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Thermodonor activation energy and mechanisms of tensoeffects in transmutation-doped γ-irradiated silicon

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Abstract. Activation energy of high temperature technological thermodonors (TD) has been determined in transmutation-doped *n*-Si(P) using the data analysis of the Hall-effect temperature dependence. Physical mechanisms of tensoeffects in *n*-Si(P) crystals doped by neutron irradiation and doped at growth were studied by the tensoeffects measurements and by analysis of the pressure dependencies of the electron concentration ratio in "upper" and "lower" Δ_1-valleys of uniaxially strained samples. Comparison of the some parameters for the crystals doped either by neutron transmutation method or in the melt is carried out.

Keywords: silicon, transmutation doping, thermodonors, gamma-irradiation.

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1. Introduction

The analysis of the tensoeffect measurement data in neutron transmutation doped (NTD) *n*-Si(P) crystals [1, 2] allows to detect the energy levels in the forbidden band which we attribute to the presence of TD defects in the crystal volume. Obviously, thermodonors in NTD *n*-Si(P) must be generated in crystals with high content of oxygen during high-temperature technological annealing. It is known, that the high-temperature technological annealing of the ingots irradiated by slow neutrons is carried out at 800÷850 °C for 1÷2 hours in order to remove radiation-induced damages of the crystalline lattice. However, a small change of the electron concentration and overlapping of ionization exponents of the TDs and phosphorous atoms in the investigated crystals [1, 2] as the temperature increases do not allow correct determination of the activation energies of the mentioned technological TDs.

In this work we present the transport phenomena measurements for a slightly neutron-irradiation doped silicon contributing to the both determination of TDs activation energies and tensoeffects mechanisms identification in high uniaxially strained NTD *n*-Si(P) crystals. Note that the NTD silicon has important applications thanks to the high homogeneity of the phosphorus dopant distribution over the crystal volume. Therefore, since in pure crystals the technology thermodonors act as a codopant, the examination of electrophysical properties of NTD n-Si(P, TD) is very important, first of all to optimize the annealing procedure. Some important parameters of the crystals doped either by slow neutrons irradiation or at the growth will be compared as well.

2. Experimental

The tensoresistivity (TR) effect, tenso Hall-effect (THE), current-voltage characteristics (ICV), as well as the temperature dependencies of conductivity, TR and THE were measured using the original installation for investigation of physical properties of solids under high uniaxial pressure [3]. For tensoeffecs measurement, samples of n-Si doped with phosphorus either at growth or by slow neutrons irradiation were used. Technological high-temperature annealing at $T = 800$ °C for 2 h was carried out in order to remove the irradiation-induced damages of the crystalline lattice in NTD *n*-Si crystals. Corresponding concentration of γ-irradiation-induced defects was achieved by choosing the proper dose exposure from a ^{60}Co source. The X-ray method of crystallographic orientation determining was used. The accuracy of this method is ±15″. After the specimen preparation and its mounting in the pressure module the precision of the sample orientation with respect to the applied stress was approximately ±30′.

3. Results and discussion

The parameters of the investigated crystals doped by various methods are listed in Table 1.

The typical pressure dependence of resistivity in uncompensated n-Si crystals doped by phosphorus from the melt (samples 1,5,7, Table 1) is characterized by the saturation of resistivity at uniaxial pressure $X \approx 0.7$ GPa (curve 2, Fig. 1). This peculiarity is determined by the Smith-Herring's dominant mechanism of TR which is defined by the redistribution of c-band electrons between the Δ_1-minima when **X**||[001] increases. On the contrary, the pressure dependencies of resistivity in NTD n-Si(P) crystals (samples 2,3,4,8,9, Table 1) are characterized by the both maximum availability on the resistivity dependencies at $X \approx 0.6$ GPa and following exponential-shape decreasing of resistivity in the pressure range 0.6÷1.2 GPa (curves 1,3, Fig. 1). Note, that the results of the corresponding calculations testify the complete transition of electrons to the "lower" valleys, since the strain-induced energy splitting of the Δ_1-valleys essentially exceeds the value of kT ($\delta\varepsilon > 10$ kT [4]). It is known that the value of energy splitting of the Δ_1-valleys in silicon in the case **X**||[001] can be determined as:

$$\partial\varepsilon = \frac{\Xi_u X}{C_{11} - C_{12}}, \tag{1}$$

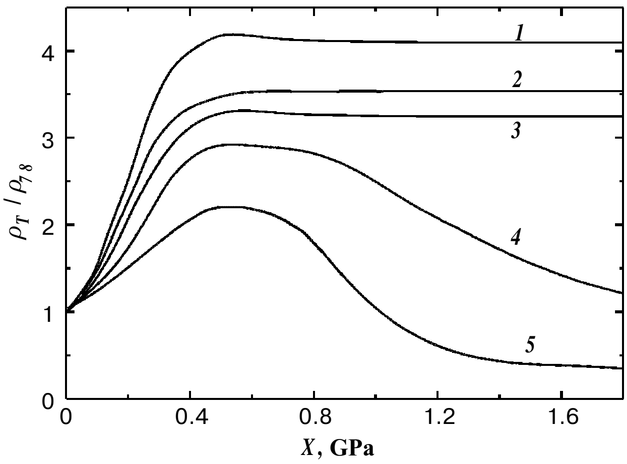

Fig. 1. Pressure dependencies of resistivity for the both neutron-transmutation-doped n-Si(P) crystals (curves 1,3,4,5, specimens 2 (NTD), 4 (NTD), 8c (NTD), 9a (NTD) respectively) and doped by phosphorus at grows (curve 2, specimen 5). **X**||[001]|| J; $T = 78$ K.

where Ξ_u is the shear deformation potential constant, C_{11}, C_{11} are the elastic constants of silicon crystal. Besides, since the main strain-induced change of the phosphorus ground state location takes place in the pressure range (0÷0.4) GPa [5,6]:

$$\delta\varepsilon(A_1) = -\frac{1}{2}\left\{\Delta_2^2 + \frac{3}{2}\Delta_2 \Xi_u (\varepsilon_{zz} - \varepsilon_{xx}) + \left[\Xi_u(\varepsilon_{zz} - \varepsilon_{xx})\right]^2\right\}^{1/2}, \tag{2}$$

we attribute the mentioned above exponential resistivity decreasing in NTD n-Si(P) in the pressure range (0.6÷1.2)

Table 1. Parameters of the investigated crystals doped by various methods

Sample	ρ_{78}, Ω×cm	μ_{78}, cm^2/V×s	$N_i = N_d + N_a$, ×10^{14} cm^{-3}	$n_e = N_d - N_a$, ×10^{14} cm^{-3}	N_d, ×10^{14} cm^{-3}	N_a, ×10^{14} cm^{-3}	$k = N_a/N_d$	Φ, ×10^{17} (quanta/cm^2)
1	15	20800	0.396	0.202	0.3	0.096	0.32	0
2(NTD)	17	21300	0.256	0.17	0.228	0.058	0.25	0
3(NTD)	1050	21500	0.21	0.19	0.2	0.01	0.05	0
4(NTD)	5.3	20500	1.84	0.58	1.2	0.62	0.52	0
5	4.55	19100	1.3	0.72	1.0	0.28	0.28	0
6	15.5	14500	5.13	0.28	2.7	2.4	0.9	0
7	3.2	17600	1.7	1.12	1.4	0.28	0.2	0
8(NTD)	1.23	16200	3.15	3.15	3.2	≈ 0.01	< 0.01	0
8a	1.43	14600	3.35	3.0	3.2	0.15	0.05	1.36
8b	1.9	14200	4.1	2.34	3.2	0.86	0.27	1.76
8c	7.75	12900	5.7	0.63	3.2	2.53	0.8	2.1
9(НЛ)	0.63	14470	7.2	7.2	7.2	≈0.01	0.01	0
9a	32.8	4750	14.0	0.4	7.2	6.8	0.94	8

GPa to the strain-induced ionization of technological TDs energy states.

In Eq. (2), Δ_2 is the singlet-doublet splitting, ε_{zz}, ε_{xx} are the components of the deformation tensor.

Great exponential decrease of resistivity in the pressure range (1÷1.8) GPa in γ-irradiated NTD n-Si(P) (curves 4,5, Fig. 1) is determined by the strain-induced increasing of ionization of the A-center (pair of vacancy-oxygen atom [7]).

The presence in the forbidden band of the energy states of the both irradiation-induced defects in NTD silicon crystals (P, A–centers) and high temperature technological TDs as well as their energy shift with pressure are clearly confirmed by the Hall-effect measurements data (curves 1–5, Fig. 2), as well.

The measurement data analysis of the temperature dependence of the Hall-effect (curve 5, Fig. 2) in slightly doped by phosphorus NTD n-Si crystal (specimen 3 NTD, Table 1) makes it possible to obtain the activation energies of the technological thermodonors states.

Two levels of thermodonors energy states were determined: $\varepsilon_1 = (78 \pm 1.5)$ meV and $\varepsilon_2 \approx 180$ meV.

It is note, that the curves of the Fig. 1 and Fig. 2 present a more characteristic behaviors measured on the silicon doped either in the melt or transmutation doped crystals and γ-irradiated ones.

Besides the representation of the discussed above examination of the tensoeffects mechanisms, the method of Ξ_u deformation potential constant determination in n-Si [8] was used for identification of the nature of the investigated phenomena.

Since according to Eq. (1) the energy splitting between the Δ_1-minima is directly proportional to the uniaxial pressure **X**||[001], the ratio of the electron concentrations in the "upper" and "lower" Δ_1-valleys in nondegenerated n-Si crystals is determined as [9]:

$$\frac{n_2}{n_1} = \exp\left(-\frac{\delta\varepsilon}{kT}\right). \qquad (3)$$

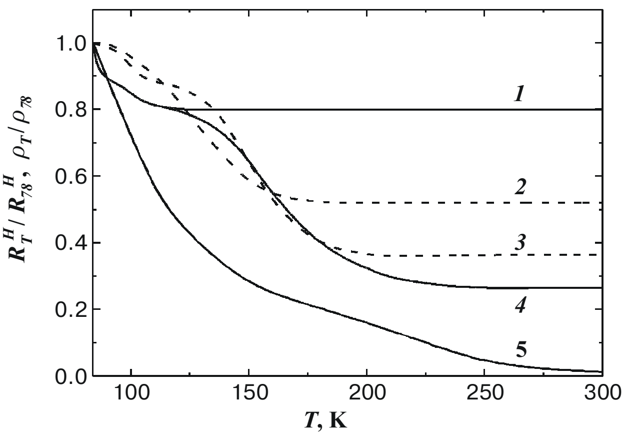

Fig. 2. Temperature dependencies of the Hall constant ratio $\left(R_T^H / R_{78}^H = f(T)\right)$ for the specimens 8 (NTD) (curves 1,2,3,4) and 3 (NTD) (curve 5). Uniaxial pressure: X = 0 (curves 1,4,5), X = 0.4 GPa (curve 3), X = 0.8 GPa (curve 2); dose of γ-radiation (quanta/cm^2): 0 (curves 1,5), 2.1×10^{17} (curves 2,3,4).

The ratio of n_2 and n_1 we can express over tensoresistivity measurement data, as:

$$\frac{n_2}{n_1} = \frac{\rho_\infty - \rho_X}{2(K\rho_X - \rho_\infty)}, \qquad (4)$$

where ρ_∞ is the resistivity of uniaxially strained crystals in the saturation range of the tensoresistivity, ρ_X is the specimen resistivity at specific value of X, K is the mobility anisotropy parameter.

Taking into account (1) and (3) we can obtain a linear dependence of the logarithm of concentration ratio lg(n_2/n_1) (expressed by TR data (4)) on X (dependence 2, Fig. 3) if the dominant TR mechanism is determined only by the intervalley redistribution of electrons (specimens 1, 5, Table 1) in silicon doped by phosphorus in the melt.

Any deviation of the dependence lg(n_2/n_1) = $f(X)$ from linearity must signify the availability of the additional physical mechanism (or mechanisms) to the Smith-Herring's one, which determines the behaviors of the TR effects in pure crystals of n-Si at T = 78 K.

As it is shown from the comparison of the curves 3,4,5,6 (Fig. 3) the deviation of the dependence lg(n_2/n_1) = = $f(X)$ from the straight line 2 (Fig. 3) increases with decreasing of the phosphorus dopant concentration in the NTD silicon.

Obviously, the contribution of an additional mechanism of tensoeffects in the TR-effect and other transport phenomena measured in silicon increases in pure crystals doped by neutron transmutation method. Thus, the physical properties of transmutation doped silicon will be determined more and more by the characteristics of technological thermodonors when concentration of phosphorus dopant decreases. Therefore, the annealing process of transmutation doped silicon crystals may be

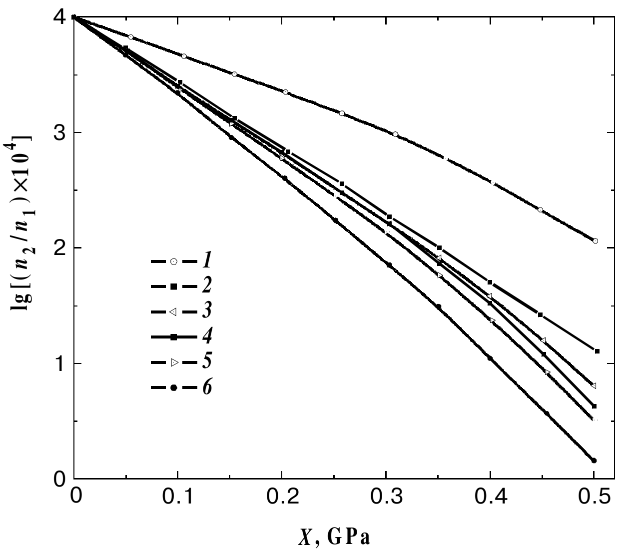

Fig. 3. Pressure dependencies of the logarithm of concentrations ratio (n_2/n_1) calculated by the Eq.(4) for the both crystals doped at grows (dependencies 1,2 specimen 1) and NTD n-Si(P) (curves 3-6, specimens 9 (NTD), 8 (NTD), 4 (NTD), 2 (NTD), respectively). T = 150 K (curve 1); T = 78 K (curves 2–6).

optimized taking into account the oxygen content in the ingots first of all.

The deviation of the dependence $\lg(n_2/n_1) = f(X)$ from linearity at $T > 120$ K in n-Si(P) doped by various methods (curve 1, Fig. 3) is determined by the both increasing of the f-transition contribution to the total scattering of electrons and strong dependence of the f-transition probability on pressure X [1,2].

4. Conclusions

The identification of the tensoeffects mechanisms in transmutation doped γ-irradiated n-Si(P) was performed using data analysis of the measurements of tensoresistivity, tenso-Hall effect, and the ratio of electrons concentration in the Δ_1-valleys of uniaxially strained crystals. An additional ionization of energy states of the both irradiation-induced defects (P, A-center) and high temperature technological thermodonors determines the essential contribution to the transport phenomena of the electron concentration increasing under increasing of the uniaxial pressure X. The remarkable strain-induced ionization of the energy states of the mentioned above crystalline lattice defects occurs in the different ranges of uniaxial pressure X (namely: 0÷0.4 GPa for the P, 0.6÷1.2 GPa for TDs, 1.0÷1.8 GPa for A-center). Essential increasing of the contribution of the electron f-transition in n-Si(P) doped by various methods takes place at the temperature increasing above $T > 120$ K.

Some parameters of the crystals doped at the growth and transmutation doped ones were compared, as well. For example the crystal fundamental parameters, namely, deformation potential constant Ξ_u, elastic constants C_{11}, C_{12} in both crystals are the same within the accuracy of the methods used for these parameters determination. The slope change of the linear part of dependencies $\lg(n_2/n_1) = f(X)$ in NTD n-Si(P) does not mean the change of the constant Ξ_u value since the tensoeffects mechanisms is not determined any more only by electrons redistribution between the Δ_1-minima. The Smith-Herring's mechanism of tensoeffects in n-Si crystals doped by shallow donors is dominant one only in the small temperature range 78–100 K and in sufficiently pure crystals ($N_D \leq 1\times10^{20}$ m^{-3}).

The two levels with the activation energies $\varepsilon_1 =$ $= (78 \pm 1.5)$ meV and $\varepsilon_2 \approx 180$ meV were detected by Hall-effect measurements and may be attributed to the energy states of high temperature thermodonors in NTD n-Si(P) formed in oxygen-containing silicon by technology heat–treatment for two hours at 800 °C. The optimization of thermal treatment regimes for NTD n-Si(P) is necessary in crystals with phosphorus dopant concentration $N_P < 1\cdot10^{19}$ m^{-3}.

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