High pressure as an external factor, effectively governing a chaotic potential of crystalline semiconductors

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Abstract
It has been revealed from pressure, temperature, magnetic and electric fields dependences of kinetic coefficients in doped compensated Ge\textsubscript{Au,Sb}, p-type InSb, InAs, CdSnAs\textsubscript{Cu} and HgTe, that the observed anomalies of electron transport in the listed above materials are linked to the presence of large-scale fluctuations of ionized impurity concentrations. It is shown, that the influence of chaotic potential begotten by these fluctuations becomes more noticeable when the temperature decreases or the pressure rises.

1. Introduction
It is known [1], that smooth large scale fluctuations of random spatial potential are being formed in doped compensated semiconductors, when concentration of free charge carriers is small in comparison with the concentration of ionized impurity centers. The influence of chaotic potential increases while temperature decreases. Obviously, it is of current importance to estimate: 1. to what extent a chaotic potential may affect the energy spectrum of charge carriers, and therefore the properties of crystal semiconductors. 2. The propriety of application of corresponding correlations in interpretation of experiments for every given case if the following inequalities take a place: $\varepsilon_F \gg \gamma$ in degenerated semiconductor and $k_B T \gg \gamma$ in nondegenerated semiconductor. Here $\varepsilon_F$ – Fermi energy, $\gamma$ - typical value of random potential amplitude, $k_B$ – Boltzman’s constant, $T$ –temperature in K. The problem becomes more complicated if we deal with correlation of distribution of impurity in doped compensated semiconductors, which stipulates a nonelectronic nature of screening [1, 2].

2. Results and discussion
Typically, pressure coefficients of energy gaps $\Delta \varepsilon$ do not depend on pressure in semiconductors [3]. As an example, let’s take so-called quasi-zero-gap semiconductors (p-InAs, p-CdSnAs\textsubscript{Cu} etc.) [4] (Figure1) which have deep impurity band near the edge of intrinsic band. It has been concluded that the use of dispersion law for ideal semiconductor in a semiconductor with random potential is correct until the dependence of energy gap on hydrostatic pressure $\Delta \varepsilon(P)$, calculated from electron transport experiments and corresponding correlation relations, is close to the linear. Increasing deviation from linearity in $\Delta \varepsilon(P)$ dependence with the temperature fall and a decrease of carrier concentration testifies a considerable influence of random potential on dispersion law.
Let’s consider the situation of quasi-gapless semiconductor p-CdSnAs₂Cu [2], where a deep acceptor level (in some cases shredded in an acceptor band) generated by cadmium vacancies, is located at the distance \( \varepsilon_A = \varepsilon_A^0 + \alpha T - \beta P \) from the bottom of the conduction band (where \( \varepsilon_A^0 = -30 \) meV, \( \alpha = 4.6 \times 10^{-2} \) meV/K, \( \beta = \frac{\partial \varepsilon_A}{\partial P} = 120 \) meV/GPa, and \( \varepsilon_g = 0.28 \) meV - width of forbidden band). Energy is counted from the bottom of the conduction band and direction inside the band is chosen to be positive. The density of states for the discussed model, in the case of the occupation parameter for acceptor band \( K_A = N_A / N_d = 0 \), is depicted in Fig.1.

![Figure 1. Density of states (schematically) of heavily doped compensated semiconductor with deep acceptor band p-CdSnAs₂Cu at atmospheric (a) and hydrostatic (b) pressures, where acceptor band occupation parameter \( K_A = 0 \). Here \( \varepsilon_v, \varepsilon_c \) – undisturbed energies of the top of valence and the bottom of the conduction bands; \( \varepsilon_A, \varepsilon_F \) – energies of deep acceptor level and Fermi level; \( \varepsilon_p, \varepsilon_c \) – energies of percolation levels for holes and electrons correspondingly. Stroke dotted line – the shape of density states for an ideal crystal. Filled states are shown shaded.](image)

Characteristic parameters of sample #10 p-CdSnAs₂Cu [2] are given in the Table 1 and Fig. 2. Here \( n, \mu_e, p_A, \mu_A \) are concentration and mobility of electrons of the conduction band and holes of the acceptor band respectively.

| T, K | P, GPa | \( R_{\sigma} \), cm/C | \( \rho_0 \), \( \Omega \) cm | \( p_{A_3} \), cm | \( \mu_A \), Cm²/V·s | \( p_A/n \), | \( \mu_e/\mu_A \), | \( K_A \) |
|------|--------|-----------------|-----------------|-------------|-----------------|---------|-----------------|-----------|
| 280  | \( 10^4 \) | -650            | 0.286           | 5.6         | 130             | 16.5    | 30              | 0.08      |
| 1.5  | -300   | 2.50            | 5.4             | 22          | 1450            | 180     | –               |           |
| \( \infty \) | 530   | 3.80            | 5.4             | 10          | \( \infty \)    | 0       | 0.10            |           |

Hereinafter, the characteristic parameters of charge carriers and pressure coefficients of energy gap \( \beta \) are calculated from temperature and magnetic field dependences of Hall coefficients, resistivity and well known values of band parameters. It is seen from Fig. 2, that pressure coefficient \( \beta \) decreases at \( P > 1 \) GPa, that is stipulated by the influence of chaotic potential on energy spectrum at \( T = 295 \) K.
Figure 2. The pressure dependences of Hall coefficient $R_0$ (curves 1, 4), resistivity $\rho_0$ (2, 5), mobilities of acceptor band holes $\mu_A$ (3, 6) in vanishing small magnetic field at $T=77.6$ K (1–3) and $T=280$ K (4–6). (7) - the pressure dependences of the deep acceptor level $\varepsilon_A$ at 280 K (sample #10 [2]).

Experimental data on pressure coefficients for the energy deep impurity centers of gold [5, 6] and copper [7] in germanium are presented in Table 2 and Fig. 3. A detailed analysis of these data has been performed earlier in [5].

**Table 2.** Pressure coefficients of the four levels due to gold in germanium

| Level | Type     | $E_C-E_i$ | $\partial(E_C-E_i)/\partial P$ | T (K)   |
|-------|----------|-----------|---------------------------------|---------|
| $E_4$ | acceptor | 0.043     | 21                              | 45–49.3 |
| $E_3$ | acceptor | 0.19      | 29 (44**)                       | 112–194 |
| $E_2$ | acceptor | 0.60      | 44                              | 170–273 |
| $E_1$ | donor    | 0.71      | 49                              | 49.5    |
| $E_v$ |          | 0.75      | 50                              |         |

We will note briefly only two factors responsible for the decreases in the pressure coefficients $\gamma_{\text{cl}}=d(E_{\text{cl}}-E_i)/dP$ and $\gamma_{\text{v}}=d(E_{\text{v}}-E_i)/dP$ in n- and p- regions, respectively. First of all, it is crucial to use the Gibbs statistics consistently, which has not been correctly done in the analysis carried out by Pel’ and others [7]. Holland and Paul [6] have taken into account the Gibbs statistics and, moreover, measured the pressure dependence of the electrical resistivity in Ge: Au at low temperatures with the aim of obtaining more reliable results. However, slightly soluble impurities (such as Au, Hg and Cu) in doped and compensated germanium can form cluster with a high probability. As the temperature decreases and the pressure increases, the concentration of free charge carriers decreases and the amplitude of a random potential and correspondingly, the degree of fluctuation bending of energy bands increases. In this situation, if the energy levels of deep impurity centers are located in the band gap, a transition to a state which is similar to a heavily doped, completely compensated semiconductor can occur [1]. This with necessity must lead to a decrease in the pressure coefficient for the energy gaps calculated from the pressure dependence of the carrier concentration, as is confirmed by the data presented in Fig. 3 and in the Table 2. It is also evident that the effect of the random potential increases with a decrease both in the temperature and in the energy separation between the deep impurity level and the edge of the intrinsic band.
In the above listed semiconductors the value of pressure coefficient of energy gap decreases, because dispersion law for ideal semiconductor was applied for the quantitative analysis. It testifies considerable influence of chaotic potential.

Unlike usual semiconductors, the influence of chaotic potential in gapless semiconductors (with inversed band structure: $\varepsilon_g=\varepsilon_{\Gamma 6}-\varepsilon_{\Gamma 8}<0$), for instance in p-HgTe, leads to an excess of pressure coefficient $\beta=\partial\varepsilon_g/\partial P$. Coefficient $\beta=\partial\varepsilon_g/\partial P$ for lightly doped sample p-HgTe-1 has been calculated according to the experimental data [8]. In slightly doped sample p-HgTe-1 at $T=295$ K and $T=77.6$ K $\beta=121$ meV/GPa, at $T=4.2$ K $\beta=220$ meV/GPa; in heavily doped sample p-HgTe-2 $\beta=85$ meV/GPa at $T=295$ K, and $\beta=210$ meV/GPa at $T=77.6$ K [9].

3. Conclusion

Hydrostatic pressure affects effectively on the electron spectrum of crystal semiconductors and allows one to determine the extent of the influence of a large scale fluctuation potential on the charge carrier energy spectrum. The latest allows one then to examine the propriety of corresponding equations for quantitative analysis of experimental results.

Acknowledgements. This work has been supported by the Russian Foundation for Basic Research (project no. 07-02-00238a).
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