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1996 J. Phys.: Condens. Matter 8 1403

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Positron transport studies at the Au–(InP:Fe) interface

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Received 3 August 1995

Abstract. Positron mobility and lifetime measurements have been carried out on semi-insulating Fe-doped InP samples with Au contacts used for electric field application. The lifetime measurements, with electric fields directed towards the Au–InP:Fe interface, reveal no component associated with interfacial open-volume sites and thus give no evidence of any positron mobility. The mobility measurements, made using the Doppler-shifted annihilation radiation technique, however, reveal a temperature independent positron mobility of about $20 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ in the range 150–300 K. These observations, together with results from I – V analysis, are discussed with reference to two possible band-bending schemes. The first, which requires an ionized shallow donor region adjacent to the Au–InP interface, seems less plausible on a number of grounds. In the second, however, an Fe^{2+} negative space charge produces an adverse diffusion barrier for positrons approaching the interface together with a non-uniform electric field in the samples capable of explaining the observed mobility results.

1. Introduction

Studying the motion of positrons in a semiconductor lattice under the action of an electric field is an important area of study. Such studies not only constitute a useful check of mobility-limiting mechanisms that are well known for electrons and holes with a particle that possesses a simpler band structure [1] but are also important for positron vacancy defect studies in semiconductors where an accurate knowledge of the positron's diffusivity in limiting trapping rate is often needed for charged defects [2]. Technologically, with the requirement for more intense low-energy positron beams growing, the search continues for moderating materials in which significant fractions of positrons can be electric field drifted micron distances into vacuum and the purity of semiconductors makes them prime candidates for investigation [3].

In terms of positron diffusivity studies, InP has received relatively little attention. A room-temperature positron mobility μ_+ of $15 \pm 5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ has been reported by Beling *et al* [1] in a study of the electric field dependent defect trapping rate of positrons in InP. Another study by Uedono and Tanigawa [4] gives the room-temperature diffusion length L_+ of positrons in InP for annealed samples as being 110 nm, a result which on using the Einstein relationship in the form $\mu_+ = L_+^2 / \tau k_B T$, with $\tau = 245 \text{ ps}$ [5] as the positron lifetime, gives a similar result for μ_+ of about $19 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. Recent work by Britton and Störmer [6] using a timed positron beam, however, suggests that these values may be too low. Working on Be-doped MBE-grown material these workers find a room-temperature positron diffusion coefficient $D_+ = 1.9 \pm 0.5 \text{ cm}^2 \text{ s}^{-1}$ corresponding to a mobility $\mu_+ = 75 \pm 20 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. In all this work, however, the possible band bending at the positron injection surface (contact) and the effect that intrinsic electric fields play have received little attention. It is the purpose of this paper to address this issue, by

in the first place looking for positron electric field drift towards an Au–InP interface using positron lifetime spectroscopy and in the second by making measurements of the positron mobility in InP using the Doppler-shifted annihilation radiation technique.

2. Experimental details

The samples employed in these studies were fabricated from Fe-doped semi-insulating InP(100) wafers of 0.5 mm thickness, supplied by ICI Wafer Technology Ltd, and had a quoted room-temperature carrier concentration of $2.5 \times 10^7 \text{ cm}^{-3}$. Two InP:Fe sample substrates were first cut into 10 mm×10 mm squares, degreased and then etched in HF:H₂O(1:1) for 1 min. Gold was then thermally evaporated to a thickness of 1000 Å in the form of a circular junction area of 0.5 cm². The front contact closest to the source was made to a thickness of only 500 Å so as to prevent positron absorption effects. The pressure in the chamber during evaporation was 10^{-6} Torr and the metallizations were not subjected to any annealing.

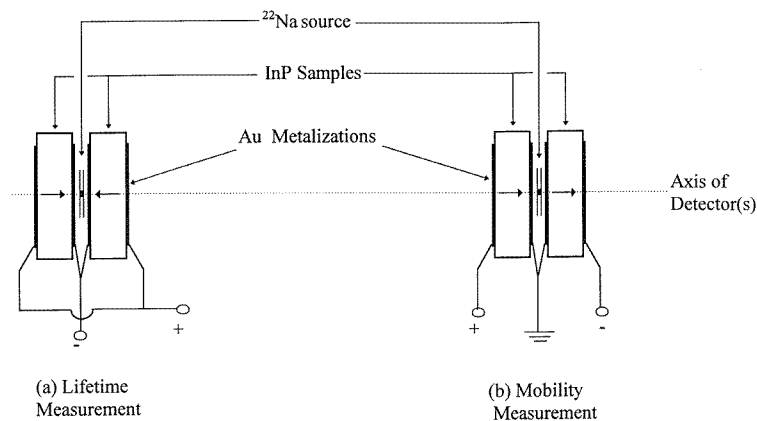


Figure 1. Schematic diagram showing the different biasing configurations required for (a) electric-field lifetime studies and (b) positron mobility studies.

The configuration of the sample biasing differed according to whether positron lifetime or mobility measurements were being made. This is shown schematically in figure 1, where it is seen that for the lifetime measurements the electric fields in both samples are antiparallel, while for mobility measurements they are parallel and in the direction of the detector axis. In both the lifetime and the mobility experiments a $10 \mu\text{Ci } ^{22}\text{Na}$ source encapsulated in Ni foils $1 \mu\text{m}$ thick was sandwiched between the samples. Voltages were applied to the Au metallizations through thin Au wires which were attached using silver paint. At room temperature the samples had quite a high leakage current. The current was typically about $30 \mu\text{A}$ at 100 V applied bias, leading to a 30 mW dissipation. To prevent damage to the Au sample contacts through thermal runaway, higher biases than 100 V were not applied. The source–sample sandwich was mounted in an Oxford Instruments liquid-nitrogen cryostat for temperature control.

For the lifetime spectroscopy studies, only DC voltages were applied to the sample sandwich. For each bias about 2×10^6 counts were collected in the spectrum. The lifetime spectrometer had a time resolution (FWHM) of 240 ps and has been described in more detail elsewhere [3]. The current through the samples was monitored routinely during the

course of the lifetime measurements.

The method employed in making the positron mobility measurements was that form of the Doppler-shifted annihilation radiation technique developed by Mills *et al* [7]. A triangular bias wave with a 1 Hz period together with its complement were applied to the sample-sandwich, thus sweeping the electric fields in the samples towards and away from the detector. The 511 keV annihilation photons, which are thus blue and red shifted at the same frequency, were detected using high-purity (HP) Ge of 1.4 keV resolution (FWHM) at the 514 keV ^{85}Sr line. The amplified 511 keV pulses were segmented using single-channel analysers into two scale rates N_1 and N_2 according to whether the pulse fell below or above the amplitude corresponding to the mean 511 keV pulse height. The pulse amplification was automatically and continuously adjusted with a slow time constant (about 100 s) so as to keep $N_1 = N_2$ while, at the much faster bias frequency, small variations ΔN_1 and ΔN_2 in N_1 and N_2 , respectively, as recorded on a synchronized multichannel scalar, monitored the mean positron velocity, v_+ given by the expression [7]

$$v_+ = \frac{1}{2}\alpha \frac{\Delta N_1 - \Delta N_2}{\langle N \rangle} \quad (1)$$

where α ($\approx 2.1 \times 10^8 \text{ cm}^{-1}$ for our set-up) is a calibration constant and $\langle N \rangle$ is the mean scalar rate of N_1 and N_2 . Owing to the detector's proximity to the sample, velocities were scaled up by a factor of 1.08 to cater for the variation in $\cos\theta$ over the active volume. A final scaling up of 1.15 was included to account for immobile source foil annihilations. The final mobility value was obtained by assuming the field in the sample to be uniform and equal to V/d , where V is the applied bias and d the thickness of the sample.

3. Results

3.1. Positron lifetime spectroscopy

Analysis of the lifetime spectra was performed using the POSITRONFIT program [8]. Without applying any source correction, it was found that the spectra could be fitted well with two lifetime components, the shorter of which was close to the accepted bulk lifetime for InP (240–252 ps) [1, 5, 6, 9] and the longer which fell in the range 350–450 ps. In order to reduce systematic errors resulting from fitting parameter correlations, the longer spectral lifetime was considered as constant and fixed for all biases at 460 ps. The results of such fitting, given in table 1, show an effectively constant long-lifetime intensity ($I_2 \approx 7\%$) and short lifetime ($\tau_1 = 242 \pm 2$ ps). The analysis reveals no evidence of any change in the positron lifetime spectra as the applied bias is changed, a fact that was subsequently confirmed by comparing overlaid spectra. In sharp contrast with the Au–GaAs interface under applied bias [10], no visual difference between any of the spectra could be found.

The long component (7% of 460 ps) found in the Au/InP spectra is so similar to the Ni foil source correction (8% of 400 ps) that within the statistical uncertainty these two may be confirmed as the same. It is concluded that, unlike the Au–GaAs interface [3], not only is there no clear evidence for any contact lifetime but also, when a bias is applied in the sense of directing positrons towards the contact, no change is observed in the expected region for microvoid-related contact lifetimes (about 400 ps). Either there really is no change or the change is very small and beyond the sensitivity of our measurements.

3.2. Positron mobility

Positron mobility measurements were performed in the temperature range 150–290 K. The results are shown by the full triangles in figure 2. It is of interest to note that the measured

Table 1. Fitting results obtained from the Au–InP:Fe positron lifetime spectra with τ_2 fixed at 464 ps.

Bias voltage (V)	τ_1 (ps)	I_1 (%)	I_2 (%)
–100	240 ± 2	93.3 ± 0.2	6.7 ± 0.2
0	243	92.6	7.4
10	241	92.5	7.5
20	244	93.2	6.8
30	242	92.7	7.3
100	241	93	7

Table 2. Positron mobility data at 270 K taken as a function of the ramping period.

Ramping period (s)	Positron mobility ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)
0.2	14.4 ± 4
1	9
2	18.2
8	11.4

positron mobility in InP is nearly constant in this range (about $16 \pm 4 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$) and is probably dropping slightly from a value of about 20 to $15 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ as the temperature is reduced. The positron mobility was measured as a function of the triangular ramp signal frequency at 270 K since such measurements in the Au/GaAs system had revealed a frequency dependence caused by the deep donor level EL2 [11]. The results obtained are given in table 2, from which it is clear that no similar frequency dependence is present in Fe-doped InP.

4. Discussion

In this section an attempt is made to understand the positron annihilation data so far presented. Two major questions emerge from the results, namely why is there no observation of a microvoid lifetime component associated with annihilations from the Au–InP:Fe interface when the electric field is directed towards it and why the observed positron mobility is independent of temperature. In an attempt to answer these questions we first review a recent finding regarding current transport through the Au–InP:Fe interface that suggests that significant band-bending occurs at such contacts when they are under bias [12].

Lee *et al* [12] discovered that the reverse I – V characteristics of the Au–InP:Fe(100) system were accurately those expected for a Schottky contact, subject to thermionic field emission (TFE) current flow, in series with the bulk resistance R_b of the compensated bulk semi-insulator. The reverse-biased current I_r through the interface was accordingly found to be given by the TFE theory of Padovani and Stratton [13] through solution of the equation [12]

$$I_r = \frac{A^* AT (\pi e E_{00})^{1/2}}{k} \left[e \left(V_r - I_r R_b - \frac{E_g}{2} + \phi_b \right) \right]^{1/2} \exp \left(\frac{-e\phi_b}{kT} \right) \quad (2)$$

where $E_{00} = h(N/4m^*\epsilon)^{1/2}$ is a tunnelling parameter with dimensions of energy, N being the concentration of ionized traps, m^* the effective carrier mass, ϵ the material permittivity,

ϕ_b the Schottky barrier height (SBH), A^* the effective Richardson constant, A the constant area, $E_g = 1.34$ eV the band gap energy, e the electronic charge and k Boltzmann's constant. The fact that equation (1) fitted not just the I - V characteristics at room temperature but also down to 230 K gave convincing evidence for a Schottky-like parabolic barrier. In [12] it was argued that the most likely form of this barrier was that for electrons as shown in case I of figure 2, where neutralized deep acceptors, Fe^{3+} , left residual donors (about 10^{14} cm^{-3}) close to the metallization exposed. It is pointed out here, however, that this is not the only possibility. With the intrinsic free-carrier concentration of $2 \times 10^7 \text{ cm}^{-3}$ it is not clear whether conduction through the sample is primarily that of holes or electrons. That raises the possibility that the observed drop in voltage across a sample contact as expressed through equation (1) could well be due to a hole barrier as shown in case II of figure 2. The negative charge responsible for such band-bending would arise from a region of ionized deep acceptors, Fe^{2+} , adjacent to the Au metallization.

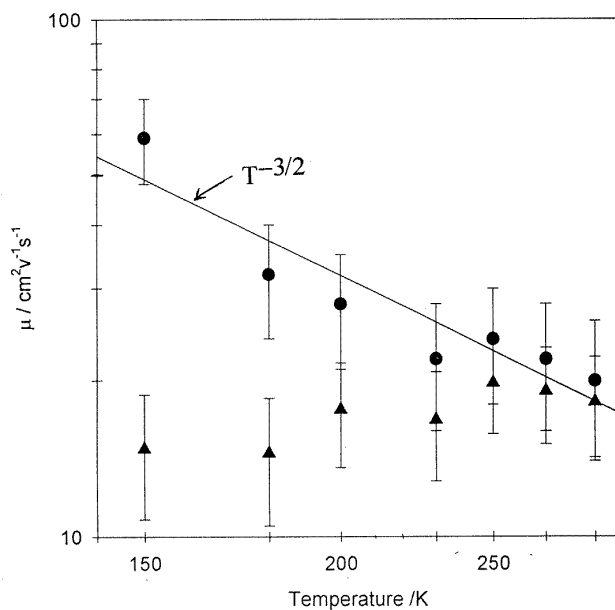


Figure 2. The observed positron mobility in InP:Fe plotted against temperature (note that the axes are logarithmic): ▲, mobility data assuming a uniform electric field of V/d across the sample; ●, data after correction has been made for the non-uniform field postulated in the band-bending case II described in the text. The approximate $T^{-3/2}$ dependence is suggestive of an acoustic-phonon-limited mobility.

As mentioned, the intrinsic nature of the InP makes it difficult to decide which of the two schemes shown in figure 2 is correct. This uncertainty is also present when considering the respective positions of the Fermi levels at the interface and in the bulk, since as measured in [12] the barrier height on the semi-insulating InP is 0.68 ± 0.05 eV, a value very close to the midgap ($E_g/2 = 0.67$ eV) and the bulk Fe^{2+} acceptor level (0.66 eV below the conduction band). The delicate balance that appears to exist makes it possible that both types of barrier could be present in our samples at the same time, one forming a barrier for electrons as in case I and the other for holes as in case II. This being the case might explain why for metal contacts on doped material the Fermi level is pinned 0.4–0.5 eV below the conduction band irrespective of whether the material is n or p type [14], whereas

for the semi-insulating InP contact it takes a value of about 0.7 eV [12]. In the latter case it could well be that the barrier heights for the hole (about 0.9 eV) and for the electron (about 0.45 eV) are being averaged through the occurrence of both types of TFE conduction in the same sample. With these facts in mind we now consider in turn cases I and case II to see which is more capable of explaining the positron annihilation results.

4.1. Case I: positive space-charge band-bending due to ionized shallow donors

In case I the description of the positron dynamics at the interface will be identical with that of the Au/GaAs system as considered by Shan *et al* [3] since the essential feature is that of a region of positive space charge adjacent to the positron injecting contact. Thus, if it is assumed, as with the Au/GaAs system, that there are microvoid interface states at the Au–InP interface capable of trapping positrons, then it will be expected that the intensity I_2 of this component will be given by [3]

$$I_2 = \frac{\alpha v_d}{\alpha v_b + \lambda_b - \lambda_2} \left\{ 1 - \frac{(\lambda_b - \lambda_2)(1 - v_b/v_d)}{\alpha v_b + \lambda_b - \lambda_2} \exp[-\alpha W(1 + \lambda_b/\alpha v_d)] \right\} \quad (3)$$

where v_b and v_d are the positron drift velocities in the compensated bulk and depleted near-surface regions, respectively, λ_b and λ_2 are the annihilation rates in the InP substrate and interfacial microvoid states, respectively, α is the positron absorption coefficient and W , the width of the depletion region, is given by

$$W = \left(\frac{2\epsilon(\phi_b - \zeta + V - I_r R_b)}{eN} \right)^{1/2} \quad (4)$$

where ζ is the energy difference between the conduction band and the bulk equilibrium Fermi level position. Following [3] the drift velocities v_b and v_d are given by the electric fields $I_r R_b/d$ and $eNW/2\epsilon$, respectively, in these regions by application of the Bardeen–Shockley [15] formula.

As has been mentioned, the fact that we observe no microvoid component could be because I_2 is smaller than our expected detection limit. To check this hypothesis the depletion width W is first computed for various donor concentrations N . These are shown in figure 4 for $N = 10^{14}$, 10^{15} , 10^{16} and 10^{19} cm⁻³, respectively, at a temperature of 290 K, where we have taken the known bulk resistance $R_b = 1.25 \times 10^7$ Ω and the current I_r , as given by equation (1). These widths should be compared with the mean implantation depth α^{-1} of positrons which according to the density of InP (4.79 g cm⁻³) should be in the range 40–45 μm [16, 3]. It is seen that, for a reasonable shallow donor concentration in the range 10^{14} – 10^{15} cm⁻³, significant fractions (10–50%) of implanted positrons will find themselves in the electric field of the depletion region. The electric fields at this donor concentration are, however, not large and do not lead to appreciable positron drift to the interface. This may be seen with reference to figure 5 where the interface intensity as computed from equation (3) is plotted against applied bias. In the calculation, the positron mobility in InP has been taken as 20 cm² V⁻¹ s⁻¹ in accordance with the room-temperature Doppler shift result (figure 2), the values of λ_b and λ_2 taken as (245 ps)⁻¹ and (460 ps)⁻¹, respectively, and the values of W as shown in figure 4. Curves are again calculated with different trap charge densities in the depletion layer. Taking a realistic lower limit for the residual shallow donor concentration of 10^{14} cm⁻³ it is noted that due to the low electric field of the depletion region the I_2 -value is only 1% at 100 V bias. As a result of an increased depletion region electric field the value rises to about 3% if the residual shallow donor concentration is taken at a more realistic value of about 10^{15} cm⁻³, the change in going from 0 to 100 V bias being only about 2.4%. Such changes should be observable

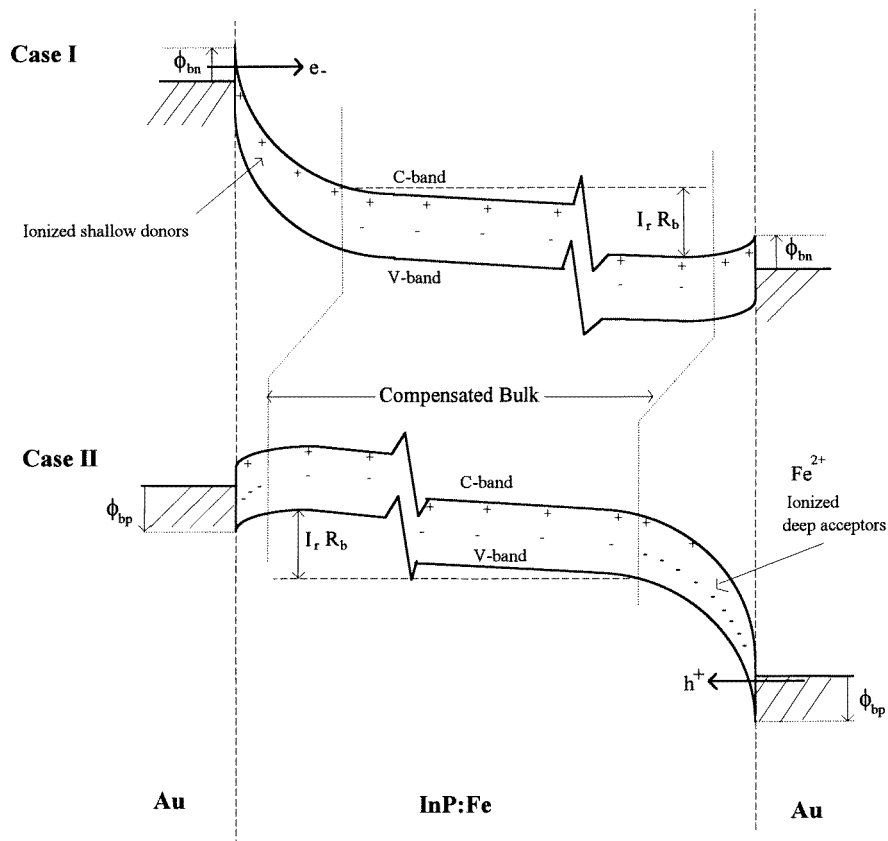


Figure 3. The two possible band-bending schemes of the Au/InP:Fe/Au system under an applied bias.

from our measurements which are estimated to have a sensitivity limit of about 0.5%. The only way of achieving I_2 -values below this limit is either for the donor concentration to be less than 10^{14} cm^{-3} or, as seen from figure 4, greater than 10^{19} cm^{-3} , and both these possibilities seem highly unlikely.

There are other possible explanations for not observing a long-lifetime component from the interface. Usually open volume defects are expected to be present at the metal–(III–V semiconductor) contact due to the lattice mismatching that occurs, and to phase segregation in the polycrystalline metal film that occurs on interdiffusion of the anion and cation components into the metal [17]. The Au–InP interface, as with the Au–GaAs interface, is well known to be diffuse in nature [18] and there is thus no obvious reason why the Au–InP interface should possess any fewer microvoid-like structures. The possibility that such defects might be present either at low concentrations or with open volumes so small that their annihilation lifetime becomes indistinguishable cannot, however, be ruled out. Another possibility is that microvoid-like defects are present at the interface, but positrons for some reason are not able to trap into them. The microvoid defects may for example be positively charged if the interfacial layer of intermixing is non-metallic in nature and if, as expected, not only positrons but also holes drift towards the contact. Such holes may, as they do in the Si/SiO₂ [19] system, be able to trap into these interface states, thus making

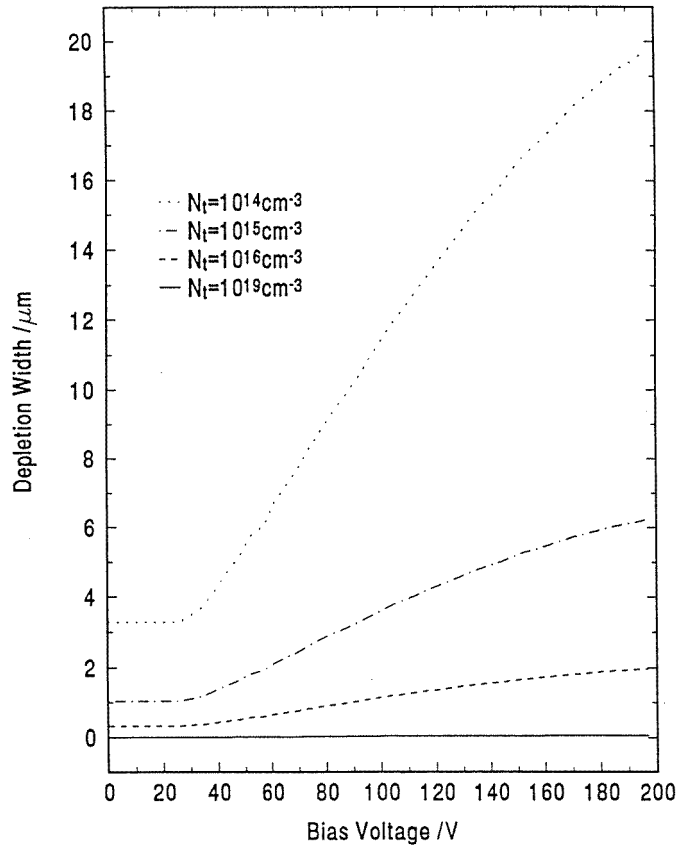


Figure 4. The expected depletion layer width W adjacent to the InP:Fe interface at 290 K for different donor (acceptor) densities plotted against the reverse bias based on the model described in the text and [3].

them positively charged and preventing the positron from trapping at the same site. Finally, it is pointed out that, within the near surface of the InP, negatively charged V_{In} could exist in sufficient concentration for positrons to be effectively trapped long before they reach the more disordered phases where microvoids exist, the latter being connected with grain boundaries of mixed phases.

With regard to the observed positron mobility it is possible that the absence of any significant temperature variation results from the presence of ionized acceptors in the InP. In addition to holes, ionized shallow acceptors in GaAs are known to shallow trap positrons as well [20]. This trapping, which becomes more dominant as the temperature is reduced, strongly inhibits the drift of positrons in the GaAs and effectively counteracts the rise in mobility resulting from phonon freeze-out, thus causing the apparent mobility to be temperature independent [11, 21]. It might be anticipated that the same process could be occurring in Fe-doped InP, in which the ionized deep acceptors, Fe^{2+} , could well act as shallow positron traps. It is difficult to confirm this hypothesis in the same way as for GaAs because the phonon-limited variation in positron mobility (or diffusivity) against temperature is not yet known in InP for the temperature range above 290 K. It is pointed out, however, that the concentration of Fe^{2+} ionized acceptors can be no more than about 10^{16} cm^{-3} , the

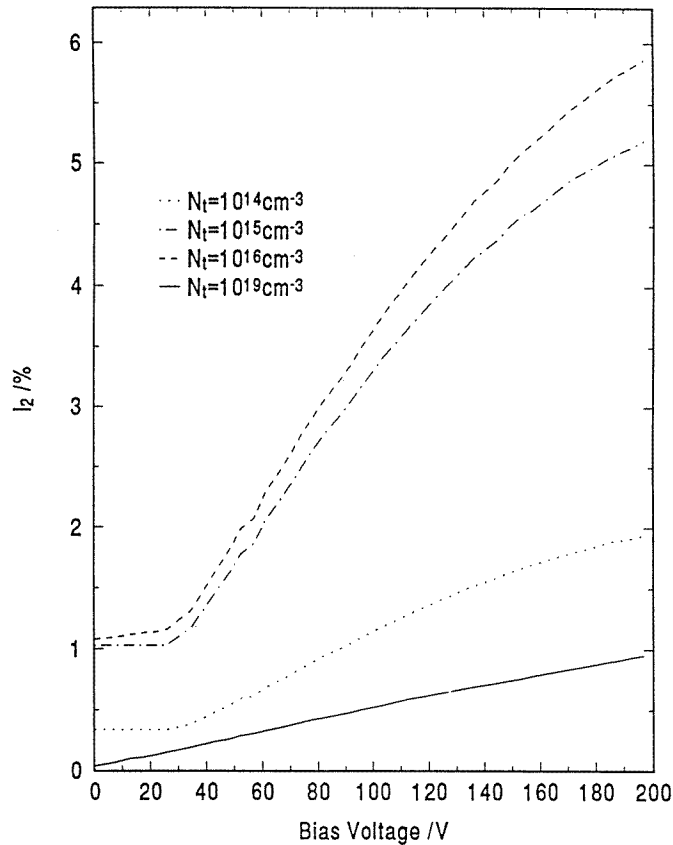


Figure 5. The intensity of the long-lifetime component I_2 plotted against the reverse bias for the Au-InP:Fe junction based upon the model described in the text and [3].

concentration of the Fe doping, and that in the compensated bulk it would be much less (about 10^{14} – 10^{15} cm^{-3}). These concentrations, being much less than the observed shallow trap concentration of about 10^{18} cm^{-3} found in semi-insulating GaAs [11], may not be sufficient to account for the observed inhibition of a phonon-limited mobility below room temperature.

4.2. Case II: negative space-charge band bending due to ionized Fe^{3+} acceptors

When considering case II, there is a clear reason why no interface microvoid component is seen. The ionized Fe^{2+} space charge adjacent to the interface here forms a potential barrier for the positron to climb. This barrier could be quite high if, as has been already supposed, the observed SBH on the Fe-doped InP is indeed due to an averaging of the SBH for holes and electrons. If we take the bulk Fermi level to be pinned at the Fe^{2+} level, i.e. about 0.65 eV below the conduction band, and assume ϕ_b through the Fermi-level-pinning phenomenon to be the same as ϕ_{bn} , the SBH on n-type material (i.e. about 0.45 eV), then we arrive at an adverse diffusion barrier of about 0.2 eV. Such a barrier would be sufficient to inhibit effectively all positron diffusion to the interface.

The presence of a negative Fe^{2+} space charge, and a rather larger SBH (about 0.9 eV)

for holes, can also explain the observed temperature-independent positron mobility, without recourse to any shallow trapping phenomenon. It may be seen with reference to figure 3 that, with this negative space-charge band-bending scheme, biasing the InP so as to drive positrons towards the (left) positron-injecting Au–InP interface causes a significant potential drop across the outside (right) Au–InP interface. This potential drop causes the injected positrons to experience an electric field smaller than that calculated V/d . The apparent electric field seen by injected positrons can be computed as $I_r R_b/d$ since we have from equation (2) the current flow I_r through the sample and know that the resistance of the compensated bulk varies as $\exp(E_g/2kT)$ [12]. When plotting the mobility as calculated using the values $I_r R_b/d$ rather than V/d it is interesting to note that the results are consistent with the $T^{-3/2}$ law characterizing acoustic-phonon-limited mobility (see figure 3).

5. Conclusions

In this paper, the transport of positrons near the Au–InP:Fe interface has been studied using the techniques of positron lifetime spectroscopy, and Doppler shift of annihilation radiation. While a positron mobility in InP of $8.2 \pm 3.5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ has been found at 280 K using the Doppler shift technique, it has not been possible to observe any drift of positrons towards the Au–InP interface when an electric field is directed towards the interface. This fact, together with the observed temperature independence of apparent positron mobility below room temperature, has a natural explanation if a negative Fe^{2+} space charge is assumed to exist adjacent to the Au–InP interface, whereas a model that supposes band-bending to be due to ionized shallow donors is less convincing. The negative Fe^{2+} space-charge conjecture is consistent with what is at present known about the Fermi-level-pinned position of Au on InP and current transport through the Au–InP contact.

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