Statistics and Size-Quantized Anisotropy of Electron States in n-Ge and n-Si Films

Bahshali KULIEV, Vugar GADJIEV
Baku State University, Physical Department Baku,
370148, Academician Z. Halilov street, 23,
Azerbaijan Republic

Abstract

The wave functions and energy spectrum of electrons in size-quantized n-Ge and n-Si films are obtained and the anisotropy of the electron state density is investigated. Also, the analytical expressions for the electronic part of heat capacity at the various approximations of electron gas degeneration are obtained.

1. Introduction

Recently, there has been growing interest in the study of physical properties of conducting films in the size-quantized conditions connected with microelectronics development. In this case the specimen sizes are of the de Broglie wave length of the current carriers, a scale at which quantum-size effects occur. If one or two specimen sizes limited the quasi-discrete nature of energy spectrum, the wave functions form changed. The influence of such size quantization on the current carrier's behavior is also naturally affected. This problem for conducting films with standard zone (simple isotropic model) has been considered by some authors, for example, in works [1-3]. As to anisotropic semiconducting films of n-Ge and n-Si type, it is assumed additional anisotropic effects appear due to film finite thickness.

2. Energy spectrum

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 the [111] axis for n-Ge and along the [100] axis for n-Si. The energy spectra near each minimum take the form:

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

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

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

$$\varepsilon_s(\vec{K}) = \frac{\hbar^2}{2}m_{\alpha\beta(s)}^{-1}K_\alpha K_\beta, \tag{2}$$

where $\alpha, \beta = 1, 2, 3$; S is the ellipsoid number, $m_{\alpha\beta(s)}^{-1}$ is the tensor of inverse effective electron masses in the new system of reference.

To solve the Schrodinger equation in the effective masses tensor approximation (when $\vec{K} \to -i\vec{\nabla}$) we assume that the film is represented as a rectangular potential pit with plane bottom and infinitely high walls:

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

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

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

$$\Psi_{n_s K_x K_y}^{(s)}(X, Y, Z) = \left(\frac{2}{L_1 L_2 d}\right)^{1/2} \sin\frac{n_s \pi}{d}z \exp[i(K_x X + K_y Y)] \times$$
$$\exp\left[-i\left(\frac{m_{13(s)}^{-1}K_x + m_{23(s)}^{-1}K_y}{m_{33(s)}^{-1}}\right)Z\right], \tag{4}$$

$$\varepsilon_s(n_s, K_x, K_y) = \frac{\hbar^2}{2}m_{33(s)}^{-1}\left(\frac{\pi}{d}\right)^2 n_s^2 + \frac{\hbar^2}{2}\bar{m}_{\gamma\delta(s)}^{-1}K_\gamma K_\delta, \tag{5}$$

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

$$\bar{m}_{\gamma\delta(s)}^{-1} = m_{\gamma\delta(s)}^{-1} - \frac{m_{\gamma3(s)}^{-1}m_{\delta3(s)}^{-1}}{m_{33(s)}^{-1}}. \tag{6}$$

One can represent expression (5) in the main ellipsoid axis's in the form:

$$\varepsilon_s(n_s, K_x, K_y) = \frac{\hbar^2\pi^2}{2m_\parallel d^2}f(\theta_s)n_s^2 + \frac{\hbar^2}{2m_\perp}\left[f^{-1}(\theta_s)K_x^2 + K_y^2\right], \tag{7}$$

1048

where θ_s is the angle between axis of rotation of the each ellipsoid and a normal to the film surface; $f(\theta_s) = 1 + (\gamma - 1)\sin^2\theta_s$; and $\gamma = \frac{m_\parallel}{m_\perp}$ is the coefficient of anisotropy.

Thus the electron state in the size-quantized n-Ge and n-Si films is essentially anisotropic, that is, reflected on discrete and quasicontinuous parts of energy spectrum.

3. State density

From expression (7) we can obtain the electron state density in the form:

$$g_f = \frac{m_\perp}{\pi d\hbar^2} \sum_{s=1}^{N} \left\{ f^{1/2}(\theta_s)\bar{n}_s \right\}, \tag{8}$$

where $\bar{n}_s = \left[\sqrt{\frac{\varepsilon_s}{\varepsilon_{1s}}} \right]$

is the integer part of number $\sqrt{\frac{\varepsilon_s}{\varepsilon_{1s}}}$, $\varepsilon_{1s} = \varepsilon_s(n_s = 1, K_x = K_y = 0)$, $N = 4$ for n-Ge and $N=6$ for n-Si.

For the fixed film thickness g_f is independent of energy until the value $\sqrt{\frac{\varepsilon_s}{\varepsilon_{1s}}}$ changes by less than unity. In this case, the leap of state density occurs and therefore its dependence on energy has a step-like character.

At the fixed energy ε_s the state density is dependent on film thickness $\sim 1/d$ until the value $\sqrt{\frac{\varepsilon_s}{\varepsilon_{1s}}}$ changes by less than unity. In this case, the leap of state density occurs again and therefore its dependence on film thickness exhibits a sawtoothed character.

Let us fix the initial film surface as the (001) surface. We will rotate the film normal by angle α around one of the crystallographic axis. We obtain for the state density:

$$g_f(\alpha) = \frac{m_\perp}{\pi d\hbar^2} \sum_{s=1}^{N} \left\{ \varphi_s(\alpha)\bar{n}_s \right\}. \tag{9}$$

With rotation of the film normal around the [100] axis the $\varphi_s(\alpha)$ functions for n-Ge assume the form

$$\varphi_{1,2}(\alpha) = \frac{1}{\sqrt{3}} \left[1 + 2\gamma + (1 - \gamma)\sin 2\alpha \right]^{1/2},$$

$$\varphi_{3,4}(\alpha) = \frac{1}{\sqrt{3}} \left[1 + 2\gamma + (\gamma - 1)\sin 2\alpha \right]^{1/2}, \tag{10}$$

and for n-Si we have

$$\varphi_{1,2}(\alpha) = \left[1 + (\gamma - 1)\sin^2\alpha \right]^{1/2},$$

$$\varphi_{3,4}(\alpha) = \left[\gamma + (1 - \gamma)\sin^2\alpha \right]^{1/2},$$

$$\varphi_{5,6} = \gamma^{1/2}. \tag{11}$$

1049

With rotation of the film normal around the [110] axis the $\varphi_s(\alpha)$ functions for n-Ge have form

$$\varphi_{1,2}(\alpha) = \left[1 + (\gamma - 1)\sin^2\left(\alpha \pm \arccos\frac{1}{\sqrt{3}}\right)\right]^{1/2},$$

$$\varphi_{3,4}(\alpha) = \left[1 + \frac{(\gamma - 1)}{3}\left(2 + \sin^2\alpha\right)\right]^{1/2}, \tag{12}$$

and for n-Si we have

$$\varphi_{1,2}(\alpha) = \left[1 + (\gamma - 1)\sin^2\alpha\right]^{1/2},$$

$$\varphi_{3,6}(\alpha) = \left[\gamma + \frac{(1 - \gamma)}{2}\sin^2\alpha\right]^{1/2}, \tag{13}$$

From expressions (9)-(13) we can obtain the electron state density expressions with the normal directed along the [001], [011] and [111] axis, respectively.

Indeed, for n-Ge, we have

$$g_f^{(001)} = \frac{4m_\perp}{\sqrt{3}\pi d\hbar^2}\left(2\gamma + 1\right)^{1/2}\bar{n},$$

$$g_f^{(011)} = \frac{2m_\perp}{\pi d\hbar^2}\left\{\left(\frac{\gamma + 2}{3}\right)^{1/2}\bar{n}_1 + \gamma^{1/2}\bar{n}_2\right\},$$

$$g_f^{(111)} = \frac{m_\perp}{\pi d\hbar^2}\left\{\bar{n}_1 + (8\gamma + 1)^{1/2}\bar{n}_2\right\}, \tag{14}$$

and for n-Si we obtain

$$g_f^{(001)} = \frac{2m_\perp}{\pi d\hbar^2}\left\{\bar{n}_1 + 2\gamma^{1/2}\bar{n}_2\right\},$$

$$g_f^{(011)} = \frac{2m_\perp}{\pi d\hbar^2}\left\{\gamma^{1/2}\bar{n}_1 + (2\gamma + 2)^{1/2}\bar{n}_2\right\},$$

$$g_f^{(111)} = \frac{2\sqrt{3}m_\perp}{\pi d\hbar^2}\left(2\gamma + 1\right)^{1/2}\bar{n}. \tag{15}$$

As it is shown from above mentioned expressions (14) and (15), the state density depends essentially on film surface orientation, i.e. state density posses so-called size-quantized anisotropy. For bulk specimen this anisotropy, evidently, vanishes.

4. Electron heat capacity

Having knowledge of the energy spectrum of electrons in the size-quantized film it is possible to calculate concrete thermodynamic functions of the system. Let us show

here expressions for the electronic part of the heat capacity for various approximations of electron gas degeneration. For arbitrary degenerated electrons we obtain:

$$C_f(\alpha) = \frac{m_\perp K_0^2 T}{\pi d \hbar^2} \sum_{s=1}^{N} \left\{ \varphi_s \{\alpha\} \sum_{n_s} \left[X_{ns} \left(F_1(\eta_{ns}) + T \frac{\partial F_1(\eta_{ns})}{\partial T} \right) + \right.\right.$$
$$\left.\left. + F_2(\eta_{ns}) + \frac{T}{2} \frac{\partial F_2(\eta_{ns})}{\partial T} \right] \right\}, \tag{16}$$

where $F_1(\eta_{ns})$ and $F_2(\eta_{ns})$ are the uniparametric Fermi integrals, $\eta_{ns} = \eta - Xns$, η is a reducible chemical potential, X_{ns} is a reducible discrete energy of spectrum (7).

From here, with the strongly degenerated electron gas approximation, we have:

$$C_f(\alpha) = \frac{m_\perp \pi K_0^2 T}{3 d \hbar^2} \sum_{s=1}^{N} \{\varphi_s(\alpha) \bar{n}_s\} = \frac{(\pi K_0)^2 T}{3} g_f(\alpha). \tag{17}$$

It is evident from this case the heat capacity has the same character for state density and posses size-quantized anisotropy.

Let us show here the heat capacity expressions for ultrathin n-Ge and n-Si degenerated films (when only one subband is filled) with definite orientations of their surface and compare them with the corresponding heat capacity C_m for bulk specimen. For n-Ge we obtain:

$$C_f^{(001)} = C_m \left\{ 1 + \frac{\gamma d^3 n_e}{2\pi \left(\frac{2\gamma+1}{3}\right)^{3/2}} \right\}^{-1/2},$$

$$C_f^{(011)} = \frac{1}{2} C_m \left\{ 1 + \frac{\gamma d^3 n_e}{\pi \left(\frac{\gamma+2}{3}\right)^{3/2}} \right\}^{-1/2},$$

$$C_f^{(111)} = \frac{1}{4} C_m \left\{ 1 + \frac{2\gamma d^3 n_e}{\pi} \right\}^{-1/2}, \tag{18}$$

where n_e is a concentration of electrons in film.

The analogous calculations for n-Si give us:

$$C_f^{(001)} = \frac{1}{3} C_m \left\{ 1 + \frac{\gamma d^3 n_e}{\pi} \right\}^{-1/2},$$

$$C_f^{(011)} = \frac{2}{3} C_m \left\{ 1 + \frac{\sqrt{2}\gamma d^3 n_e}{\pi (\gamma+1)^{3/2}} \right\}^{-1/2},$$

$$C_f^{(111)} = C_m \left\{ 1 + \frac{\sqrt{3}\gamma d^3 n_e}{\pi (2\gamma+1)^{3/2}} \right\}^{-1/2}. \tag{19}$$

The analysis of expressions (18) and (19) for C_f shows that depending on ultrathin film surface orientation the contributions into the heat capacity give different number of ellipsoids. Only at the definite film surface orientations ($C_f^{(001)}$ for n-Ge and $C_f^{(111)}$ for n-Si) the heat capacity of electron gas conditioned by all ellipsoids. It is also a consequence of the energy spectrum anisotropy in n-Ge and n-Si films.

For the nondegenerated electron gas from (16) we obtain:

$$C_f(\alpha) = K_0 n_e \sum_{s=1}^{N} \left\{ \varphi_s(\alpha) \sum_{ns} \left[1 + (1 + Xns) \left(1 + Xns - \ell n \frac{\pi d \hbar^2 n_e}{m_\perp K_0 T A(\alpha)} \right) \right] \times \frac{\exp(-Xns)}{A(\alpha)} \right\}, \tag{20}$$

where $A(\alpha) = \sum_{s=1}^{N} \left\{ \varphi_s(\alpha) \sum_{ns} \exp(-X_{ns}) \right\}$.

As it is shown in this case, heat capacity also depends on film surface orientation. But $C_f(\alpha)$ behavior in nondegenerated n-Ge and n-Si films become more complicated than in degenerated films.

References

[1] V. B. Sandomirsky, J. Eksp. I Teor. Fiziki, 52 (1967) 158 (in Russian).

[2] B. A. Tavger, V. N. Demihovsky, Uspehi Fiz. Nauk, 96 (1968) 61 (in Russian).

[3] B. M. Askerov, Electron Transport Phenomena in Semiconductors, World Scientific, Singapore (1994) 374.