THE ENERGY SPECTRUM AND STATISTICS OF ELECTRONS IN THE SIZE-QUANTIZED ANISOTROPIC FILMS

B.I. KULIEV, V.M. GADJIEV
Baku State University Named After M.E. Rasulzade,
Academician Z.Khalilov str. 23, Baku-370148
(Received 04.01.96)

The wave functions and energy spectrum of electrons in the size-quantized n-Ge and n-Si films are obtained in the effective masses tensor approximation for an arbitrary orientation of the film surface. On the basis of the obtained spectrum the density of the electron states is analysed. The expressions for the electron concentration and electronic part of heat capacity are obtained in various approximations.

1. At the last time thin films are intensively investigated in the size-quantized conditions that is connected with the requirement of compactness of devices on the basis of semiconductor materials. At the size-quantized conditions an essential change in the energetic spectrum and mechanisms of scattering occurs and, as a result, quantum sized effects are observed. The investigations of these effects give us valuable information about zone structure, mechanisms of interactions of elementary excitements and etc. The theory of quantum sized effects in the semiconductors with standard zone has been developed in the works [1,2]. As to semiconductors with anisotropic many-valley zone, for example n-Ge and n-Si, the consistent theory of the quantum sized effects for them has not been worked out yet.

In the present work the energy spectra of electrons in size-quantized films of n-Ge and n-Si are obtained and the density of states and statistics of the electron gas are investigated. As an example of application of these spectra for the calculation of concrete effects the analytic expression for the electronic part of heat capacity in various approximations is obtained.

2. As it is known the energy spectra of n-Ge and n-Si are anisotropic. The isoenergetic surfaces near the minimum of conducting zone are rotational ellipsoids with axis of rotation directed along axis of the type $|111|$ for n-Ge and the one of the type $|100|$ for n-Si.

In the own system of reference their energy spectra near each minimum take the form:

$$\varepsilon(\vec{K}') = \frac{\hbar^2}{2}\left(\frac{K_x'^2 + K_y'^2}{m_\perp} + \frac{K_z'^2}{m_\parallel}\right) \quad , \qquad (1)$$

where $m_\perp$ and $m_\parallel$ are transverse and longitudinal effective masses of electron respectively.

In the following it is necessary to make transformation of the expression (1) into the one for the system of reference connected to the film with surface of arbitrary orientation with respect to the crystallographic axes. The spectrum obtained in the new system of reference for each ellipsoid is written as:

$$\varepsilon_s(\vec{K}) = \frac{\hbar^2}{2} m^{-1}_{\alpha\beta(s)} K_\alpha K_\beta \quad , \qquad (2)$$

where $\alpha, \beta = 1,2,3$, s is the ellipsoid number, $m^{-1}_{\alpha\beta(s)}$ is the inverse tensor of the electrons' effective masses in the new system of reference.

To solve the Schrödinger equation in the effective masses tensor approximation (when $\vec{K} \to -i\vec{V}$) we assume that the film is represented as a rectangular potentional pit with plane bottom and infinitely high walls [3],

$$U(z) = \begin{cases} 0 & \text{for } 0 < z < d \\ \infty & \text{for } z < 0,\ z > d \end{cases} \quad , \qquad (3)$$

where d is the thickness of the film and on the (xy)-plane $U(x,y) = const$.

Then for the wave functions and energy spectrum the following expressions are obtained:

$$\Psi^{(s)}_{n_z K_x K_y}(x,y,z) = \left(\frac{2}{L_1 L_2 d}\right)^{1/2} \sin\frac{n_z \pi}{d} z \exp\left[i(K_x X + K_y Y)\right] \exp\left[-i\frac{m^{-1}_{13(s)}K_x + m^{-1}_{23(s)}K_y}{m^{-1}_{33(s)}} Z\right] \quad , \qquad (4)$$

$$\varepsilon_s(n_z, K_x, K_y) = \frac{\hbar^2}{2} m^{-1}_{33(s)} \left(\frac{\pi}{d}\right)^2 n_z^2 + \frac{\hbar^2}{2} \overline{m}^{-1}_{\gamma\delta(s)} K_\gamma K_\delta \quad , \qquad (5)$$

where $\gamma, \delta = 1,2$, L_1 and L_2 are the corresponding sizes of the basic domain of the film on the (xy)-plane, $n_z = 1,2,3\ldots$ is the sized quantum number, while $\overline{m}^{-1}_{\gamma\delta(s)}$ has the form:

$$\overline{m}^{-1}_{\gamma\delta(s)} = m^{-1}_{\gamma\delta(s)} - \frac{m^{-1}_{\gamma 3(s)} m^{-1}_{\delta 3(s)}}{m^{-1}_{33(s)}} \quad . \qquad (6)$$

We see that the electron states are determined by three quantum numbers (n_s, K_x, K_y), one of which takes discrete positive values. Therefore, the state of the electron in two-dimensional $\vec{K}$-space (K_x, K_y) is quasicontinuous while on the third direction the spectrum becomes discrete. Thus, the energy spectrum of the electrons in the films is divided on separate overlaring two-dimensional subzones corresponding to fixed values of n_s. The characteristic feature of the film spectrum is finite minimal energy

$$\varepsilon_{1s} = \varepsilon_s\left(K_x = K_y = 0, n_s = 1\right) = \frac{\hbar^2}{2} m^{-1}_{33(s)} \left(\frac{\pi}{d}\right)^2 . \quad (7)$$

3. Let us define now the density of states. To do this we calculate the full number of the electron states per unit volume with energy less than ε_s (for each ellipsoid)

$$Z_s(\varepsilon_s) = \frac{2}{V} \sum_{n_s K_x K_y} \Rightarrow \frac{1}{2\pi^2 d} \sum_{n_s} \int dK_x dK_y \quad , \quad (8)$$

where multiplier 2 is spin degeneration of states, $V = L_1 L_2 d$ is the volume of the film basic domain.

The integral of two-dimensional $\vec{K}$-space is calculated easily and for the density of states we obtain:

$$g_t^{(s)}(\varepsilon_s) = \frac{\left(\overline{m}^{-1}_{11(s)} \overline{m}^{-1}_{22(s)} - \overline{m}^{-2}_{12(s)}\right)^{-1/2}}{\pi d \hbar^2} \left[\sqrt{\frac{\varepsilon_s}{\varepsilon_{1s}}}\right] , \quad (9)$$

where $\left[\sqrt{\frac{\varepsilon_s}{\varepsilon_{1s}}}\right]$ is the integer part of number $\sqrt{\frac{\varepsilon_s}{\varepsilon_{1s}}}$, that is the average number of subzones with the bottom below ε_s. Evidently to obtain the full density of the electron states it is necessary to sum up over all ellipsoids corresponding to the first Brillouin zone, i.e.

$$g_t = \sum_s g_t^{(s)}(\varepsilon_s) \quad , \quad (10)$$

As seen from (9), for the fixed film thickness $g_t^{(s)}(\varepsilon_s)$ is independent on the energy until the value $\sqrt{\frac{\varepsilon_s}{\varepsilon_{1s}}}$ does not change by one. Therefore $g_t^{(s)}(\varepsilon_s)$ is a step function. The leap occurs every time when the energy ε_s coincides with the bottom of the next subzone, i.e. $\varepsilon_s = \varepsilon_{ns} = \varepsilon_{1s} n_s^2$. At these values of the energy the density of states in the film coincides with that in bulk specimen: $g_t^{(s)}(\varepsilon_s) = g_m^{(s)}(\varepsilon_s)$.

It is easy to show that the dependence on the density of states (9) of thickness at fixed energy ε_s also has nonmonotonous character. At the thicknesses d_{ns} when $\sqrt{\frac{\varepsilon_s}{\varepsilon_{1s}}}$ is integer, i.e. when the bottom of some subzone coincides with ε_s, $g_t^{(s)}(\varepsilon_s, d_{ns}) = g_m^{(s)}(\varepsilon_s)$. At other thicknesses when d increases the density of states $g_t^{(s)}(d)$ decreases as $1/d$ until the number of subzones below ε_s does not change by one. It is just such nonmonotonous behaviour of the density of states on energy and thickness that is the reason of peculiarities of the physical phenomena in thin films.

Let us calculate now the concentration of electrons. For each ellipsoid at an arbitrary temperature we get:

$$n_1^{(s)} = \frac{\left(\overline{m}^{-1}_{11(s)} \overline{m}^{-1}_{22(s)} - \overline{m}^{-2}_{12(s)}\right)^{-1/2}}{\pi d \hbar^2} \sum_{n_s} \left[\xi - \varepsilon_{n_s} + k_0 T \ln\left(1 + \exp\left(\frac{\varepsilon_{ns} - \xi}{k_0 T}\right)\right)\right] \quad . \quad (11)$$

In order to obtain the full concentration of electrons it is necessary to sum up (11) over all ellipsoids corresponding to the first Brillouin zone.

It is interesting to consider the electron concentration in the cases of the degenerated and nondegenerated electron gases. In the case of the degenerated electron gas we obtain:

$$n_1^{(s)} = \frac{\left(\overline{m}^{-1}_{11(s)} \overline{m}^{-1}_{22(s)} - \overline{m}^{-2}_{12(s)}\right)^{-1/2}}{\pi d \hbar^2} n_{0s} \left[\xi_F - \frac{\varepsilon_{1s}\left(n_{0s} + 1\right)\left(2n_{0s} + 1\right)}{6}\right] \quad , \quad (12)$$

where $n_{0s} = \left[\sqrt{\frac{\xi_F}{\varepsilon_{1s}}}\right]$ is the integer part of number $\sqrt{\frac{\xi_F}{\varepsilon_{1s}}}$. After summing up over all ellipsoids we obtain the expression for the concentration of the degenerated gas n_{en} which relates n_e to the Fermi level ξ_F for the films of arbitrary thickness. From this expression we can find ξ_F in the cases of superthin $(n_{0s}=1)$ and thick $(n_{0s}>>1)$ films. We note that in the limit $n_{0s}>>1$ (12) turns into the corresponding expression for the bulk specimen.

In the case of the nondegenerated electron gas we obtain:

$$n_1^{(s)} = \frac{\left(\overline{m}_{11(s)}^{-1}\overline{m}_{22(s)}^{-1} - \overline{m}_{12(s)}^{-2}\right)^{-1/2} k_0 T}{\pi d\hbar^2} \sum_{n_z} \exp\left(\frac{\xi - \varepsilon_{n_z}}{k_0 T}\right) \quad . \tag{13}$$

After summing up over all ellipsoids an expression for the chemical potential ξ in the limits of superthin and thick films can be also obtained. In the thick film limit we obtain for (13) in the first approximation the result of bulk specimen while in the next approximation a quantum correction due to the size quantization can be found.

4. As an example of application of the results obtained above let us show here the concrete expressions for the heat capacity of electrons in the film.

For the strongly degenerated electron gas we obtain:

$$C_s = \frac{\left(\overline{m}_{11(s)}^{-1}\overline{m}_{22(s)}^{-1} - \overline{m}_{12(s)}^{-2}\right)^{-1/2} \pi k_0^2 T}{3d\hbar^2} n_{n_z} \quad , \tag{14}$$

and for the nondegenerated electron gas we have:

$$C_s = \frac{\left(\overline{m}_{11(s)}^{-1}\overline{m}_{22(s)}^{-1} - \overline{m}_{12(s)}^{-2}\right)^{-1/2}}{\pi d\hbar^2} \sum_{n_z} \left\{ \left[2\left(\varepsilon_{n_z} + k_0 T\right) - \xi + \frac{\varepsilon_{n_z}}{k_0 T}\left(\varepsilon_{n_z} - \xi\right) \right] \exp\left(\frac{\xi - \varepsilon_{n_z}}{k_0 T}\right) \right\} \quad . \tag{15}$$

As we see from (14) and (15) at the size-quantized conditions the heat capacity of electrons becomes nonmonotonous function of the film thickness and also depends on orientation of the film surface with respect to the crystallographic axises.

[1] *V.B.Sandomirsky.* JETF,1967,v.52,p. 158 /inRussian/.

[2] *B.A. Tavger, V.N. Demikhovsky.* UFN,1968,v.96,p.61 /inRussian/.

[3] *B.M. Askerov.* The electrons transpore phenomena in the semiconductors,Moscow, "Nauka", 1985, § 26, p. 295 /inRussian/.

B.İ. Quliyev, V.M. Hacıyev

ÖLÇUYƏ GÖRƏ KVANTLANMIŞ ANİZOTROP NAZİK TƏBƏQƏLƏRDƏ ELEKTRONLARIN ENERJİ SPEKTRİ VƏ STATİSTİKASI

Səthi ixtiyari yönəlmiş n-Ge və n-Si nazik təbəqələrində ölçüyə görə kvantlanma halında effektiv kütlə tenzoru yaxınlaşmasında elektronların dalğa funksiyaları və enerji spektri üçün ifadələr alınmışdır. Alınan spektr əsasında hal sıxlığı funksiyası təhlil olunub. Müxtəlif yaxınlaşmalarda elektron qazının konsentrasiyası və istilik tutumu üçün ifadələr alınmışdır.

Б.И. Кулиев, В.М. Гаджиев

ЭНЕРГЕТИЧЕСКИЙ СПЕКТР И СТАТИСТИКА ЭЛЕКТРОНОВ В РАЗМЕРНО-КВАНТОВАННЫХ АНИЗОТРОПНЫХ ПЛЕНКАХ

Получены волновые функции и энергетический спектр электронов в размерно-квантованных пленках n-Ge и n-Si в приближении тензора эффективных масс при произвольной ориентации поверхности пленки. На основе полученного спектра проанализирована плотность состояний электронов. Получены выражения для концентрации электронов и электронной части теплоемкости в различных приближениях.

Редактор: Р.Р. Гусейнов