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Electrical resistivity of bismuth implanted into silicon

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We investigate the electrical properties of Bi-doped Si samples, prepared by ion implantation, in a range of concentrations around and above the metal–nonmetal transition. Comparison between experimental and theoretical values of the resistivity brought out that in these samples a similar behavior is observed as for other n-doped Si, thus confirming the results obtained in the same range of impurity concentration, i.e., $\rho(\mathrm{Sb})<\rho(\mathrm{P})<\rho(\mathrm{As})<\rho(\mathrm{Bi})$. © *1996 American Institute of Physics.* [S0021-8979(96)05404-X]

INTRODUCTION

The theoretical and experimental investigations of the transport properties of heavily doped semiconductors continue to be a topic of considerable interest.[1–13] Recently the systems Si:P,[2–5,10–13] Si:As,[3,12,13] Si:Sb,[3] Si:Bi,[3] Si:B,[1,9] and Si doubly doped with P and As donors (Si:P, As),[6] and P donors and B acceptors (Si:P,B),[6–8] and other pair systems[6,14,15] have again demonstrated the interest of such investigations. Nevertheless, some lack of experimental and theoretical information exists, particularly for Bi, the last dopant of the V column of the periodic table, which has been observed to have a low equilibrium solid solubility limit in silicon crystal.[3,16] It is worthwhile to point out that the Si:Bi system has not been given much attention probably because of its large ionization energy and smaller effective Bohr radius, i.e., $E_I=71$ meV and $a^*=8.9$ Å, respectively, compared to the three donors, P, As, and Sb. With such values of E_I and a^* the theory of the effective mass was expected to be less applicable to the Si:Bi system.[3] Owing to the smaller value of a^* one expects that a higher donor concentration will be required to reach a metallic regime, i.e., above the metal–nonmetal (MNM) transition.

The aim of this work is to investigate the Hall mobility μ_H and resistivity ρ of Si:Bi in a range of doping around and above the MNM transition. The experimental procedure is at room temperature with the samples prepared by ion implantation, which is an important method of making semiconductor devices.[16]

The theoretical calculations are carried out at a similar doping regime. The impurity critical concentration N_c for the MNM transition has been proposed to describe the specific feature of the transition. The values of N_c were found to vary from 1.0 to 1.8×10^{19} cm^{-3}.[3]

In the measured resistivity of the Si:Bi system we observe a continuous increase of resistivity around N_c, going below the metallic region. This behavior is more accentuated in Si:Bi compared to other n-type-doped Si systems.[3,10–13,17,18] In Si:P, for instance, increasing temperature, from 4.2 to 300 K, results in a lower resistivity below the MNM transition.[19,20] There is a crossover of ρ around N_c for this range of temperatures. Above this value ρ, at 4.2 K, presents a similar behavior for those higher temperatures, i.e., 77 and 300 K, respectively.[12,19,20] The results obtained confirm the general features of the resistivity, i.e., $\rho(\mathrm{Sb})<\rho(\mathrm{P})<\rho(\mathrm{As})<\rho(\mathrm{Bi})$.[3,21,22]

EXPERIMENTAL DETAILS

The Si wafers used in this work were of p type and (100) oriented with resistivity in the range of 16–25 Ω cm Van der Pauw structures[23] having low sheet resistance areas (<20 Ω/□, phosphorus doped) were implanted at nominal room temperature with Bi±. Five implantations with energies of 35, 70, 120, 200, and 360 keV were accumulated in each sample with proper doses to result in a plateaulike depth profile of Bi with ~5% deviation up to the depth of 0.15 μm, according to TRIM simulation.[24]

Samples with Bi concentrations of 5×10^{17}, 5×10^{18}, 1×10^{19}, 5×10^{19}, 1×10^{20}, and 5×10^{20} cm^{-3} were prepared and labeled as samples 1, 2, 3, 4, 5, and 6, respectively. For sample 6 the implanted Bi doses are 5×10^{14} cm^{-2} (at 35 keV), 7×10^{14} cm^{-2} (at 70 keV), 8×10^{14} cm^{-2} (at 120 keV), 1.4×10^{15} cm^{-2} (at 200 keV), and 2.5×10^{15} cm^{-2} (at 360 keV). For the samples 1, 2, 3, 4, and 5 these doses were reduced by a factor of 1000, 100, 50, 10, and 5 times, respectively.

The damage annealing and the electrical activation of Bi was performed at 600 °C for 30 min in an inert atmosphere. Since Bi+ doses for samples 1, 2, and 3 were below the threshold for amorphization a second annealing step at 900 °C for 60 s was performed to enhance the electrical activation of Bi.

The van der Pauw devices were electrically characterized by sheet resistivity $R(\Omega/\square)$ and Hall measurements at room temperature.

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TABLE I. Room-temperature measurements of Si:Bi.

Sample	R ($\Omega/\hbar$)	μ ($cm^2/V\,s$)	n_s (cm^{-2})	N_d (cm^{-3})	ρ (Ω cm)
1	3424	535	3.4×10^{12}	3.0×10^{17}	0.039
2	1112	277	2.0×10^{13}	1.8×10^{18}	0.012
3	708	189	4.7×10^{13}	4.0×10^{18}	0.0083
4	302	77	2.7×10^{14}	2.2×10^{19}	0.0037
5	187	59	5.7×10^{14}	4.8×10^{19}	0.0022
6	99	38	1.7×10^{15}	1.4×10^{20}	0.0012

RESULTS AND DISCUSSION

The room-temperature impurity resistivity is calculated from the generalized Drude approach (GDA),[25,26]

$$\rho(w)=\frac{-im^*w}{N_de^2}+i\frac{2}{3\pi N_dkw}\int_0^\infty dq\ q^2\left(\frac{1}{\epsilon(q,w)}-\frac{1}{\epsilon(q,0)}\right). \tag{1}$$

This expression is assumed to be valid for all frequencies w, especially for zero frequency which is the limit of interest here. In Eq. (1) $\epsilon(q,0)$ is the static temperature-dependent random-phase-approximation (RPA) dielectric function of the donor electrons, m^* is the effective mass, and k is the dielectric constant of the material.[25,26]

For the sake of comparison the low-temperature impurity resistivity $\rho=1/\sigma$ (inverse of the conductivity σ) is also calculated from the Sommerfeld expansion, where we keep only the lower-order terms. Therefore, we can use such an expansion for $T<10$ K, which is the validity of this calculation, to obtain[3,5]

$$\sigma=\sigma_0+\Delta\sigma, \tag{2}$$

where σ_0 is the zero temperature conductivity derived from the Kubo formalism, given by[3,5]

$$\sigma_0=\frac{eN_v}{3\hbar}\int\sum(E_F,N_d)\left(\frac{df(E)}{dE}\right)dE \tag{3}$$

and

$$\Delta\sigma=f[T,D(E_F)]. \tag{4}$$

In the above equations, N_V is the number of valleys of the conduction band ($N_V=6$ for Si),[3] N_d is the donor impurity concentration, E_F is the Fermi energy, $D(E_F)$ is the density of states at E_F, and $f(E)$ is the Fermi distribution function.

For the MNM transition four criteria have been used to determine N_c, based mainly on use of a regular lattice, a randomlike distribution of impurities, a disordered one-band model, and the Hubbard model. The values of N_c vary from 1.0 to 1.8×10^{19} cm^{-3}.[3] The latter value of N_c, corresponding to the two first criteria, is closer to the value obtained from the general expression of the Mott criterion (i.e., $N_c^{1/3}a^*\cong0.25$) for the MNM transition.[27] We adopt this value.

In Table I we show the measured values of the samples with concentration varying from 3.0×10^{17} to 1.4×10^{20} cm^{-3}. The resistivity is calculated by $\rho=1/q\mu N$ and the Hall coefficient by the relation $R_H=1/Nq$, where q is the electrical charge. It means that the Hall scattering factor $A=1$, which is a good approximation for heavily doped semiconductors.[13] The carrier concentration N is identified with N_d.

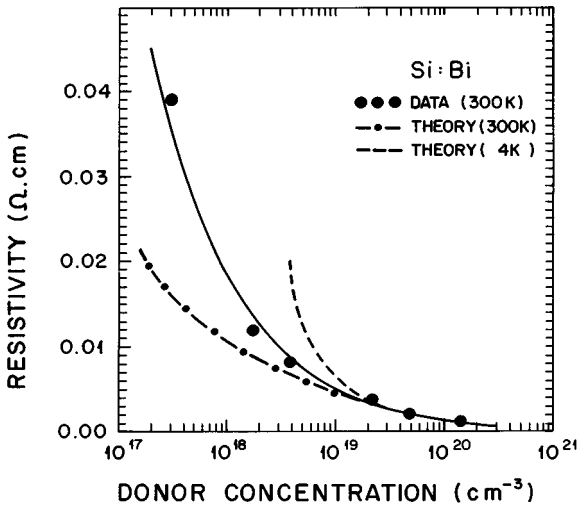

FIG. 1. The room-temperature resistivity ρ of Si:Bi as a function of donor impurity concentration N_d. The dotted-dashed and dashed lines represent our calculations at 300 and 4 K, using Eqs. (1) and (2), respectively.

In Fig. 1 we plot the resistivity of Si:Bi as a function of impurity concentration for both experimental and theoretical results. The experimental data, at room temperature, are represented by solid circles. The line joining the circles is obtained by fitting of the equation

$$\rho=bN^{-a}, \tag{5}$$

where $a=0.5517$ and $b=1.582\times10^{-8}$. We observe a continuous increase of the resistivity with decreasing doping regime around 2×10^{19} cm^{-3}, where, at very low temperature, one expects a MNM transition.[3]

This continuous increase of resistivity at room temperature is more accentuated than, for instance, in the Si:P

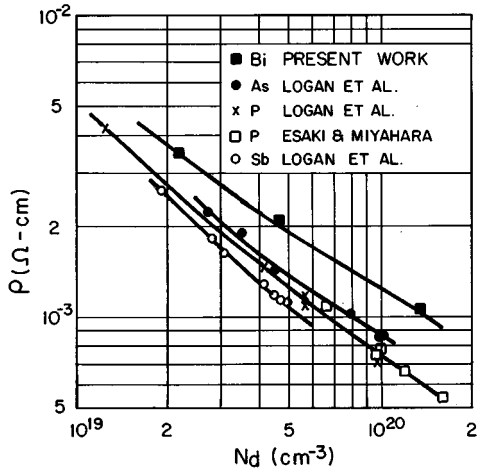

FIG. 2. Log–log plot of resistivity vs impurity concentration at room temperature, for silicon samples doped, respectively, with bismuth, arsenic, phosphorus, and antimony. The data of (●) As, (×) P, and (○) Sb are from Logan and co-workers (Ref. 21) and (□) P are from Ref. 22.

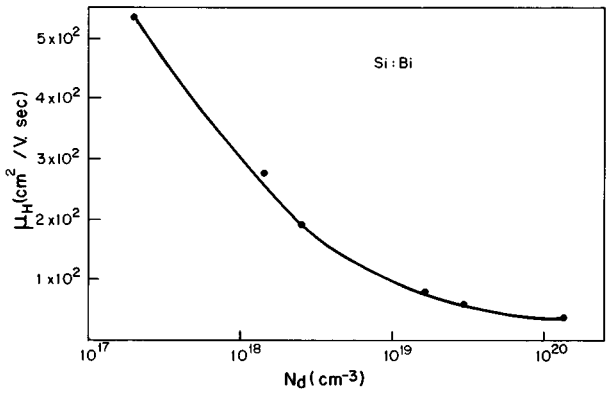

FIG. 3. Hall mobility μ_H vs donor impurity concentration of Si:Bi at room temperature.

system.[19,20] We may argue that this is due to its low ionization energy of 71 meV, compared to 45 meV of Si:P, which will lead to higher values of N_c at the MNM transition.

In Fig. 1 we also observe a similar behavior above the MNM transition for both calculations, i.e., 300 K and 4 K, using Eqs. (1) and (2), respectively, as one expects for the metallic regime. For the temperature of 300 K the agreement between theory and experiment, above 10^{18} cm^{-3}, looks quite good.

The doping of Si with Sb, P, As, or Bi gives rise at low concentrations to a set of discrete donor levels with bound states whose ionization energies (which directly determine their effective Bohr radia) are about 43, 45, 53, and 71 meV, respectively.[3,28] Their respective effective Bohr radia are about 16, 15, 13, and 9 Å.[3,28] As the concentration of donors is increased, the overlap and hopping between nearby states and the random arrangements of adjacents centers cause the bound-state energies to be spread into a band which is eventually separated from the host conduction band. Considering the effective Bohr radius to vary from the lower to the larger value, i.e., a^* (Bi) to a^* (Sb), σ moves toward larger values in the following order: $\sigma(\mathrm{Sb})>\sigma(\mathrm{P})>\sigma(\mathrm{As})>\sigma(\mathrm{Bi})$. This is as expected because a large a^* (i.e., small ionization energy) causes a larger overlap and, consequently, a bigger conductivity. As a consequence N_c moves toward lower values, i.e., $N_c(\mathrm{Sb})<N_c(\mathrm{P})<N_c(\mathrm{As})<N_c(\mathrm{Bi})$, where $N_c(\mathrm{Sb})=3.0\times10^{18}$ cm^{-3}, $N_c(\mathrm{P})=3.7\times10^{18}$ cm^{-3}, $N_c(\mathrm{As})=(6.4-8.5)\times10^{18}$ cm^{-3}, and $N_c(\mathrm{Bi})=1.8\times10^{19}$ cm^{-3}.[3,28]

In Fig. 2 we compare the resistivity versus the impurity concentration, at 300 K, for the Si:Bi system with those of the other three systems, i.e., Si:As, Si:P, and Si:Sb. Above 10^{19} cm^{-3} we confirm the general feature observed for resistivity, i.e, $\rho(\mathrm{Bi})>\rho(\mathrm{As})>\rho(\mathrm{P})>\rho(\mathrm{Sb})$.[3,21]

Figure 3 shows the room-temperature Hall mobility as a function of bismuth concentration. We observe that the qualitative and quantitative values, above 10^{17} cm^{-3}, are similar to those obtained by Mousty, Ostoja, and Passan for Si:P.[29] Above $N_d=2\times10^{19}$ cm^{-3} the values of $\mu_H=\mu q\approx10^2$ cm^2/V s are close to the theoretical prediction.[3]

In the absence of a complete study in Si:Bi comparable, at least, to the Mousty and co-workers work[29] in Si:P, we conclude that further analysis of this system is certainly very interesting. Such work is under consideration even at very low temperature and will be reported in the near future.

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