Interaction of positrons with the surface of a silicon single crystal

V. I. Gol'danskiĭ, Yu. A. Novikov, A. V. Rakov, and V. P. Shantarovich
Institute of Chemical Physics, Academy of Sciences of the USSR

(Submitted 4 April 1988)
Pis'ma Zh. Eksp. Teor. Fiz. **47**, No. 10, 522–524 (25 May 1988)

The existence of bound states of positrons at a silicon surface has been observed. Such states are possible only for p-type silicon, produced by doping with boron, beginning at carrier densities $p \approx 10^{16}$ cm^{-3}. These states are explained in terms of a change in the sign of the positron work function φ_+ upon a change in the carrier density.

Several recent papers[1-3] have reported the observation of narrow peaks at $\theta = 0$ mrad in the angular distributions of the annihilation γ rays from certain metals (θ is the extent by which the angle between the emission directions of the annihilation γ rays differs from π). The appearance of such a peak is linked with the filling of stationary states in a one-dimensional potential well at the surface of the metal[4] under the condition that the positron work function of the metal satisfies φ_+ (Me) $\geqslant 0$. In the case φ_+ (Me) $\langle 0$, on the other hand, a bound state might be filled if a converter were used[3] and if the positron work function of the metal were related to the converter φ_+ (Conv) by the relation

$$0 > \varphi_+(Conv) > \varphi_+(Me).$$

There is accordingly much interest in studying the interactions of positrons with the surfaces of semiconductors. Semiconductors have a unique ability to undergo a change in electronic properties when small amounts of some other substance are added (doping). The sign of the charge carriers may also change.

The electronic properties vary smoothly as a function of the dopant concentration, and the change in the probability for the appearance of a peak in the angular distribution of annihilation γ rays of semiconductors (β_S) may be manifested in a narrow interval of the values of φ_+ (as φ_+ crosses 0).

The maximum integral contribution of the peak is determined by the probability for the escape of positrons to the surface[5]:

$$P_S \doteq \frac{L/l}{1+L/l}, \tag{1}$$

where $L = \sqrt{D\tau}$ is the positron diffusion length, D is the diffusion coefficient, τ is the positron lifetime, and l is the positron absorption thickness in the substance of interest.

For the experiments we selected single crystals of KÉF silicon (phosphorus-doped n-type silicon) and DKB silicon (boron-doped p-type silicon) with a (100) surface orientation and with resistivities of 4.5 Ω·cm (KÉF-4.5), 15 Ω·cm (KÉF-15),

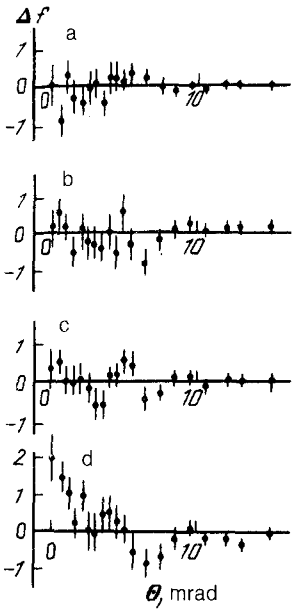

FIG. 1. Differences between the angular distributions of annihilation γ rays, $\Delta f(\theta) = f_2(\theta) - f_1(\theta)$ (in arbitrary units). As $f_1(\theta)$, the angular distribution for KÉF-4.5 has been used. As $f_2(\theta)$, the angular distributions of (a) KÉF-15, (b) high-resistivity silicon, (c) KDB-4, and (d) KDB-1 have been used.

12 kΩ·cm (compensated, high-resistivity), 4 Ω·cm (KDB-4), and 1 Ω·cm (KDB-1). The samples had dimensions of $15\times30\times0.3$ mm. The angular distributions of the annihilation γ rays were measured on an apparatus with a parallel-slit geometry (angular resolution of 0.7 mrad). The positron source was the isotope ^{22}Na with an activity of 10 mCi. We used an optimization procedure in the course of the measurements.[6]

Figure 1 shows differences in the angular distributions of the annihilation γ rays $[\Delta f(\theta) = f_2(\theta) - f_1(\theta)]$. In all cases, we used as $f_1(\theta)$ the angular distribution of the annihilation γ rays for the KÉF-4.5 silicon (in connection with Refs. 1–3 and 6, very accurate measurements have been carried out for this type of silicon, with an error $\sim0.2\%$ at the maximum of the angular distribution); as $f_2(\theta)$ we used that for KÉF-15 (Fig. 1a), high-resistivity silicon (Fig. 1b), KDB-4 (Fig. 1c), and KDB-1 (Fig. 1d). We see that for all the silicon samples, except the KDB-1 we have $\Delta f(\theta) = 0$, within the error. For the pair KDB-1, KÉF-4.5, $\Delta f(\theta)$ takes the form of a narrow peak near $\theta = 0$ mrad. Under the assumption that this peak is determined by the annihilation of positrons (or of positronium atoms) from surface states in the KDB-1, and under the assumption that the magnitude of this peak is determined by the diffusion of positrons to the surface, we find [with $l(\mathrm{Si}) = 110\ \mu$m; Ref. 5]

$$L(\text{KDB-1}) = 0.38 \pm 0.11\ \mu\text{m}.$$

This figure agrees within the error with the value $L = 0.49 \pm 0.08\ \mu$m, found from the data of Ref. 4.

Our experimental results thus confirm that there is a threshold for the appearance of the peak in the angular distribution of annihilation γ rays from silicon in the dopant concentration. This threshold lies in the region of p-type silicon [for the (100) surface orientation], at a hole concentration $p \approx 10^{16}$ cm^{-3}. Consequently, in p-Si(100) at $p > 10^{16}$ cm^{-3} we have φ_+ (Si) > 0; i.e., all the positrons that reach the surface fill surface states. In n-Si(100), i-Si(100), and p-Si(100) with $p < 10^{16}$ cm-3, we have φ_+ (Si) < 0, and all the positrons that emerge at the surface escape from the silicon into vacuum.

In this connection, we can write the angular distributions of the annihilation γ rays from silicon in the general form

$$f(\theta) = (1 - \beta_S) f_B(\theta) + \beta_S f_S(\theta) , \tag{2}$$

where $f_B(\theta)$ is the angular distribution for silicon if the surface is ignored [this distribution is the same as that for the phosphorus-doped n-type silicon with the (100) surface orientation], $f_S(\theta)$ is the angular distribution in the case of annihilation from surface states, and β_S is the probability for the filling of surface states, given by

$$\beta_S = \begin{cases} 0, & \text{при} \quad \varphi_+ < 0 \\ P_S, & \text{при} \quad \varphi_+ \geqslant 0 . \end{cases}$$

To verify this conclusion, we carried out some experiments with a converter. Specifically, we used wafers of Si(100), types KÉF-4.5 and KDB-1, with respect to thicknesses of 300 and 200 μm, as converters. The angular distributions of the anni-

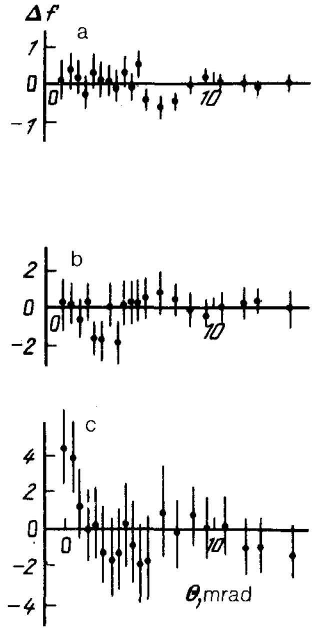

FIG. 2. Differences between the angular distributions of annihilation γ rays, $\Delta f(\theta)$ (in arbitrary units). As $f_1(\theta)$, the angular distribution for KÉF-4.5 has been used. As $f_2(\theta)$, the angular distributions of samples with a chromium film on a KÉF-4.5 substrate have been used, (a) from measurements without a converter, (b) from measurements with a KDB-1 (100) converter, and (c) from measurements with a KÉF-4.5 (100) converter.

hilation γ rays were measured for a sample with a chromium film 0.3 μm thick on a KÉF-4.5 (100) substrate.

Figure 2 shows the differences between the angular distributions, $\Delta f(\theta)$, where we have used the angular distribution for KÉF-4.5 (100) as $f_1(\theta)$, while as $f_2(\theta)$ we have used the angular distribution for a sample with a chromium film in measurements without a converter (Fig. 2a) and with converters of KDB-1 (100) (Fig. 2b) and KÉF-4.5 (100) (Fig. 2c). We see quite clearly that in the measurements without a converter (Fig. 2a) there is no narrow peak in the angular distribution from chromium. This result is explained[1] on the basis of a negative positron work function of chromium [$\varphi_+(\mathrm{Cr}) = -1.7 \pm 0.2$ eV; Ref. 7]. There is again no peak in the measurements with the KDB-1 converter (Fig. 2b), as follows from the results reported above on the measurements of the angular distribution for KDB-1. In experiments in which we used KÉF-4.5 (100) as a converter, there was a peak in $\Delta f(\theta)$ (Fig. 2c). According to Refs. 3 and 5, its relative contribution to the angular distribution of chromium is described by the expression

$$\beta = \frac{L/l}{1 - L/l}, \tag{3}$$

where β is the probability for annihilation from surface states of the chromium film. In (3), in contrast with (1), L is the diffusion length, and l is the absorption length of the positrons in the converter, not in the substance whose angular distribution is being measured. We then find

$$L(\text{KÉF-4.5}) = 0.43 \pm 0.14\,\mu\text{m}.$$

in good agreement with the data of Ref. 4 and the results which we reported above for L (KDB-1).

Two mechanisms are thus operating in the interaction of positrons with the surface of a silicon single crystal with a (100) surface orientation. The first of these mechanisms, which operates in n-Si, i-Si, and p-Si with $p < 10^{16}$ cm^{-3}, consists of the emission into vacuum of slow positrons which have reached the surface. The second mechanism, manifested in p-Si with $p > 10^{16}$ cm^{-3}, consists of the capture in surface states of positrons which have emerged at the surface of the silicon single crystal.

---

[1] K. A. Valiev, V. I. Gol'danskiĭ, Yu. A. Novikov *et al.*, Pis'ma Zh. Eksp. Teor. Fiz. **45**, 296 (1987) [JETP Lett. **45**, 373 (1987)].

[2] L. G. Aravin, K. A. Valiev, V. I. Gol'danskiĭ *et al.*, Proceedings of the European Meeting on Positron Studies of Defects (PSD-87), GDR 2, Part 2, 1987, p. 29.

[3] Yu. A. Novikov, A. V. Rakov, and V. P. Shantarovich, Dokl. Akad. Nauk SSSR (in press).

[4] P. Hautojärvi (editor), Positrons in Solids (Topic in Current Physics, Vol. 12), Berlin, 1979.

[5] Yu. A. Novikov, A. V. Rakov, and V. P. Shantarovich, Preprint, Institute of General Physics, Academy of Sciences of the USSR, 1988.

[6] L. G. Aravin, Yu. A. Novikov, M. K. Filimonov, and V. P. Shantarovich, Poverkhnost', No. 4, 77 (1987).

[7] A. P. Mills, P. M. Platzman, and B. L. Brown, Phys. Rev. Lett. **41**, 1076 (1978).

Translated by Dave Parsons