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Strain-Induced MI Transition in n-Si and n-Ge: Physical Mechanisms and Transport Phenomena

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The analysis of experimental data on the pressure and temperature dependences of conductivity, the current–voltage characteristics (IVC), and the pressure dependence of the activation energy in n-Si and n-Ge crystals in the region of strain-induced metal–insulator transition (MIT) is presented. A remarkable change of the effective mass of carriers in semiconductors caused by strain-induced transformation of the energy band structure is the main necessary condition for realization of this kind of metal–nonmetal transition.

Introduction The metal–insulator transition in semiconductors is usually realized due to the change of dopant concentration. In the case of increasing dopant concentration, the overlapping of the wave function of donors or acceptors increases and results in the delocalization of carriers when a critical doping concentration (N_c) is achieved. It was found that the value of N_c can be changed by applying high magnetic field [1, 2] or uniaxial pressure [3]. In barely metallic crystals, the N_c change leads to the transition to activation-type conductivity at low temperature and high magnetic field [1, 2]. In slightly insulating crystals n-Si(P), the transition to metallic-type conductivity is realized at a random orientation of uniaxial pressure which, in turn, leads to a decrease of valley-orbital splitting [3]. The parameters of the conduction band do not change under the influence of such a type of deformation. In magnetic field, the electrons also move on the isoenergetical surface without changing the effective mass. At the same time, in Si and Ge there is a certain possibility of a crucial transformation of the conduction band under high uniaxial pressure [4]. In this case, for n-Si at orientation of the deformation axis along [111] direction and for n-Ge at $\mathbf{X} \parallel [100]$ a remarkable increase of the electron effective mass is observed that leads to a transition from metallic to activation type conductivity in the region of concentrations which essentially exceed the critical

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concentration N_c [4, 5]. Obviously, different reasons of effective mass increasing in n-Si and n-Ge under uniaxial strain could lead to different mechanisms of MI transition in these crystals. Because the MIT for both crystals is caused by an increase of electron effective mass m_e and their localization on donor atoms, the common peculiarities of the strain-induced MIT should take place. Thus, for the n-Si and n-Ge the uniaxial pressure increase results in (i) an increase of the activation energy E_a; (ii) the linear $I-V$ characteristics (IVC) is transformed to a non-linear S-shape IVC; (iii) weak localization is replaced by a strong localization of electrons on impurity centers, etc. Analysis of the mentioned above peculiarities of MIT in highly strained n-Si and n-Ge crystals depends on the transformation of the energy spectrum of C-band presented in this work.

Experimental An original equipment for investigations of physical properties of solids at extremely high uniaxial pressure up to 6–7 GPa was utilized for measurements of transport phenomena in the region of strain-induced MIT [6]. A specially developed electronic circuit allows to measure dependences in the investigated sample at the constant current condition. A fixed value of current could be adjusted on the necessary level in the range 0.1 μA to 20 mA. An experimental methodology also enables to measure IVCs under the condition of low-temperature impact ionization of the dopant by fixed values of uniaxial pressure. According to measured effect, two types of samples were used: with prism and dumb-bell shape. The dimensions of the prism specimens are $\approx (0.6 \times 0.6 \times 7)$ mm^3. Cylindrical dumb-bell specimens were used in order to avoid a surplus carrier injection and the influence of high pressure on current contact properties. The dimensions of the sample were approximately 0.25 mm^2 $\times$ 2.5 mm for the thin isthmus and 5 mm^2 $\times$ 2.5 mm for the thicker parts at both ends of the specimens. The current contacts were removed from the region of direct application of mechanical stress to the crystal.

The accuracy of the X-ray method of crystallographic orientation was $\pm 15''$. Disorientation of the applied stress with respect to the crystallographic axis was better than $\pm 30'$. To avoid specimen heating, the pulse regime of $I-V$ characteristics measurement was used as well.

Results and Discussion In monocrystalline semiconductors doped by shallow impurities the critical concentration N_c of MIT is determined by the well known Mott criterion:

$$N_c^{1/3} a_B \approx 0.25 \,. \tag{1}$$

In the crystal for hydrogen-like impurities the Bohr radius a_B is determined as

$$a_B = \frac{h^2 \chi}{m^* e^2} \,, \tag{2}$$

where χ is the dielectric permittivity, m^* is the effective mass of carriers.

In the condition of strain-induced MIT caused by the change of m^* and considering relationship (1) we obtain

$$N_c^{1/3} a_B = N_{c_1}^{1/3} a_{B_1} \,. \tag{3}$$

The change of critical concentration, which is determined by the dependence of effective mass m^* on pressure X, equals:

$$\frac{N_{c_1}}{N_c} = \left(\frac{m_X}{m_0}\right)^3 . \qquad (4)$$

Evidently, even insignificant changes of the carrier effective mass must lead to an appreciable change of critical concentration of the dopant which determines the MIT. Thus, an increase of electron effective mass which occurs for both n-Si and n-Ge crystals because of C-band transformation [4] is the principle of strain-induced MIT [4, 5]. An essential decrease of free electrons concentration due to their localization in region of strain-induced MIT gives rise to an observable decrease of the crystal dielectric constant [2], and leads to more effective localization of electrons on the impurity atoms.

Therefore, in n-Si an increase of the electron effective mass at increasing uniaxial pressure $\mathbf{X} \parallel [111]$ due to the strain-induced non-parabolicity of the Δ_1-valleys [8], determines the physical mechanism of the MIT in high strained degenerative crystals [9]. In germanium, a substantial increase of the electron effective mass due to $L_1-\Delta_1$ inversion of the conduction band minima [10] also leads to strain-induced MIT under the condition $\mathbf{X} \parallel [001]$ [9]. In the region of the MIT, the measurements were performed on temperature dependences of the crystal resistivity at various pressure (Fig. 1a for n-Si(P); Fig. 1b for n-Ge(Sb)) to determine the appearance and increase of activation energy under uniaxial pressure.

An appearance in n-Ge and n-Si of activation energy with increasing pressure indicates the localization of an electron on the impurity center and, in both crystals, the transition to ε_2-conductivity (Fig. 1a, b). So, an increase of the electron effective mass and the corresponding decrease of Bohr radius, lead to strain-induced MIT at constant level of doping of n-Si and n-Ge crystals in the region of substantial degeneracy at $X = 0$.

Thus, the structure of the dependences of activation energy on pressure in n-Ge and in n-Si is substantially different for these crystals [9]. So, the different behavior of the $\varepsilon_a = f(X)$ dependences indicates different transformation regularities of C-band in silicon and germanium for specific directions of the deformation axis [4]. On the other hand, for both n-Ge and n-Si the region of strong localization of electrons, with increasing doping level shifts towards higher pressure [9].

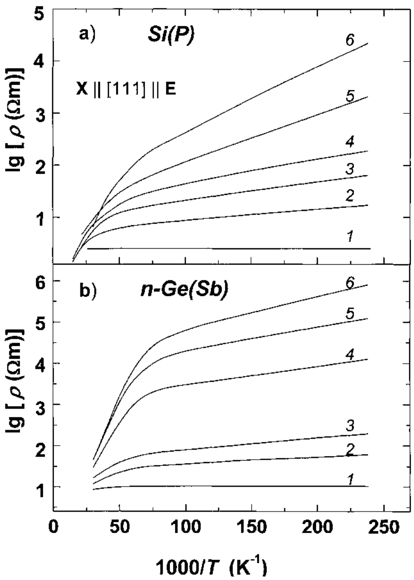

Fig. 1. Temperature dependence of resistivity for different values of uniaxial pressure X (GPa). a) n-Si(P): (1) 0 , (2) 2.4, (3) 2.6, (4) 2.81, (5) 3.0, (6) 3.2 GPa; $N_P = 4.7 \times 10^{24}$ m^{-3}. b) n-Ge(Sb): (1) 0, (2) 1.0, (3) 1.8, (4) 1.9, (5) 2.0, (6) 2.1 GPa; $N_{Sb} = 1.8 \times 10^{23}$ m^{-3}

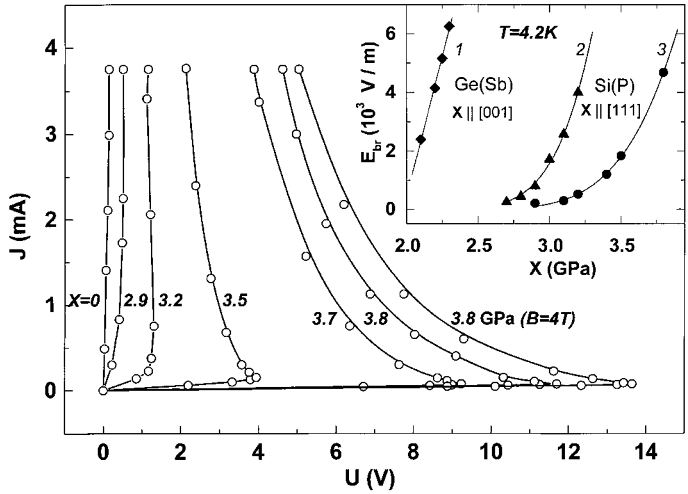

Fig. 2. Change of current–voltage characteristics for n-Si(P) crystals measured in pulse regime under variation of uniaxial stress ($N_P = 4.7 \times 10^{24}$ m^{-3}, $T = 4.2$ K). The inset shows the dependences of breakdown field of shallow-donor localized states vs. uniaxial pressure for Ge(Sb): $N_{Sb} = 1.8 \times 10^{23}$ m^{-3} (1); and Si(P): $N_P = 4.2 \times 10^{24}$ m^{-3} (2), $N_P = 6.2 \times 10^{24}$ m^{-3} (3)

Figure 2 shows the assemblage of IVCs which were measured at different values of pressure for n-Si doped with phosphorous ($N_P = 4.7 \times 10^{24}$ m^{-3}). The change of low-stress linear IVCs into S-like shape in the region of MIT also indicates the transition to ε_2-conductivity at high uniaxial pressure. Impact ionization of the electrons localized on impurity atoms in the region of strain-induced MIT occurs in the range of electric fields of 5×10^2 to 6×10^3 V/m (curves 1 to 3 in the inset to Fig. 2). Magnetic field with intensity 4 T leads to the same increase of the breakdown field as uniaxial pressure $X = 0.1$ GPa. Insignificant influence of magnetic field on additional electron localization is related to low mobility of electrons in the region of ε_2-conductivity. Experimental data demonstrate that ε_2-conductivity is a key type of conductivity in the region of strain-induced MIT at $T = 4.2$ K in n-Si and n-Ge degenerately doped with shallow donors. Obviously, at milli-Kelvin temperatures a strain-induced transition to the hopping conductivity would be observed.

In conclusion, the transport phenomena have been investigated in highly, uniaxially strained silicon and germanium with concentration levels which remarkably exceed the critical concentration of MIT. The mechanisms of strain-induced MIT determined by transformation peculiarities of C-band energy spectra of Si and Ge at specific orientation of deformation axis, **X** || {111} and **X** || {100} respectively, are discussed. These mechanisms of strain-induced transition from the metallic type conductivity to the activation type one differ from the common investigated mechanisms with the pressure-related change of main characteristics of the energy band: effective mass of carriers, anisotropy of effective mass K_m, density of states, ionization energy of shallow impurities and others. The main statements of the effective-mass–donor concept for hydrogen-like impurities were verified from the experimental data for the principal behavior of strain-induced transitions in heavy doped monocrystalline semiconductors. Analysis of tensoresistive effect investigations, of the temperature dependence of resistance, the dependence of activation energy on uniaxial pressure, and the IVC transformation under pressure, reveal the transition to ε_2-conductivity in degenerately doped n-Si and n-Ge crystals under specific orientation of uniaxial pressure. A strong influence of the strain-induced increase of electron effective mass on the change of critical concentration of MIT was demonstrated in n-Si and n-Ge in the high uniaxial pressure region.

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