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The diffusion length of positrons in different Si wafers

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The diffusion length of positrons in many Czochralski (Cz)-grown Si wafer from different sources has been measured by a monoenergetic positron beam in order to look for a new way for the detection of a small amount of crystalline defects. From the observed relationship between the change in the diffusion length of positrons and that in the capture rate of them, it was found the diffusion length is dominated rather strongly by the presence of shallow traps than that of deep traps. Deep traps can provide a very strong effect on the positron annihilation characteristics as compared with that on the diffusion length. In turn, shallow traps can provide a very strong effect only on the diffusion length without any effect on the annihilation characteristics. On the basis of this new finding, a new way by means of the positron annihilation technique to extract the information on the nature of shallow positron traps and their concentration in Si is proposed.

1. INTRODUCTION

In semiconducting materials, atomic or point defects are electrically active and dominate often the electrical and optical properties. Because of the small size, their direct observation by conventional techniques can be impossible. It has been well established that the positron annihilation technique is very powerful for the study of atomic or point defects in materials[1-4]. Because of the positive charge, positrons are strongly repelled by the positive ion cores in solids. Open volume defects like vacancies and negatively charged impurities are attractive trapping centers for positrons. As a result of trapping, the annihilation characteristics change very sensitively. This uniqueness of positrons has made the technique one of a very few method which can detect point defects in solids. Since the negative values of positron work function for many solid surface were discovered, the generation of low energy positron beam was realized. The low energy positron beams opened a new era for the positron spectroscopy. By means of this new technique, we can now measure the diffusion length of positron in solids. As described later, the diffusion length also tells us the information on point defects. Particularly, in semiconducting materials, the information on the shallow positron traps can be also derived.

In the present work, we measured the Doppler broadening profiles of annihilation radiation as a function of incident positron energy in many Cz-Si wafers from different sources by means of an energy variable positron beam and determined the diffusion length of positron for many different Cz-Si wafers. Based on the experimental results, a systematic interpretation on the effect of point defects on the diffusion length of positrons will be shown.

2. EXPERIMENTAL PROCEDURE AND RESULTS

The monoenergetic positron beam (0-50 keV) used for the present experiment has been reported elsewhere[5]. The Doppler broadening profiles of annihilation radiations were measured as a function of incident positron energy for commercially available Cz-Si from different sources. The lineshape of the spectrum was characterized by a lineshape parameter S which is defined as the counts for a fixed region in the central part of the spectrum divided by the total counts.[4, 5] Figure 1 shows the lineshape parameter S as a function of incident positron energy, i.e., the $S(E)$ response for 12 different Cz-Si wafers. The value of S decreases monotonically with increasing the incident energy for each specimen. The observed energy dependence of S can be well explained as follows[5-8]: implanted positrons not only annihilate in the Si substrate but also diffuse back to the surface, because of the negative work function of a positron for Si. The positrons diffusing back to the surface annihilate at the surface trapped state or positronium state. This behavior can be expressed as

$$S(E) = S_S F_S(E) + S_B F_B(E), \qquad (1)$$

where S_S and S_B are the characteristic values of S for the bulk annihilation and the surface annihilation and $F_S(E)$ and $F_B(E)$ are the fractions of annihilation from respective states. From the one dimensional diffusion model[4], $F_S(E)$ can be given by [6–8]

$$F(E) = \int_0^\infty P(x,E)\exp(-x/L)\,dx, \qquad (2)$$

where $P(x,E)$ is the positron implantation profile and L is the diffusion length of positrons in the substrate. In Fig. 1, the value of S at the energy higher than 20 keV is constant and takes nearly the save value for all the examined specimens. In order to look different manners in the tailing of $S(E)$ for different specimens, Fig. 1 is replotted as Fig. 2 by shifting data points by a constant value among each other. Table 1 lists the determined value of L for 12 different Cz-Si wafer. The specimen dependence of the diffusion length was found to be surprisingly big. Hitherto, the diffusion length of positrons L has been recognized to bear the following relation to the diffusion coefficient of positrons D_0, the bulk annihilation rate λ_B and the trapping rate $\mu_D C_D$:

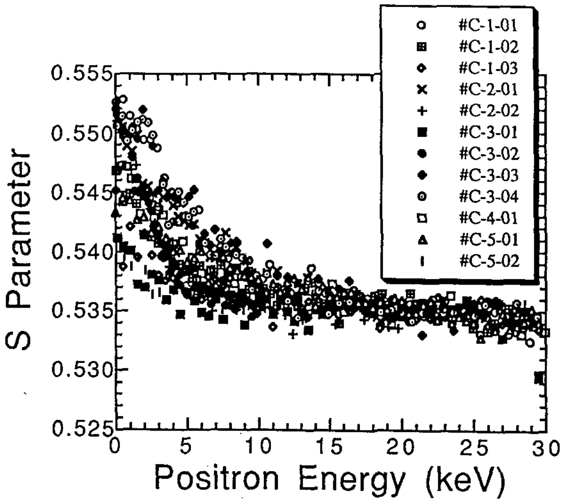

Figure 1. Lineshape parameter S as a function of incident positron energy for 12 different Cz-Si wafers

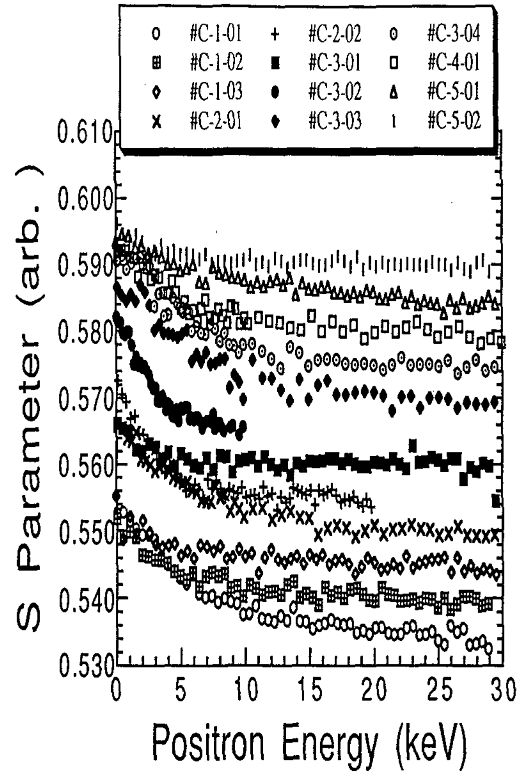

Figure 2. Replotted $S(E)$ response in figure 1 by shifting data points by a constant value among each other.

$$L = [D_0/(\lambda_B + \mu_D C_D)]^{1/2}. \qquad (3)$$

The present experimental results, however, refuse the the validity of the above relation. That is, if L varies between 340 nm and 55 nm, $\mu_D C_D$ in the specimen with the shortest value of L should be 35 times higher than λ_B. Such a high trap-

Table 1
Diffusion length of positrons in Si from different sources.

Specimens	L (Å)	Std. Deviation
# C-1 -01	2955	228
# C-1 -02	1648	225
# C-1 -03	944	183
# C-2 -01	3018	284
# C-2 -02	841	87
# C-3 -01	546	186
# C-3 -02	853	90
# C-3 -03	3438	303
# C-3 -04	2908	255
# C-4 -01	2232	238
# C-5 -01	3293	419
# C-5 -02	1270	141

ping would provide a remarkable increase in S at the Si substrate region comparable to the saturation level. It is not the case. In order to solve this puzzling behavior, we propose a new picture of the effect of defects on the diffusion length of positrons as described in the next section.

3. THE EFFECT OF POINT DEFECTS ON THE DIFFUSION LENGTH OF POSITRONS

In semiconducting materials, two kinds of point defects should be considered to fully explain the trapping behavior of positrons. That is, deep traps and shallow traps. The former group of traps affect both the annihilation characteristics like S_B and the diffusion length of positrons. The latter group, however, affect only the diffusion length. As described briefly in the paper by the present author[9] about no effect of donor doping on positron annihilation in Si, the dielectric constant takes an important role in the trapping mechanism of positrons. This idea is now well established as the positron Rydberg state[10]. That is, charged particles in semiconductors can form hydrogen-like Rydberg states around oppositely charged ions. The value of static dielectric constant in Si is 11.7. So, the radius of the Rydberg states ranges around 3-10 nm. As a result, the annihilation characteristics from the Rydberg states is just the same as the bulk annihilation. Rydberg states affect only the diffusion process of positrons. In the following, we propose a new systematic picture of the positron trapping by both deep traps and shallow traps. The diffusion of positron can be expressed as follows:

$$D_0\nabla^2 n(x,t) - \lambda n(x,t) = \partial n(x,t)/\partial t, \qquad (4)$$

where $n(x,t)$ is the positron probability at the depth x and at the time t, λ is the escape rate of positrons from the diffusion process. We now examined two cases and derived the following relations:

(i) only with deep traps

$$\lambda = \lambda_B + \mu_D C_D \qquad (5)$$

$$\mu_D C_D = \lambda_B[(L_0/L)^2 - 1] \qquad (6)$$

L_0 = diffusion length in a perfect lattice

(ii) only with shallow traps

$$n_S/n_B = (L_0/L)^2 - 1 \qquad (7)$$

n_B = the fraction of positrons in the free state

n_S = the fraction of positrons in the Rydberg state

In the case of (i), the annihilation characteristics like S should vary directly with the change in L. On the other hand, in the case of (ii), only the diffusion length can vary with the presence of shallow traps. The present experimental results can be explained by the case (ii). Therefore, the measurement of the $S(E)$ response can provide the information on both deep and shallow traps. The temperature dependence of n_S/n_B should be important at low temperatures, because the fraction of Rydberg states can be dominated by $n_S/n_B = \exp(E_S/kT)$ and the magnitude of E_S might be around 10 meV. The present experiment and analysis will open a new era for the study of shallow traps in semiconductors which can not be detected by the measurement of annihilation characteristics in them.

4. CONCLUSION

The specimen dependence of diffusion length in Cz-Si wafers can be attributed to the trapping of positrons by shallow traps or the formation of positron Rydberg states. Hitherto, the trapping of positrons by deep traps has made the technique a very sensitive, specific and selective method for point defects. The present new finding added a new way to detect shallow traps by positrons. The detailed description of our systematic picture will be published in a separate paper.

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