and the shape of the 511-keV annihilation line is measured. The annihilation line shows Doppler broadening originating from the momentum of the annihilating electron-positron pairs. The line shape is described by the parameter S defined as the relative area of a fixed central region 511 keV $\pm\Delta E$ ($\Delta E=0.87$ keV) of the annihilation line. Hence the S parameter represents the fraction of electron-positron pairs with a momentum component $p_L\leq 2\Delta E/c$. As positrons either annihilate in Si or drift to the interface and annihilate there, the experimental line-shape parameter reads as

$$S(E,V_b)=J(E,V_b)S_i+[1-J(E,V_b)]S_b\,. \tag{1}$$

Annihilation at the interface gives rise to a well-defined value of the line-shape parameter (S_i) which is different from that in bulk Si (S_b). They can both be determined experimentally, as all positrons can be made to annihilate either in bulk Si or they can be drifted to the interface before annihilation.[10] The probability J of positron drifting to the interface is a function of the incident positron energy E, which determines the range during slowing down, and the electric field $\mathcal{E}$ in the space-charge region of the metal-semiconductor contact. The field is varied by applying an external voltage V_b to the contact. To relate $J(E,V_b)$ to the positron mobility μ_+, positron transport is described within the drift-diffusion approximation. The mobility can then be deduced by carrying out a fitting procedure in which μ_+ is a free parameter.[10]

The Schottky diodes were prepared by evaporating a 100-Å Au layer of 8-mm diameter on a P-doped floating-zone refined Si wafer. The capacitance-voltage (C-V) measurement of a 1.2-mm-diam diode, in which the Au layer is much thicker, gives the carrier concentration of 4.0×10^{14} cm^{-3} and the barrier height 0.74 eV. The current-voltage (I-V) curve measured *in situ* gives the barrier height 0.78 ± 0.05 eV. The ideality factor n defined by $I=I_S\exp(qV/nk_BT)$ was found to be 1.02. The series resistance of 25 Ω in the Ga contact in the back side of the Si crystal was estimated from the current at forward bias voltages $V_b>0.20$ V. For the reverse bias $|V_b|\leq5$ V the current was less than 0.5 μA. All these values are for $T=295$ K.

The measurements were carried out using the positron beam at Helsinki University of Technology.[11] The incident energy of the positron beam having a diameter of 4 mm and an intensity of 10^6 e^+/s was varied from 0.1 to 27 keV. The annihilation line was recorded with a high-purity Ge detector mounted perpendicular to the direction of the electric field, and the spectra were acquired using a digitally stabilized multichannel-analyzer system. At each incident-positron energy, typically 10^6 counts were collected to the annihilation peak. The sample temperature was controlled with a closed-loop He cryocooler and electron-beam heating. The stability of the temperature measured with an Au(0.07% Fe)/NiCr thermocouple was better than ±1 K above 80 K. The lowest temperature the sample could attain was 30 ± 3 K.

Figure 1 shows the line-shape parameter S as a function of the incident-positron energy at 80 and 295 K. The external bias voltage was applied to produce the same electric field at both temperatures. The field in Si and, consequently, the positron-drift velocity are directed towards the interface. Annihilation at the interface clearly leads to a smaller line-shape parameter than in bulk Si. The difference between the two curves demonstrates a higher fraction of positrons drifting to the interface at 80 K compared to that at 295 K due to a higher positron mobility.

The solid lines in Fig. 1 correspond to the least-squares fits to the drift-diffusion model of positron transport. The data at the incident-positron energies below 9 keV was omitted, and the dashed lines are guides for the eye. The peak at the incident energies < 2.5 keV is independent of the external voltage, and we ascribe it to implantation and subsequent annihilation in the Au overlayer and also to emission of nonthermal positrons. The drift-diffusion approximation comprises the positron velocity

$$\mathbf{v}_+ = \mathbf{v}_d - \frac{D_+}{n_+(\mathbf{r},t)} \nabla n_+(\mathbf{r},t) . \qquad (2)$$

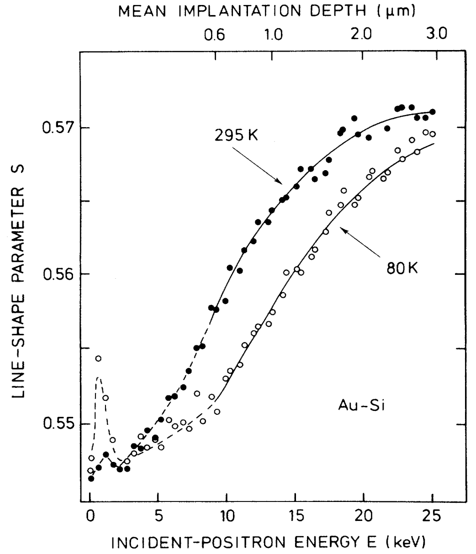

FIG. 1. The line-shape parameter S as a function of the incident-positron energy at 80 and 295 K. An external voltage was applied to produce approximately the same electric fields (maximum field 5.3×10^3 V cm^{-1}, depletion layer 0.89 μm). The solid lines are fits to the drift-diffusion model corresponding to the positron mobilities 950 ± 100 and 115 ± 10 cm^{2}V^{-1}s^{-1}. The mean range, given for the incident energies $E \geq 9$ keV, is for the stopping profile in Si.

In the linear-response regime the drift velocity is $\mathbf{v}_d = \mu_+ \mathcal{E}$, and the mobility is independent of the field $\mathcal{E}$. In this approximation the flux of positrons to the interface is solved from the equation

$$D_+ \nabla^2 n_+(\mathbf{r}) - \lambda n_+(\mathbf{r}) - \nabla \cdot [n_+(\mathbf{r}) \mathbf{v}_d] + P_E(\mathbf{r}) = 0 . \qquad (3)$$

In Eq. (3), $P_E(\mathbf{r})$ is the positron stopping profile, or more rigorously the introduction rate of positrons, which represents the initial distribution $n_+(\mathbf{r}, t=0)$. This model assuming diffusive motion is valid if the range of positrons during slowing down is several scattering mean free paths, and it can be applied except at very low incident positron energies or sample temperatures.[12] As the drift length $l_+ = \tau v_d$ (τ is the positron lifetime of 217 ps in Si) is large compared to the diffusion length, it was not possible to determine the diffusion coefficient independently. Therefore it was expressed in terms of the mobility through the Einstein relation $D_+ = (k_B T/e) \mu_+$.

In a metal-semiconductor contact, the diffusion potential, or the built-in potential, is equal to

$$qV_{\mathrm{bi}} = \phi_b - (E_C - E_F) , \qquad (4)$$

where ϕ_b is the Schottky-barrier height, and $(E_C - E_F)$ is the Fermi-level position in Si measured from the bottom of the conduction band. The electric field $\mathcal{E}(x)$, where x denotes the distance from the interface, was calculated under the abrupt depletion-layer approximation. In this standard model, the field decreases linearly from its maximum value at the interface to zero at the end of the depletion layer. Alternatively, the Poisson equation including the carrier contribution in addition to the impurity concentration in the space-charge region was integrated numerically. The effect of the different approximations of the field is discussed below.

There are a number of parameters inherent in the analysis. For the carrier concentration and the surface-barrier height we use the values 4.0×10^{14} cm^{-3} and $\phi_b = 0.78$ eV based upon the C-V and I-V measurements at room temperature. The surface barrier was assumed to be independent of temperature. The characteristic line-shape parameter for annihilation at the interface $S_i(T)$ was estimated from the experimental data at each temperature. At 295 K the line-shape parameter S_b in bulk Si was extracted from $S(E)$ measured at that temperature. At low temperatures the positron mobility increases, and some positrons always drift to the interface before annihilation if the incident-positron energy is 30 keV or below. The line-shape parameter $S_b(T)$ in bulk Si was determined from a conventional measurement using a ^{22}Na source. From 30 to 500 K in 10^4 Ω cm Si, a linear increase of 0.072% per 100 K compared to S at 300 K was found.[13]

The main source of error comes from the uncertainty in the positron stopping profile. We have used the stopping profile based upon the Monte Carlo simulation of positron slowing down.[14] As a function of incident-positron energy, the mean implantation depth increases as $\langle x \rangle \propto E^n$. At 300 K, the value $n = 1.60 \pm 0.02$ was estimated from the positron diffusion data at different electric fields,[10] in good agreement with the simulations and experimental studies of multilayer structures.[15] Positron stopping is definitive much before slowing down to thermal energies, and temperature bears no influence on the average range.[16] The effect of the Au layer was included by requiring the positron transmission to be continuous (for details of the stopping profile, see Ref. 10). In the analysis, the incident energies below 9 keV were omitted. At incident energies $E > 9$ keV, stopping in the Au layer becomes negligible, and the average range in Si is > 0.5 μm.

Figure 2 shows the positron mobility as a function of temperature from 30 to 300 K. At 80 K and above, the line-shape parameter $S(E)$ was measured at three or four different voltages V_b. The maximum electric field was changed from 4×10^3 to 9×10^3 V cm^{-1}, and the width of the depletion layer varied from 0.8 to 2.0 μm, respectively. The values given in Fig. 2 are the average values of μ_+ measured at different electric fields, and the errors indicated correspond to the 95% confidence level. The mobility at 30 K is from a measurement at $V_b = 0.70$ V. All the results correspond to the electric field $\mathcal{E}(x)$ solved from the Poisson equation including the contribution from the carriers and ionized donor atoms. At 110 K and above the difference due to the different approximations of the field is 10% or less and it does not bear any effect on the temperature dependence. At 30 and 80 K, where P atoms are only partly ionized, the more accurate calculation of the electric field results in a smaller positron mobility.

Since the drift velocity in the linear-response (Ohmic) regime should be small compared to the thermal velocity, this approximation becomes increasingly poor as the temperature is lowered. Comparing with the time-of-flight measurements of the drift velocity of holes in Si,[17] the Ohmic region above 100 K is reached if the drift velocity is approximately 1×10^6 cm s^{-1} or below. For $T \geq 110$ K, the mobility in Fig. 2 corresponds to the average drift velocity $v_d \leq 2\times10^6$ cm s^{-1}. In this temperature region the experiment does not show any dependence of μ_+ on the field. It is still a reasonable approximation to introduce a field-independent mobility to the drift-diffusion model. At 80 K the drift velocity is already comparable to the thermal velocity and the model becomes more approximate.

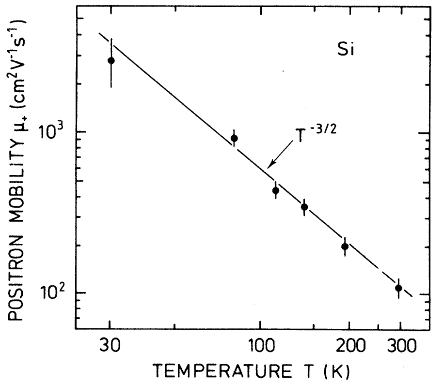

FIG. 2. Positron mobility as a function of temperature. At 80 K and above, the mobility is the average value from the fits of the drift-diffusion model to the experimental line-shape parameter $S(E,V_b)$ at different external voltages V_b. The errors indicated correspond to the 95% confidence level. At 30 K the mobility is from a single measurement of $S(E,V_b)$ with $V_b = 0.70$ V. The solid line stands for the temperature dependence $T^{-3/2}$.

At 30 K, the external voltage $V_b = 0.70$ V corresponds to the electric field of approximately 2 kV/cm at the interface. In this case, however, the region of the depleted layer where the Ohmic condition clearly fails is narrow (the region where $v_d > 1\times10^6$ cm s^{-1} is less than 0.3 μm) compared with the positron drift length (~ 10 μm) in that area. As a result the probability of drifting to the interface is not too much affected even if the approximation of the positron transport in this high-field area is not valid. There is, however, another difficulty. Because of the high mobility and the necessity to go to small electric fields, small errors in the field become increasingly significant at 30 K. The independence of the mobility on the external voltage at 80 K and above indicates that the calculation of the field is approximately correct at those temperatures.

At 295 K, we find the positron mobility $\mu_+ = 110 \pm 10$ cm^{2}V^{-1}s^{-1}. This result is equal to that measured previously.[10] The experimental results in Fig. 2 were fitted to the temperature dependence $\mu_+ = \mu_0(T/300\text{ K})^{-\alpha}$ from 80 to 300 K. As a result, we find $\alpha = 1.52 \pm 0.12$. The mobility 2800 ± 1000 cm^{2}V^{-1}s^{-1} at 30 K is consistent with the same temperature dependence, but the experimental uncertainty is much larger. As already noted, the positron stopping profile affects the absolute value of the experimental mobility. However, the temperature dependence of μ_+ is far less sensitive to the stopping profile. Assuming $n = 1.55$ or 1.65, which represent a rather large change in the stopping profile compared to $n = 1.60 \pm 0.02$ estimated at 300 K, the temperature dependence changes, respectively, to $\alpha = 1.45$ and 1.62.

There are two previously reported measurements of positron mobility from 80 to 300 K in Si. From the direct measurement of positron drift velocity by observing the Doppler shift of the annihilation radiation, Mills and Pfeiffer[18] found the mobilities 460 ± 20 and 173 ± 15 cm^{2}V^{-1}s^{-1} at 80 and 184 K. Simpson *et al.*[19] have reported the values 370 ± 80 and 68 ± 1 cm^{2}V^{-1}s^{-1} at 104 and 295 K. Although these values are somewhat smaller than the present ones, the overall agreement is reasonable.

The positron mobility 110 ± 15 cm^{2}V^{-1}s^{-1} at 300 K corresponds to the diffusion constant $D_+ = 2.8 \pm 0.3$ cm^{2}s^{-1}. This is in good agreement with $D_+ = 3.1 \pm 0.2$ cm^{2}s^{-1} measured in a high-purity Si sample in which the electric field can be neglected, and also with $D_+ = 2.70 \pm 0.2$ cm^{2}s^{-1} reported by Schultz *et al.*[9] The mobility at 80 K, 920 ± 150 cm^{2}V^{-1}s^{-1}, corresponds to the diffusion constant $D_+ = 6.3 \pm 1.0$ cm^{2}s^{-1}.

The carrier mobility can usually be described by the temperature dependence $\mu \propto T^{-\alpha}$, and the value of α is typical of the scattering mechanisms limiting the carrier mobility. The deformation-potential approximation for coupling to the long-wavelength acoustic phonons gives the temperature dependence $T^{-3/2}$ also shown in Fig. 2. There is a good accordance of the experimental positron mobility with $\alpha = \frac{3}{2}$. This suggests that coupling with longitudinal-acoustic phonons is the prevailing lattice scattering mechanism which limits the positron motion at 300 K and below. The same is found in metals in a wide temperature region from 20 K to the onset of positron trapping at thermal vacancies.[3]

It is also interesting to compare the results with the theoretical deformation potential. Boev, Puska, and Nieminen[20] have calculated the positron and electron energy levels in Si at 300 K, and from those band-structure calculations the acoustic deformation-potential constant is $E_d = -6.19$ eV. Within the deformation-potential approximation, it gives the diffusion constant $D_+ = 3.05$ $\mathrm{cm^2 s^{-1}}$ at 300 K, in good agreement with the present experiments. There is, however, some uncertainty in the effective positron mass which complicates the comparison. In Ref. 20 the effective mass $1.5m_e$ was assumed. Estimates for m_{eff} vary between $1.2m_e$ and $1.6m_e$.[21] The effective mass of $1.2m_e$–$1.6m_e$ gives the deformation-potential constant in good agreement with the band-structure calculations in various metals.[3]

Other scattering mechanisms include electron scattering, impurity scattering, and coupling to optical- and transverse-acoustic phonon modes. Simple estimates of scattering rates indicate that scattering from electrons and also from neutral or ionized impurities are small compared to phonon scattering.[7] Up to 300 K, we do not find any indications of positron coupling to optical phonons. This is partly due to the high energy (63 meV) of longitudinal-optical phonons in Si. There is, however, another possible cause of this. Band-structure calculations show a rather free-particle-like lowest positron band at the Γ point with s-like orbital character. The symmetry restrictions imply a zero optical deformation potential at $k = 0$, and zero-order optical-phonon processes are weak (see, e.g., Ridley[22] and references therein). To see the importance of optical modes in positron scattering the measurement must be extended to higher temperatures.

In conclusion, positron mobility in Si is measured from 30 to 300 K in the electric field in a surface-barrier diode. At 300 K the mobility is $110 \pm 15\ \mathrm{cm^2 V^{-1} s^{-1}}$, and at 30 K it increases to $2800 \pm 1000\ \mathrm{cm^2 V^{-1} s^{-1}}$. The temperature dependence is in good agreement with $T^{-3/2}$, which imposes the temperature dependence of the diffusion constant $D_+ \propto T^{-1/2}$. This is typical of scattering from longitudinal-acoustic phonons.

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