Influence of Pressure on the Temperature Dependence of Quantum Oscillation Phenomena in Semiconductors

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The influence of pressure on the oscillations of Shubnikov-de Haas (ShdH) and de Haas-van Alphen (dHvA) in semiconductors is studied. Working formula for the calculation of the influence of hydrostatic pressure on the Landau levels of electrons is obtained. The temperature dependence of quantum oscillations for different pressures is determined. The calculation results are compared with experimental data. It is shown that the effect of pressure on the band gap is manifested to oscillations and ShdH and dHvA effects in semiconductors.

1. Introduction

Currently a variety of experimental methods for the study of influence of pressure on the oscillations ShdH and dHvA are tested in new types of semiconductors. Most quantum oscillation phenomena in semiconductors are due to oscillation density of energy states in a strong magnetic field [1–5].

The works of [6, 7] studied the temperature dependence of the density of states in quantizing magnetic fields. These studies showed that the continuous spectrum of the density measured at the temperature of liquid nitrogen at low temperatures turns into discrete Landau levels. Mathematical modeling of processes using the experimental values of the continuous spectrum of the density of states makes it possible to calculate the discrete Landau levels. The work of [8] examined the effect of temperature on the oscillation dHvA effect using this model. Here, the obtained oscillation dHvA effects take into account the thermal broadening of the Landau levels. However, these studies did not consider the effect of pressure on the effects of oscillations ShdH and dHvA in semiconductors.

The aim of this work is a theoretical study of the influence of hydrostatic pressure on the quantum oscillation phenomena in semiconductors.

2. Method of Calculation of the Density of the Energy States

Consider the dynamics of the free electron gas in a quantizing magnetic field. In the presence of a magnetic field parallel to the z direction, the energies of electrons and holes in the conduction bands and valence bands are as follows:

\[ E_c (N, k_z) = E_g + \left( N + \frac{1}{2} \right) \hbar \omega_c + \frac{\hbar^2 k_z^2}{2m_c} \pm \frac{1}{2} s g \mu_B B \]  

(1)

\[ E_v (N, k_z) = - \left( N + \frac{1}{2} \right) \hbar \omega_v - \frac{\hbar^2 k_z^2}{2m_v} \pm \frac{1}{2} s g \mu_B B. \]  

(2)

Here, \( \omega_c \) and \( \omega_v \) represent cyclotron frequency of electrons and holes, \( s \) represents spin quantum number, and \( B \) represents the magnetic field induction.

For parabolic zone [9], \( E = \hbar^2 k^2 / 2m \) and \( S = \pi k^2 = \pi (k^2 - k^2_z) \).

Hence, the cyclotron mass

\[ m_c = \frac{\hbar^2}{2\pi} \left( \frac{\partial S}{\partial E} \right) = m. \]  

(3)

We now find the number of states in the interval between two Landau levels. Using expression (3), let us find the
difference between the areas of cross-sections of two equal-energy surfaces, which differ in energy $\Delta E = \hbar \omega_c$:

$$\Delta S = \frac{2\pi m_e}{\hbar^2} \Delta E = \frac{2\pi m_e}{\hbar^2} \hbar \omega_c. \quad (4)$$

For the determination of the oscillation effects of ShdH and dHvA in the conduction band, primarily we must calculate the oscillations of the density of energy states in quantizing magnetic field. We will consider a box with large but finite sides $L_x, L_y, L_z$ (the main area of the crystal) [9]. As you can see from expressions (1), the second term is called the energy of the electron motion in the plane $xy$ and changing discretely. Hence, the number of states per unit area in a plane $k_x k_y$ will be $L_x L_y / (2 \pi)^2$. That is, the number of states between two quantum orbits equals

$$L_x L_y / (2 \pi)^2 \Delta S = \frac{m \omega_c}{c^2} L_x L_y. \quad (5)$$

Then the total number of quantum states with energies less than $E$ is equal to

$$N(E) = \frac{L_x L_y L_z m^{3/2}}{\pi^2 \hbar^3} \hbar \omega_c \sum_{N=0}^{N_{max}} \frac{1}{\sqrt{E - \left( E_g + \hbar \omega_c (N + 1/2) \right)}}. \quad (9)$$

As is known, the band gap depends on the magnetic field, temperature, and pressure. The dependence of the semiconductor band gap at hydrostatic pressure changes as follows [10, 11]:

$$E_g(P) = E_g(0) - \beta P. \quad (11)$$

Here, $\beta$ represented pressure coefficients, characterizing the change in position of the edges of the valence band and the conduction band with pressure.

The dependence of the Fermi level from pressure can be written in the following form:

$$E_F(P, T) = -E_g(P) + \frac{3}{4} kT \ln \left( \frac{m^*}{m_e} \right). \quad (12)$$

Then the derivative with respect to the energy from Fermi-Dirac distribution function has the following form:

$$\frac{\partial f_0(E, E_F(P, T), T)}{\partial E} = \frac{1}{kT} \left[ \frac{1}{1 + \exp \left( E - \left( -E_g(P)/2 + (3/4) kT \ln \left( m^*/m_e \right) \right) / kT \right) \right] \left( \frac{m^*}{m_e} \right). \quad (13)$$

3. Influence of Pressure on the Oscillations Effects of ShdH and dHvA in Semiconductors

It is known that in the case of the density of states Landau quantization is a periodic function of the magnetic field. This leads to oscillations ShdH and dHvA that are periodic in the strong magnetic field. The relaxation time takes the following form: $\tau = \tau_0 e^{E'/T}$. The exponent $r$ has different values for different scattering mechanisms. For example, in the case of scattering by acoustic vibrations of impurity ions, the exponent is equal to $-1/2$ and $3/2$ [12]. Naturally, the effects of oscillations ShdH and dHvA appear on the change in the density of energy states in semiconductors. Hence, we define
Figure 1: Comparison of oscillation effects of ShdH in Si at different pressures.

the dependence of the oscillation effects of ShdH [9] and dHvA [12] on the full pressure with the help of expressions (10)–(15):

$$\sigma_{zz}(B, T, P) = A \cdot \hbar \omega_z(P)$$

$$\cdot \int_{\hbar \omega_z(P)}^{\infty} \sum_{N} \tau_N(E) \left( -\frac{\partial f_0(E, E_F(P, T), T)}{\partial E} \right) dE,$$

and longitudinal resistance $\rho_{zz}(B, T, P) = 1/\sigma_{zz}(B, T, P)$. Here, $A = -(2m)^{1/2} e^2/\pi^2 \hbar^3$.

$$\chi(B, T, P) = 2\mu_B^2 \int_{0}^{\infty} \sum_{N} \frac{1}{E - \left( E_F(P) + \hbar \omega_z(P) (N + 1/2) \right)}$$

$$\cdot \left( -\frac{\partial f_0(E, E_F(P, T), T)}{\partial E} \right) dE.$$  

Here, $\mu_B$ represents Bohr magneton. $\chi$ represents magnetic susceptibility.

Now, we must determine the critical pressure ($P_k$) in a strong magnetic field. If the pressure is equal to or greater than the critical value ($P \geq P_k$), the Landau levels begin to shift from the edges of the conduction band. For the calculation of critical pressure, consider the simplest case:

$N = 0, (1/2)\hbar \omega_z - \beta P_k = 0$, or $P_k = (1/2\beta)\hbar \omega_z$. Consider estimation for semiconductor Si: ($\beta = -1.5 \cdot 10^{-11}$ eV/Pa) at $B = 2$ T (20 kGs) [10, 11]. $P_k = (1/2\beta)\hbar \omega_z \approx 2 \cdot 10^8$ Pa. This means that, for Si, if the pressure of $P \geq 2 \cdot 10^8$ Pa, it will change shape oscillation ShdH and dHvA.

Now, we get the graphics effects oscillations ShdH and dHvA by means of formulas (16) and (17). Figure 1 shows the dependence of the oscillations effects of ShdH and dHvA on the hydrostatic pressure in Si at low temperatures. As seen from these figures, with increasing pressure, the shape of the Landau levels strongly changes. In Figures 2 and 3, three-dimensional image oscillations ShdH and dHvA are shown at different pressures in Si. With increasing pressure to $5 \cdot 10^8$ Pa semiconductors Si was observed a decrease the number of Landau levels oscillations ShdH and dHvA at $T = 5$ K. Figure 4 shows the oscillations of the longitudinal magnetoresistance in Si at different temperatures and pressures. With increasing temperature, the pressure of the Landau levels is noticeably reduced. From Figure 4 it is seen that without pressure and at a temperature of 40 K Landau levels are manifested, but $P = 6 \cdot 10^8$ Pa and $T = 40$ K oscillations disappear. Figure 5 shows the influence of pressure on the temperature dependence of the oscillations ShdH in the three-dimensional image.

4. Influence of Nonparabolicity Energy Bands on the Oscillations Longitudinal Magnetoresistance in Narrow-Gap Semiconductors

The work of [4] investigated the oscillations longitudinal magnetoresistance at hydrostatic pressures up to 1 GPa in
Figure 4: Influence of pressure on the temperature dependence of the oscillations ShdH in Si.

Figure 5: Temperature dependence of the oscillations ShdH in Si. (a) At no pressure; (b) at the pressure, $P = 6 \cdot 10^8$ Pa.

HgSe$_{1-x}$S$_x$. In this work, the quantum oscillations of ShdH were observed at $T = 4.2$ K. Figure 6 shows the oscillations ShdH of pressure $P = 0.38$ GPa in the samples with $x = 0.104$ [4]. In these semiconductors bandgap varies from 0.1 eV to 0.4 eV, for different values of $x$ [4, 13]. An important feature of the semiconductor with a narrow band gap is a strong nonparabolicity conduction band [13]. The limiting case of Kane’s model is realized. The low value of the band gap narrow-gap semiconductors leads to its stronger dependence on pressure, temperature, and external fields. The work of
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Figure 6: Oscillation effects of ShdH in HgSe$_{0.896}$S$_{0.104}$ at $T = 4.2$ K. (a) Experimental data [4]; (b) calculated from formula (19).

[14] obtained a formula for the density of energy states in a quantizing magnetic field with Kane dispersion law:

$$N_n^S(E, H) = \frac{(n!)^{3/2}}{(2)^{1/2} \pi^2 \hbar^3} \sum_{N=0}^{N_{max}} \frac{2E/E_g + 1}{\sqrt{E^2/E_g + E - (N + 1/2) \hbar \omega_c}}. \quad (18)$$

Here, $N_n^S(E, H)$ refers to the density of energy states in a quantizing magnetic field with Kane dispersion law. $E_g$ refers to band gap without pressure. $E$ represents energy free electrons in the conduction band. Influence of pressure on the oscillations effect of ShdH with the Kane dispersion law according to formula (18) is determined from expression (16):

$$\sigma_z^N(B, P) = A \cdot \hbar \omega_c \int_{\hbar \omega_c(P)}^{\infty} \sum_{N} \frac{2E/E_g(P) + 1}{\sqrt{E^2/E_g(P) + E - (N + 1/2) \hbar \omega_c(P)}} \tau_N(E) \left( -\frac{\partial \rho_0(E)}{\partial E} \right) dE. \quad (19)$$

Here, $\sigma_z^N(B, P)$ stands for longitudinal conductivity with a nonparabolic dispersion law.

As a result, we obtain graph dependence of the effect of oscillations ShdH on the pressure in HgSe$_{1-x}$S$_x$ with nonquadratic dispersion law. Figure 6(b) shows oscillation longitudinal resistance in HgSe$_{0.896}$S$_{0.104}$ at $P = 0.38$ GPa. These figures show the oscillations effects of ShdH at low constant temperatures. The working equation (19) makes it possible to build charts oscillations ShdH of the sample at different temperatures and pressures.

5. Conclusion

The influence of pressure and temperature on the oscillations effects of ShdH and dHvA is considered in semiconductor. An analytical expression for the longitudinal magnetoresistance in semiconductors with Kane dispersion law for electrons is obtained. The calculation results are compared with experimental data. It is shown that the effect of pressure on the band gap is manifested to oscillations ShdH and dHvA effects in semiconductors. The above results are valid when there is no Lifshitz transition or any other pressure-induced phase transition.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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