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Investigations of physical mechanisms of metal-insulator transition in highly strained *n*-Si and *n*-Ge crystals

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Abstract. Analysis of experimental results on transport phenomena is presented for highly uniaxially strained silicon and germanium crystals heavily doped by shallow donors. Possible mechanisms of the strain induced metal-insulator (MI) transition determined by peculiarities of the c-band energy spectrum transformation in *n*-Si and *n*-Ge are discussed. The main statements of the effective mass-donor concept for hydrogen-like impurities in monocrystalline semiconductors were verified.

Keywords: many-valley semiconductors, metal-insulator transition, effective-mass theory, high uniaxial pressure

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1. Introduction

Results of long-period investigations of a band structure of semiconductors allowed to determine its characteristic peculiarities and to define fundamental parameters of the energy spectrum. Therefore, heavily doped semiconductors are most commonly used for analysis of the metal-insulator transition mechanisms [1,2]. The insulator-metal transition is usually realized in the range of very low temperatures ($T \to 0$) by increasing the doping concentration. It leads to wave functions overlap increase and, as a consequence, to delocalization of electrons when so-called critical concentration of the MI transition is achieved [3]:

$$a_B N_c^{1/3} \approx 0.25 \quad (1)$$

Universality of the Mott criterion (1) was confirmed experimentally for various materials with the critical concentration of the MI transition varying by 8 orders of magnitude ($10^{20} \div 10^{28}$) m^{-3} [4]. However, long-time experimental and theoretical researches on the MI transition phenomenon show that we still have some unsolved problems. They are connected not only with some quantitative discrepancies between the theoretical calculation results and respective experimental data. More surprising result is the opposite changes of a critical concentration value of the MI transition that were obtained from theoretical calculations [5] and found experimentally in uniaxially strained *n*-Ge (As) [6] and *n*-Si (P) [7] heavily doped by shallow donors. It was found [5] that the theoretically calculated sign reverse of the critical concentration change occurring at increasing of uniaxial pressure is opposite to the experimentally measured one. For example, the strain induced transition from the activation type conductivity (insulator) to the metallic type conductivity was observed in slightly-insulating highly doped by phosphor monocrystalline silicon at millikelvin temperatures (3÷35 mK) and pressure $X \approx 0.8$ Gpa [7]. Thus, experimental data show a decrease of the MI transition critical concentration value N_c with an increase of uniaxial pressure (insulator-metal transition) while according to the calculations based on the effective mass theory (EMT) an increase of uniaxial pressure should cause the increase of the critical concentration value N_c (metal-insulator transition).

Obviously, comparison of theoretically predicted change of the MI transition critical concentration with increasing uniaxial pressure X and appropriate experi-

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mental data for semiconductors highly doped by shallow donors (*n*-Si, *n*-Ge) can be correctly realized in the case of appreciable electron effective mass variation under high uniaxial pressure. Experimental data analysis of the energy band spectrum transformation in highly strained *n*-Si and *n*-Ge crystals [8] allowed to define the characteristic deformation orientations that lead to an appreciable increase of the electron effective mass value: **X** || [111] – in *n*-Si, and **X** || [001] – in *n*-Ge. This paper reviews mechanisms of the strain-induced metal-insulator transitions in *n*-Si and *n*-Ge associated with the electron effective mass variation under high uniaxial pressure.

2. Experimental results and discussion

The MI transitions in highly uniaxially strained n-Si and n-Ge crystals were realized at much higher (comparably to [7]) temperatures (4.2÷60 K). An original setup for investigations of physical properties of semiconductors at extremely high uniaxial pressure [9] was utilized for measurements of the MIT phenomenon. Cylindrical dumb-bell specimens were prepared using an originally designed equipment. Dimensions of samples were approximately (0.5÷0.6) mm in diameter with the length (1.5÷2.0) mm for the thin isthmus and ≈ 2.5 mm in diameter and with a length ≈ 2 mm for the thicker parts at the both ends of the specimens.

In Fig. 1 and Fig. 2, temperature dependencies of resistivity at various values of uniaxial pressure are shown for *n*-Ge(Sb) and *n*-Si(P) crystals, respectively. The dopant concentrations on these crystals markedly exceed the corresponding critical concentrations of the insulator-metal transition which is realized due to the increase of shallow dopant concentration. Obviously, the value of N_D / N_{Dc} is equal approximately to 1.6 for *n*-Ge(Sb) and 1.4 for n-Si(P), respectively. Therefore, the metallic type conductivity is realized in unstrained crystals. These specimens are degenerated and the activation energy of conductivity at low temperatures (curves 1 in Figs 1 and 2) tends to zero. Appearance in *n*-Ge at **X** || [001] and in *n*-Si **X** || [111] of activation energy e_2 that increases with increasing pressure is shown in Fig. 1 and Fig. 2, (curves 2–7 respectively). Since, for the both *n*-Ge at **X** || [001] and *n*-Si at **X** || [111] the electron effective mass increases due to the strain-induced transformation of the energy band structure [8], the critical concentration of the MI transition according to the Mott criterion must increase, as well. According to the effective mass concept, the Bohr radius a_b of electron localized on shallow donor is determined as:

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

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

According to Eq. (1), a continuous increase of the free electron effective mass at the increase of uniaxial pressure and the corresponding decrease of the Bohr radius leads to the localization of electron on the donor atom providing thus the strain-induced metal-insulator transition realization. Taking into consideration Eqs. (1) and (2), the increasing of critical concentration of the MI transition is defined as:

$$N_c(X) = N_c(0)\left(\frac{m_X^*}{m_0^*}\right)^3 \tag{3}$$

Increasing the electron effective mass at uniaxial pressure results in increasing the critical concentration value which corresponds to the transition from the metallic type conductivity to the activation type one. This is in agreement with the effective mass concept findings and is con-

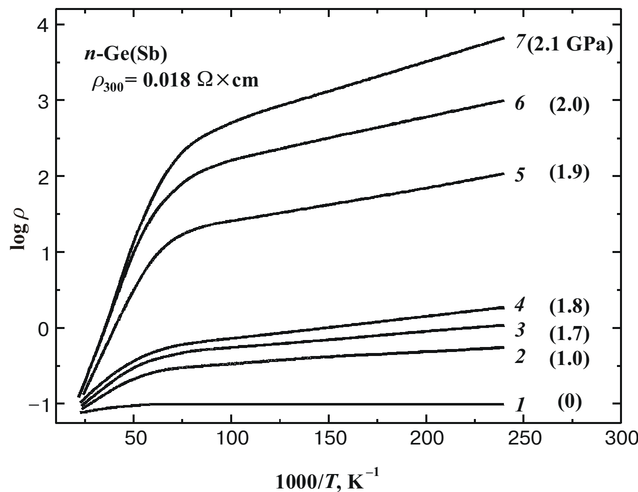

Fig. 1. Temperature dependencies of the specific resistance for *n*-Ge(Sb) crystals at various values of the uniaxial pressure **X** || [100].

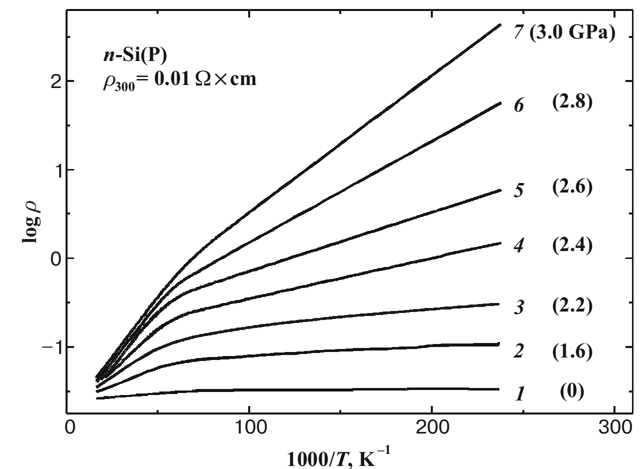

Fig. 2. Temperature dependencies of the specific resistance for *n*-Si(P) crystals at various values of the unixial pressure **X** || [111].

firmed by experimental data on the strain-induced MI transitions in the initially degenerated n-Ge(Sb) (Fig. 1) and n-Si(P) (Fig. 2) crystals. Analysis of experimental results on the MI transition in highly strained crystals with account for the transformation of the linear I–V characteristics at $X = 0$ to the S-like ones on the insulator side of the MI transition at high pressures evidences that the strain-induced MI transition is the transition to the ε_2-conductivity which occurs at 4.2÷20 K.

Thus, the strain-induced MI transition is realized in impurity band of Si and Ge that is formed by the donor sublattice in the crystals with high level of doping [10,11]. Note, that according to analysis of infrared reflection spectra in n-Si(P) crystals, the MI transition is realized in the impurity-band [12].

At the higher temperatures ($T \approx$ 25÷60 K), contribution of the ε_1- conductivity to the crystal conductance is observed in both n-Si(P) and n-Ge(Sb) crystals. The pressure dependence of the ε_1-conductivity activation energy is also defined by the increase of the electron effective mass in accordance with the effective mass-donor concept for hydrogen-like impurities [13]:

$$\varepsilon_1 = -\frac{m^* e^4}{2\hbar^2 \chi^2} \tag{4}$$

In fact, temperature dependencies of crystal resistivity show that in the both n-Ge(Sb) and n-Si(P) (Fig. 1, Fig. 2) the strain-induced increase of the electron effective mass leads to the increase of the ε_I- activation energy as well.

Since in n-Si at **X** || [111] and in n-Ge at **X** || [001] many-valley degeneracy of Δ_1-valleys and L_1-valleys, correspondingly, is not removed, the change of the activation energy caused by the valley-orbit splitting change [6, 7] does not occurs.

In n-Ge at **X** || [001] in the pressure range $X \approx (1.5\div2.1)$ GPa the L_1-Δ_1-inversion of the absolute minima type takes place [8]. In this case Ψ-function of the electron localized on the shallow donor is described by the linear combination of the Bloch functions of four L_1-valleys and two Δ_1-valleys [14-16]:

$$\Psi = \sum_{\vec{k}} \left(C_{L\vec{k}} \Psi_{L\vec{k}} + C_{\Delta\vec{k}} \Psi_{\Delta\vec{k}} \right) \tag{5}$$

Therefore, the change of ε_2-conductivity activation energy in n-Ge which occurs in the pressure range 1.5 GPa < X < 2.2 GPa is characterized by the pressure dependence of the relative contributions of the L_1- and Δ_1-valleys Bloch wave-functions to the localized electron wave function. Evidently, the Ψ-function is determined only by the L_1-valleys Bloch functions contribution in the pressure range X < 1.5 GPa while the Ψ-function is determined by the Δ_1-valleys Bloch functions contribution in the pressure range X > 2.2 GPa. Thus, the inversion of the Ge conduction band absolute minimum in the pressure range X >2.2 GPa leads to the silicon-like conduction band. In consequence of L_1-Δ_1 – inversion the electron effective mass m_e^* increases while effective mass anisotropy $K_m = m_\parallel^* / m_\perp^*$ decreases. The density of states distribution changes in the both conduction band and impurity band. Therefore, according to the main statements of the effective mass-donor concept, the activation energy of ε_1 and ε_2-conductivity should change as well. A correlated increase of the activation energy of the ε_1 and ε_2-conductivity at increasing uniaxial pressure X is confirmed by the experimental data of strain induced metal-insulator transition caused by the increasing of the electron effective mass in n-Ge(Sb) crystals.

At the **X** || [111] (Fig. 2), the transverse component of electron effective mass $m_\perp^*$ increases due to the removing of degeneracy of the Δ_1 and Δ_1' branches of the conduction band at the edge of the Brillouin zone in silicon. The strain-induced increase of the $m_\perp^*$ causes the metal-insulator transition (Fig. 2, curves 1–7) in high pressure range according to the effective mass-donor concept (1) – (4)) as well.

3. Conclusions

The purpose of this paper was to study the physical mechanisms of the strain-induced metal-insulator transition in n-Si(P) and n-Ge(Sb) degeneratively doped crystals. Extensive measurements of the tensoresistive effect, temperature dependencies of resistivity and current-voltage characteristics at different values of uniaxial pressure were performed. Appearance of an activation energy in n-Ge and n-Si in the range of strain-induced MI transition indicates that the localization of electron on impurity center takes place as a consequence of an appropriate transformation of the energy spectrum of the both conduction band and impurity band of Si and Ge, which is characterized by the increase of the effective mass of electron. The similar behaviors and different ones of strain-induced transitions phenomenon in n-Si and n-Ge were observed and analyzed. The main statements of the effective mass-donor concept for hydrogen-like impurities in semiconductors were verified on the basis of the experimental investigations of the metal-insulator transition in high uniaxially strained monocrystalline silicon and germanium.

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