Low-temperature positron transport in semi-insulating GaAs

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Positron diffusion and drift in semi-insulating (SI) GaAs in the temperature range of 50–300 K were studied by the slow-positron beam technique. Both the temperature-dependent positron diffusion coefficient and positron mobility were measured independently using the method reported recently [Y. Y. Shan *et al.*, Phys. Rev. B **54**, 1982 (1996)]. The experimental results are consistent with the Einstein relation. The diffusion coefficient and mobility approximately follow $D_+(T) = 9400 T^{-\beta}$ cm^2 s^{-1}, and $\mu_+(T) = 10^8 \times T^{-\sigma}$ cm^2 V^{-1} s^{-1}, with $\beta = 1.5 \pm 0.1$, and $\sigma = 2.5 \pm 0.2$, respectively in the temperature range of 50–300 K. The results are consistent with scattering from optical-phonon modes as the dominant scattering process for positron transport in GaAs (SI) in this temperature range. No trapped positron states were observed to 50 K. [S0163-1829(97)00716-9]

I. INTRODUCTION

Carrier transport measurements are of interest for understanding the mechanisms of phonon and impurity interactions in solids. As a positive carrier of electric charge, the positron has a simpler band structure and relatively larger effective mass than electrons and holes in common semiconductors.[1] The study of positron motion provides unique information about lattice scattering in solids, which is essential to many applications of the positron annihilation technique.[2]

The positron motion can be characterized by measuring its diffusion coefficient D_+, and mobility μ_+. There are several methods used to determine these two quantities. Mills and co-workers studied positron mobility by measuring its drift velocities based on the very small changes in the Doppler shift of the annihilation radiation.[3,4] The positron lifetime method has been carried out to measure positron mobility in Si (Ref. 5) and GaAs.[6] The positron beam technique has been effectively used to determine positron diffusion coefficients in metals[7] and semiconductors.[8–14] In these methods, either D_+ or μ_+ can be obtained experimentally. If one is determined, the other is deduced via Einstein relation. So far, few measurements of independently determining both the positron mobility and diffusion coefficient have been reported.

GaAs, as an important semiconductor compound, has been extensively studied. The positron mobility value of 35 ± 10 and 60 ± 20 cm^2 V^{-1} s^{-1} at room temperature were reported by the drift velocity technique and lifetime technique, respectively,[15,16] which, using the Einstein relation, relate to diffusion coefficients of 0.9 ± 0.3 and 1.6 ± 0.5 cm^2 s^{-1}, respectively. Using the slow positron beam technique, diffusion lengths of 1800 ± 140 and 1500 ± 100 Å were reported for n-type GaAs at 300 K, which correspond to positron diffusion coefficients of 0.9–

1.4 cm^2 s^{-1}.[17,18] Soininen *et al.* reported a diffusion coefficient of 1.6(2) cm^2 s^{-1} in semi-insulating (SI) GaAs at 300 K.[15] More recently, a diffusion coefficient of 1.8(2) cm^2 s^{-1} and a mobility of 70 ± 10 cm^2 V^{-1} s^{-1} in GaAs (SI) were obtained independently at room temperature.[19]

Measurements of the temperature effect on positron diffusion showed that scattering from acoustic phonons is predominant in cubic metals (20–1400 K),[7] Ge (>500 K),[14] and Si (30–500 K).[14,20,21] The diffusion coefficient follows the $T^{-1/2}$ power law. While in GaAs (SI), the diffusion coefficient exhibits a weak temperature dependence and does not follow the $T^{-1/2}$ power law in the temperature of 300–1000 K.[14] In n-type GaAs, clear deviations from $T^{-1/2}$ was observed in the temperature of 100–300 K.[18] It was attributed to positron shallow traps, possibly from negative compensating centers, where the positron is localized in Rydberg states.

In this study, monoenergetic positron beam measurements are provided for both the positron diffusion and drift in GaAs (SI) in the low-temperature range 50–300 K. The temperature dependence of the positron diffusion coefficient and mobility are independently determined. The results are consistent with the Einstein relation. The diffusion coefficient approximately follows the power law $D_+ \propto T^{-3/2}$, indicating that positron motion is largely limited by optical-phonon scattering in this temperature range according to the calculation of the momentum relaxation time using the deformation-potential approximation.[14,22–25]

II. EXPERIMENT

The sample used in our experiments were undoped liquid-encapsulated-Czochralski-grown semi-insulating GaAs(100), grown by the ICI Wafer Technology Ltd. The room temperature resistivity of the sample was 10^8 Ω, and the thickness was 0.5 mm. The substrate was annealed at

500 °C for an hour to reduce possible positron trapping defects inside the bulk. This was confirmed by positron lifetime measurement in a previous work.[26] It was then degreased in acetone and ethanol prior to being etched in standard solutions of $NH_4OH:H_2O_2:H_2O(3:1:90)$ and $H_2SO_4:H_2O_2:H_2O(8:1:1)$ for 1 min, respectively. A 1000-Å gold layer was evaporated onto each side of the sample to form a circular spot with 8-mm diameter. A dc bias was applied across the sample for the positron drift measurements.

Doppler broadening measurements of positron annihilation radiation were performed with a magnetically guided positron beam at Brookhaven National Laboratory. Fast positrons from a 50 m Ci ^{22}Na source was moderated in a 1-μm-thick W(100) single crystal foil in transmission geometry. The beam intensity was about $3 \times 10^5 e^+$/s, and its diameter was 4 mm. The sample was mounted on the coldfinger of a closed-cycle He refrigerator cryostat for low-temperature measurements and the pressure during the measurements was 10^{-8} mbar. The incident positron beam energy was varied from 0.1 to 50 keV. A high-purity Ge detector was used to detect the positron-electron annihilation gamma spectra. A total of 1×10^6 counts were collected under the 511-keV annihilation photopeak using a digitally stabilized multichannel analyzer.

III. METHOD OF MEASURING BOTH TEMPERATURE-DEPENDENT POSITRON DIFFUSION COEFFICIENT AND MOBILITY

Positrons thermalize rapidly (~ 10 ps) after they are implanted into solids.[27] Thermal positron transport can be modeled using the drift-diffusion equation.[1,28] In our case, the system can be approximately treated as a semi-infinite space with a perfectly absorbing boundary at the Au/GaAs interface. The drift-diffusion equation can be solved with proper boundary and initial conditions.[19] By integrating the positron current density at the Au/GaAs interface, the fraction of positrons reaching this interface ($z=0$) can be obtained as[19,29]

$$F_{in} = \int_0^\infty P_E(z)e^{-z/L_{eff}}dz, \quad (1)$$

where z denotes the distance from the interface along the positron beam entering direction. $P_E(z)$ is the implantation profile for a two layer structure, given as[20,30–34]

$$P(z) = m\frac{(z+a)^{m-1}}{z_0^m}\exp\left[-\left(\frac{z+a}{z_0}\right)^m\right], \quad (2)$$

where $a=(\rho_{Au}/\rho_{GaAs})\Delta$, ρ_{Au} and ρ_{GaAs} are densities (in g cm^{-3}) of Au overlayer and GaAs crystal, respectively. Δ is the thickness of the Au layer. The parameters are taken as $\alpha=450$ Å g cm^{-3}, $m=2.0$, $n=1.6$.[32–36] $z_0=(\alpha/\rho_{GaAs})E^n$, and the beam energy E is in keV. The electric field is not expected to distort the implantation profile of the keV positrons. The positron mean implantation depth is $z_0\Gamma(1+1/m)$.

The effective diffusion length

$$L_{eff}(T,V) = \left\{\frac{\nu_+(V)}{2D_+(T)} + \left[\frac{1}{D_+\tau} + \left(\frac{\nu_+}{2D_+}\right)^2\right]^{1/2}\right\}^{-1} \quad (3)$$

depends on both the temperature T and the applied bias V across the sample. ν_+ is the positron drift velocity, D_+ is the positron diffusion coefficient, and τ is the positron lifetime. The measured line-shape parameter $S(E)$ can be expressed as[37]

$$S(E) = F_{Au}S_{Au} + (1-F_{Au})[F_{in}S_{in} + (1-F_{in})S_b], \quad (4)$$

where F_{Au} is the fraction of positrons annihilated in gold overlayer. S_{Au}, S_{in}, and S_b are the specific S parameters of the Au overlayer, Au-GaAs interface, and bulk GaAs (SI). Thus an experimental value of the fraction of positrons reaching the absorbing boundary for beam energy E at temperature T under a bias of V can be obtained as

$$F_{in}(E,T,V) = \frac{1}{S_b(T) - S_{in}(T)}$$
$$\times \left[S_b(T) - \frac{S(E,T,V) - F_{Au}S_{Au}(T)}{1-F_{Au}}\right]. \quad (5)$$

When no bias is applied across the sample, i.e., $V=0$, the electric field throughout the sample is zero, expect in the narrow Au/GaAs contact region where a small ''built-in'' contact potential exists. Since the ''built-in'' potential of Au/GaAs is very small (~ 0.3 eV), this field effect in the contact region is neglected in our analysis and will not seriously influence the positron motion in the bulk. Under this approximation, from Eqs. (1) and (3), the fraction of positron diffusing back to the interface is

$$F_{in}(E,T,0) = \int_0^\infty P_E(z)e^{-z/L_{eff}(T,0)}dz, \quad (6)$$

where $L_{eff}(T,0) = [D_+(T)\tau(T)]^{1/2}$. By fitting Eq. (6) to the experimental data, the temperature-dependent positron diffusion coefficient $D_+(T)$ can be obtained.

When a bias of V is applied across the sample, the bias will drop mainly across the wide depletion region of the Au/GaAs Schottky contact, creating a large electric field. The mean electric field in the depletion region is[38]

$$E_d(V) = \left[\frac{eN_D(\phi_{bi} + V - IR_b)}{2\varepsilon_0\varepsilon_r}\right]^{1/2}, \quad (7)$$

where I is the current flowing through the sample. R_b is the bulk resistance. ε_r is relative permittivity, and N_D is the concentration of deep donor EL2 in GaAs (SI). ϕ_{bi} is the ''built-in'' contact potential given by $e\phi_{bi} = \phi_b - (E_c - E_f)$, ϕ_b is the Schottky barrier height. $E_c - E_f$ is the bulk Fermi level measured from the bottom of the conduction band. Compared to the positron mean implantation depth of beam energy less than 50 keV in this study, the wide depletion region (~ 3 μm) created by a large reverse bias (~ 25 V) can be approximately treated as infinity. Thus the fraction of positron drift to the interface is

$$F_{in}(E,T,V) = \int_0^\infty P_E(z)e^{-z/L_{eff}(T,V)}dz, \quad (8)$$

where

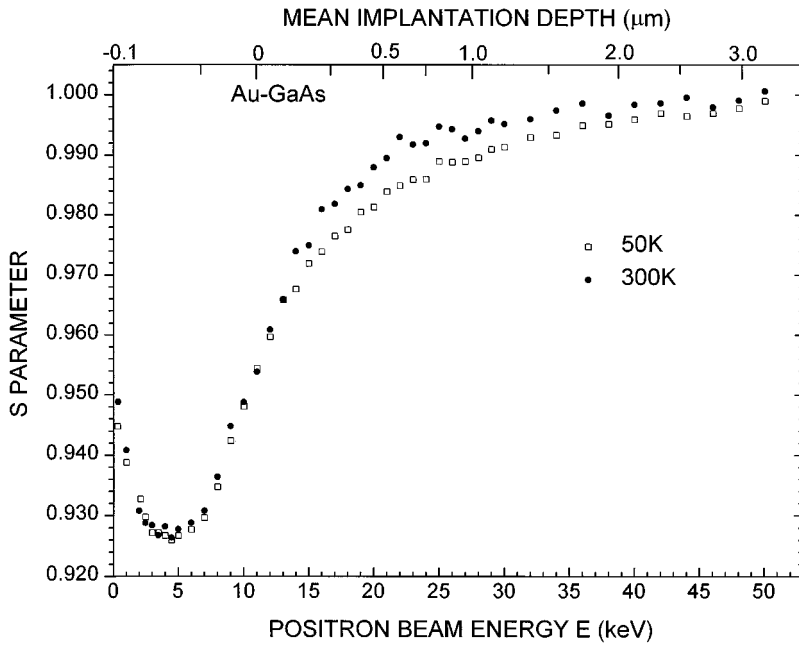**MEAN IMPLANTATION DEPTH (μm)**

FIG. 1. The line-shape S parameter as a function of the incident positron beam energy at temperatures 50 and 300 K. The mean implantation depth for incident energies $E < 11$ keV and $E \geq 11$ keV, represents positron implantation mainly in the 1000-Å overlayer and in bulk GaAs, respectively.

$$L_{\text{eff}}(T,V) = \left\{ \frac{\mu_+ E_d(V)}{2D_+(T)} + \left[\frac{1}{D_+\tau} + \left(\frac{\mu_+ E_d}{2D_+} \right)^2 \right]^{1/2} \right\}^{-1} . \qquad (9)$$

By fitting Eq. (8) to the experimental data with a bias applied, a temperature-dependent positron mobility $\mu_+(T)$ can be obtained. Therefore, both temperature-dependent positron diffusion coefficient and mobility are determined experimentally. By comparing the obtained $D_+(T)$ and $\mu_+(T)$, a way to check the consistency of the Nerst-Einstein relation for positron transport in a wide temperature range can be provided.

IV. RESULTS AND DISCUSSIONS

Figure 1 shows the measured S parameter values as a function of positron incident energy at 50 and 300 K. The S values are normalized to the bulk GaAs S value of 0.4985.

The mean implantation depth is indicated on the upper axis. The smaller $S(E)$ values at 50 K indicate more positron diffusing to the Au/GaAs interface at lower temperature because the interface S value is smaller and the bulk S value almost temperature independent, as presented in Fig. 2. The merge of the two $S(E)$ values at around 12 keV indicates the Au/GaAs is a perfect absorbing boundary, which means that all the positrons diffusing back to the interface are trapped and annihilate in the interface. This is in agreement with the lifetime measurements.[26]

Figure 2 shows the S parameter as a function of temperature for several incident-beam energies. The measured S value of 0.4985(5) at a beam energy of 50 keV is assumed to be the bulk S value of GaAs (SI), which shows a nearly temperature-independent behavior, and is in good agreement with other works.[18,39] All the S values are normalized to this bulk value. The constant S value at 50 keV indicates that no
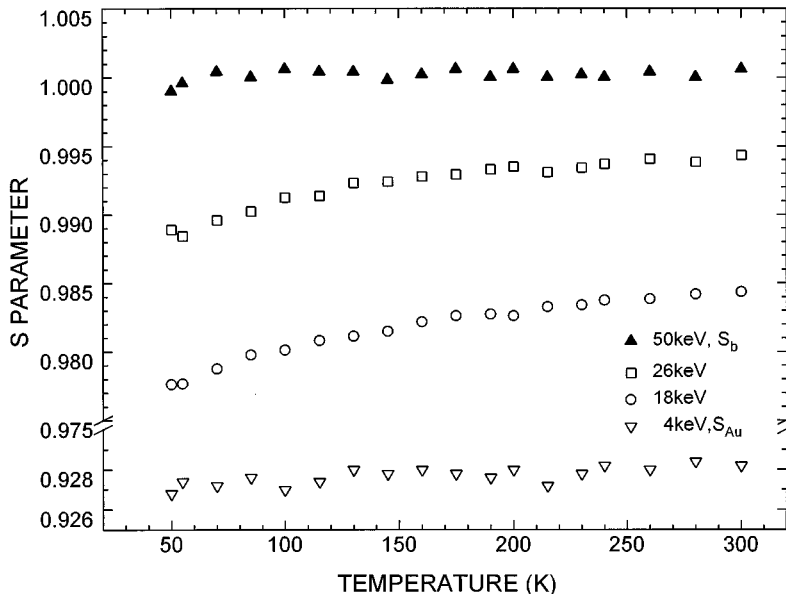

FIG. 2. Doppler broadening line-shape S parameter as a function of sample temperature for incident positron energies of 4, 18, 26, and 50 keV, corresponding to the cases of positrons implanted meanly in the Au overlayer, in the region of GaAs close to Au/GaAs interface, and in bulk GaAs.
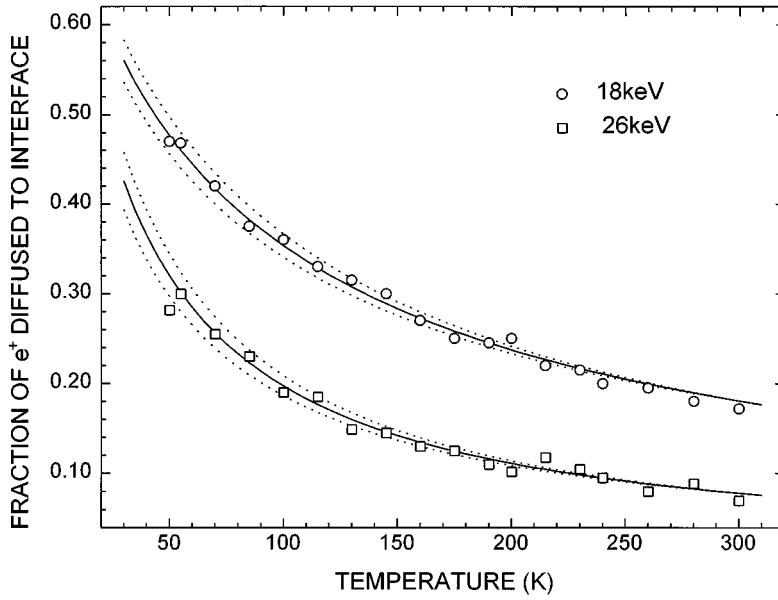
FIG. 3. The fraction of the positron diffusing back to the Au/GaAs interface as a function of temperature for positron beam energies of 18 and 26 keV, respectively. The solid and dotted lines are the calculations from Eq. (8), corresponding to diffusion coefficient $D_+(T) = 9400T^{-\beta}$ cm^2 s^{-1}, $\beta = 1.5 \pm 0.1$.

trapping at vacancy-type defects occurs in the studied temperature range. The S value of 0.9265(5) for a beam energy of 4 keV characterized the Au overlayer, which shows a very small linear increase possibly due to lattice expansion. So the specific S values characterizing bulk GaAs (S_b), Au/GaAs interface (S_{in}), and Au overlayer (S_{Au}) were all assumed to be temperature independent, and were taken as 1.0, 0.9729, and 0.9265, respectively, in our data analysis. The interface S value can be obtained by fitting the S-E curve.[19] For incident energies of 18 and 26 keV, positrons are mainly implanted into the bulk region close to the interface. Consequently, a large amount of positrons will diffuse to the interface and annihilate there. Since diffusion is temperature dependent, the measured S value as the function of temperature will characterize the temperature-dependent positron diffusion. When temperature decreases from 300 to 50 K, S values decrease from 0.9843(5) to 0.9775(5), and from 0.9944(5) to 0.9890(5) for beam energies of 18 and 26 keV, respectively. Although a measurement at a single energy value is sufficient to yield D_+ and μ_+, we used two beam energy values to obtain a more robust result.

Figure 3 shows the fractions of the positron F_{in} diffusing back to the Au/GaAs interface as a function of temperature. F_{in} increases when the temperature decreases. By fitting Eq. (6) to the data, the temperature-dependent positron diffusivity D_+ of 9400 T$^{-\beta}$ cm^2 s^{-1}, with $\beta = 1.5 \pm 0.1$, was obtained. This result is consistent with the calculation of momentum relaxation time due to optical-phonon scattering using the deformation-potential approximation.[14,22–25] Unlike cubic systems with only one atom in its primitive cell, zinc-blende lattice GaAs has two different atoms in its primitive cell. For each wave vector there are three acoustic-phonon modes and three optical-phonon modes. Optical-phonon scattering is important for positron diffusion in GaAs. As shown in earlier works, acoustic-phonon scattering alone could not explain the experimental results.[14,15,18]

In the above data analysis, the fraction of positron annihilated in the Au overlayer is calculated by

$$F_{\text{Au}} = \int_{-a}^{0} P_E(z)\,dz. \qquad (10)$$

The implanted thermalized positrons in the evaporated Au overlayer can be assumed to be trapped, and to annihilate inside the Au layer where significant defects are present. Table I lists the values of the parameters used in the calculations.

When a reverse bias is applied across the sample, the bias drops mainly across the Au/GaAs Schottky barrier region, forming a wide depletion region with very strong electric field ($\sim 10^5$ cm V^{-1}). Positrons implanted into the depletion region will drift back to the Au/GaAs interface. The drift effect depends on the positron mobility and the electric field it experiences. Figure 4 shows the S parameter as a function of temperature under a reverse bias of 25 V for positron energies of 18 and 26 keV. Also, data for no bias are pre-

TABLE I. The values of the parameters used in the calculation fitting to the experimental data.

Relative permittivity of GaAs	ε_r	13.2 [a]
Sample resistance at 300 K	R^b	9.95×10^6 Ω
Thickness of the Au layer	Δ	1000 Å
Density	ρ_{Au}	19.3 g cm^{-3}
	ρ_{GaAs}	5.32 g cm^{-3}
Deep donor concentration	N_D	1.5×10^{16} cm^{-3}
Built-in potential	ϕ_{bi}	0.3 eV [b]
Potential across the sample	V	25 V
	IR_b	7.5 V
Implantation profile	α	450 Å g cm^{-3}
	m	2.0
	n	1.6
Positron lifetime	τ (300 K)	230 ps
	$\Delta\tau$ (ps/100 K)	0.6 [c]

[a]Sze (Ref. 38).

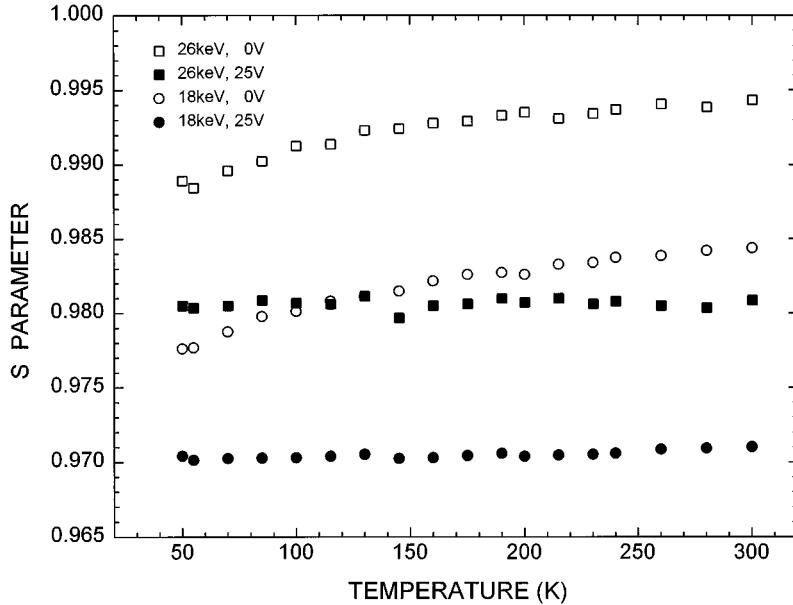[b]Rhoderick and Williams (Ref. 40).

[c]Soininen et al. (Ref. 14).

FIG. 4. The comparisons of zero-biased and 25-V reverse-biased line-shape S parameters as a function of temperature for beam energies of 18 and 26 keV, respectively.

sented for comparison. Smaller and less temperature-dependent S values were obtained, comparing to those without bias. This can be understood because a large fraction of positrons implanted in the high-field depletion region will drift back to the interface of low-S value when the contact is reverse biased. Since the electric field is very large ($\sim 10^5$ cm V^{-1}), saturation of positron drift can be easily achieved.

Figure 5 shows the fraction of positron drifting back to the interface as a function of temperature under a reverse bias of 25 V for beam energies of 18 and 26 keV, respectively. By fitting Eq. (8) to this experimental data, a positron mobility $\mu_+(T)$ of about $10^8 T^{-\sigma}$ cm^2 V^{-1} s^{-1} with $\sigma = 2.5 \pm 0.2$ was obtained. The electric field experienced by positron and the effective positron diffusion length were found by using Eqs. (7) and (9). The values of the parameters used in the calculation are listed in Table I. Because of the saturation in drift, F_{in} cannot be enhanced much by decreasing the temperature if an appropriate reverse bias is applied. A possible high-efficiency positron moderator using GaAs (SI) can be operated at room temperature.[16] On the other hand, σ will not be sensitive to the above fitting when positron drifting is saturated. A more sensitive way of determining the temperature-dependent positron mobility is suggested. If an Ohmic metal-GaAs (SI) contact is prepared instead of a rectifying contact used in our measurements, a small and uniform electric field can be established across the sample. In such case, no saturation drift will happen, and a more accurate σ value can be obtained. This may also be the way to improve positron mobility measurement using drift velocity method in which a uniform electric field is used.[15]

Figure 6 shows the consistency between the Einstein relation and the relation of the obtained positron diffusion coefficient and positron mobility in our measurements. The data points represent cases of the largest deviation from Einstein relation when $(\sigma - \beta) = 1.0 \pm 0.3$ is obtained from the
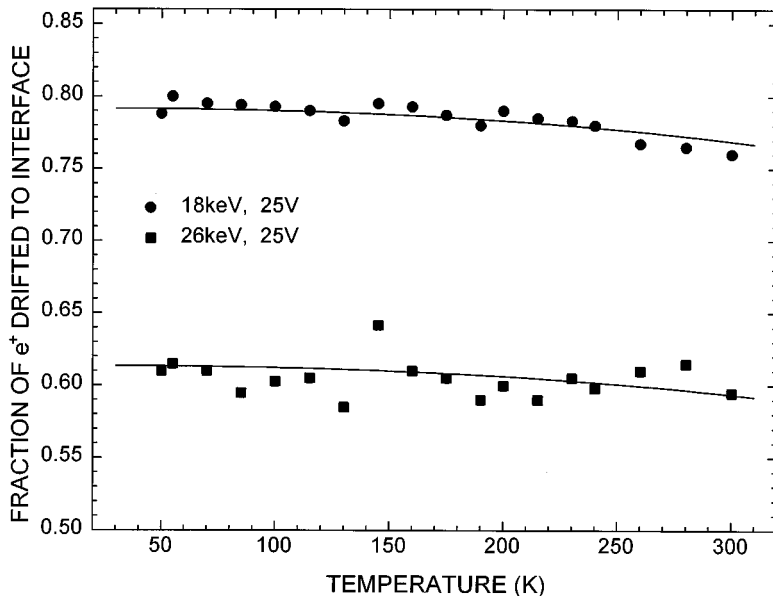

FIG. 5. The fraction of positrons drifting back to the Au/GaAs interface under 25-V reverse bias as a function of temperature with positron incident energies of 18 and 26 keV, respectively. The solid lines are the calculations from Eq. (10), with positron diffusion coefficient of $D_+(T) = 9400 T^{-\beta}$ cm^2 s^{-1}, $\beta = 1.5$, and positron mobility of $\mu_+(T) = 10^8 T^{-\sigma}$ cm^2 V^{-1} s^{-1}, $\sigma = 2.5$.
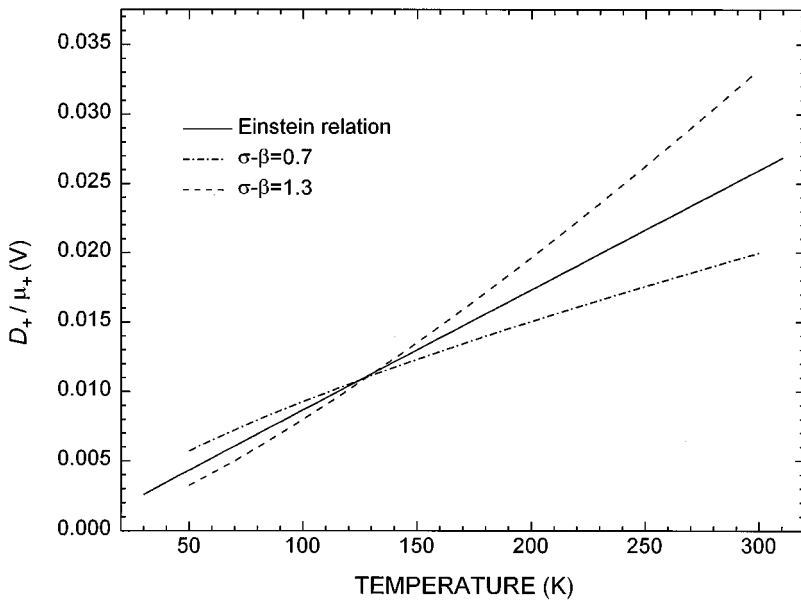
FIG. 6. Comparison between the experimental results of positron diffusion coefficient and mobility with the Einstein relation.

previous fitting shown in Figs. 3 and 5. The agreement in the low-temperature range supports that positron diffusion coefficient follows the $T^{-3/2}$ power law, i.e., the main scattering is from optical phonons in GaAs (SI) in the temperature range of 50–300 K.

V. CONCLUSIONS

A monoenergetic positron beam of 0.1–50 keV was used to study positron transport in semi-insulating GaAs in the temperature range of 50–300 K. Low-temperature effects on positron diffusion and drift were observed. The nearly temperature-independent bulk S value is interpreted that no vacancy-type trap is present at low temperatures. Both temperature-dependent diffusion coefficient and mobility can be experimentally determined for positrons without resorting to the Einstein relation. A positron diffusion coefficient of 9400$T^{-\beta}$ cm^2 s^{-1} and a positron mobility of 10$^8 T^{-\sigma}$ cm^2 V^{-1} s^{-1} in GaAs (SI), with $\beta = 1.5 \pm 0.1$ and $\sigma = 2.5 \pm 0.2$, were obtained in the temperature range of 50–300 K. A way to check the consistency of the Einstein relation for positron motion was provided in this work. The fact that the positron diffusion coefficient and mobility follow the above-temperature power law suggests optical-phonon scattering is the main scattering mechanism in GaAs (SI) in the temperature range studied.

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