THE INFLUENCE OF SIZED QUANTIZATION ON THE KINETIC COEFFICIENTS IN n-Ge AND n-Si FILMS

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The behaviour of the kinetic coefficients in dependence on orientation of n-Ge and n-Si films surface is investigated. Expressions for the relaxation time including mechanisms of scattering on acoustical and non-polar optical phonons are obtained. Also the expressions for the Hall constant and thermopower in n-Ge and n-Si films plane in a weak magnetic field are obtained in various approximations of electron gas degeneration.

At the present time thin semiconducting films are intensively investigated in the size-quantized conditions that is connected with the microelectronics development. When the specimen sizes are de Broglie wave length of the current carriers the quantum sized effects are occurred. In this case the quasi-discrete nature of energy spectrum is occurred and the wave functions form is changed. Some thermodynamic and kinetic properties for conducting films with standard zone have been considered in the works [1-4]. In the works [5,6] the electron states in anisotropic size-quantized n-Ge and n-Si films have been considered and dependence of physical values on film surface orientation has been predicted, so-called the size-quantized anisotropy of thermodynamic properties of system. Evidently that such dependence also can be observed in kinetic characters of n-Ge and n-Si films.

In the present work the behaviour of the kinetic coefficients in dependence on orientation of n-Ge and n-Si films surface is investigated. Expressions for the relaxation time including mechanisms of scattering on acoustical and non-polar optical phonons are obtained. Also the expressions for the Hall constant and thermopower in n-Ge and n-Si films plane in a weak magnetic field are obtained in various approximations of electron gas degeneration.

1. The wave functions and the energy spectrum of electrons in size-quantized n-Ge and n-Si films have form [6]:

$$\Psi^{(S)}_{n_z K_x K_y}(x,y,z)=\left(\frac{2}{L_x L_y d}\right)^{1/2} \sin\frac{\pi n_z}{d} z \exp[i(K_x x+K_y y)]\times \exp\left[-i\frac{m^{-1}_{13(S)}K_x+m^{-1}_{23(S)}K_y}{m^{-1}_{33(S)}}z\right], \quad (1)$$

$$\varepsilon_s(n_z,K_x,K_y)=\frac{\hbar^2}{2m_\parallel}\left(\frac{\pi}{d}\right)^2\varphi_s^2(\alpha)\,n_z^2+\frac{\hbar^2}{2m_\perp}[\varphi_s^{-2}(\alpha)K_x^2+K_y^2], \quad (2)$$

where $m_\parallel$ and $m_\perp$ are longitudinal and transverse effective masses of electron respectively, $m^{-1}_{13(S)}$ $(i=1,2,3)$ are components of the inverse tensor of electron effective masses in film, L_x and L_y are the corresponding sizes of the basic domain of the film, d is the film thickness, S is the ellipsoid number, n_z=1,2,3,... is the sized quantum number, α is the angle of rotation of a normal to the [001] film surface, $\varphi_s(\alpha)$ are the functions that characterize of ellipsoids orientation as regards to the system of reference and depend on anisotropy parameter of effective masses (see [6]).

Let us consider some kinetic effects in nonquantized magnetic field that directed along a normal to the film surface. For it we decide two-dimensional Boltzmann transport equation in n-Ge and n-Si films plane. If the nonequilibrium distribution function of electrons is represented in form:

$$f_1=\left(-\frac{\partial f_0}{\partial\varepsilon_s}\right)(\vec{V}\ \vec{P}), \quad (3)$$

then the next decision of equation is obtained:

$$\vec{P}=\frac{1}{1+\nu^2}\left\{\hat{\tau}\vec{\Phi}_0+\frac{e}{c}\hat{\tau}[\vec{H}\hat{M}^{-1}(\hat{\tau}\vec{\Phi}_0)]\right\}, \quad (4)$$

where f_0 is the function of Fermi-Dirac distribution, $\nu=\frac{e|\hat{\tau}|^{1/2}}{c|\hat{M}|^{1/2}}H$, $\vec{\Phi}_0=-e\vec{E}-\frac{\varepsilon_s-\xi}{T}\vec{\nabla}T$, $\hat{\tau}$ is the tensor of relaxation time, $\hat{M}^{-1}$ is the inverse tensor of electron effective masses, $|\hat{\tau}|$ and $|\hat{M}|$ are determinants of the relaxation time and effective masses tensors respectively.

If we consider the electrons scattering on acoustical and non-polar optical phonons then for the relaxation time τ_s in film surface we have:

$$\tau_s^{-1}(\varepsilon_s)=\sum_{\beta,s'}W_{\beta,\beta,s'}\left(1-\frac{K'_xK_x+\varphi_s^4(\alpha)K'_yK_y}{K_x^2+\varphi_s^4(\alpha)K_y^2}\right), \quad (5)$$

where $W_{\beta\beta'_z}$ is probability of transition from state $\beta_z=(n_z,K_x,K_y)$ to state $\beta'_z=(n'_z,K'_x,K'_y)$ or back, having the form:

$$W_{\beta\beta'_z}=\sum_q W_q\left\{N_q\delta_{K'_x,K_x-q_x}\delta_{K'_y,K_y+q_y}\delta(\varepsilon_{\beta'_z}-\varepsilon_{\beta_z}-\hbar\omega_q)+\right. \quad (6)$$
$$\left.+(N_q+1)\delta_{K'_x,K_x-q_x}\delta_{K'_y,K_y-q_y}\delta(\varepsilon_{\beta'_z}-\varepsilon_{\beta_z}+\hbar\omega_q)\right\}\left|I_{n'_z n_z}\right|^2$$

where N_q is the Planck function, ω_q is the dispersion of phonons, and the form of ω_q functions are the same as for corresponding one in bulk specimen[7].

Taking into consideration the wave functions anisotropy we have for $I_{n'_z n_z}(q_z)$ function:

$$I_{n'_z n_z}(q_z)=\frac{2}{d}\int_0^d \exp(iq_z z)\sin\frac{\pi n'_z}{d}z\sin\frac{\pi n_z}{d}z\times \quad (7)$$
$$\times\exp\left(-i\frac{m^{-1}_{13(z)}(K'_x-K_x)+m^{-1}_{23(z)}(K'_y-K_y)}{m^{-1}_{33(z)}}z\right)dz$$

Then for the relaxation time τ_z the next result is obtained;

$$\tau_z(\varepsilon_z)=\tau_0\varphi_z^{-2}(\alpha)\left(\bar{n}_z+\frac{1}{2}\right)^{-1} \quad (8)$$

where $\bar{n}_z=\left[\sqrt{\frac{\varepsilon_z}{\varepsilon_{1z}}}\right]$ is an integer part of number $\sqrt{\frac{\varepsilon_z}{\varepsilon_{1z}}}$, $\varepsilon_{1z}=\varepsilon_z(n_z=1,\ K_x=K_y=0)$. τ_0 are the multipliers that don't depend on energy and proportional to the analogous expressions in bulk specimen[7].

From (8) one can see that τ_z depends on energy only through $\bar{n}_z$. Moreover τ_z essentially depends on n-Ge and n-Si films surface orientation and in the $\bar{n}_z>>1$ case result for bulk specimen is obtained.

2. Having known decision of transport equation and expression for the relaxation time one can calculate the current and the energy stream densities and then we can determine the components of kinetic tensors. On this base we can calculate all kinetic effects under various conditions. Let us show some of them in a weak magnetic field ($\nu<<1$) at the conditions of electrons scattering on acoustical and non-polar optical phonons.

So, for the Hall constant in this case we obtain:

$$R_y=-\frac{1}{n_e ec}\frac{\sum_{z=1}^{g}\left\{\varphi_z\sum_{n\sigma}F_1(\eta_{n\sigma})\right\}\sum_{z=1}^{g}\left\{\varphi_z^{-3}\left(\bar{n}_z+\frac{1}{2}\right)^{-2}\sum_{n\sigma}F_1(\eta_{n\sigma})\right\}}{\left[\sum_{z=1}^{g}\left\{\frac{(\varphi_z^{-2}+1)}{2}\left(\bar{n}_z+\frac{1}{2}\right)^{-1}\sum_{n\sigma}F_1(\eta_{n\sigma})\right\}\right]^2} \quad (9)$$

where n_e is the concentration of electrons in film, N=4 (n-Ge) and N=6 (Si).

For the thermopower we have:

$$\alpha_{zz}=-\frac{k_0}{e}\left\{\alpha_0+\alpha_1\tilde{\nu}^2\right\} \quad (10)$$

where $\tilde{\nu}=\frac{\tau_0 eH}{m_\perp c}$,

$$\alpha_0=\frac{\sum_z\left\{\frac{(\varphi_z^{-2}+1)}{2}\left(\bar{n}_z+\frac{1}{2}\right)^{-1}\sum_{n\sigma}\left[F_2(\eta_{n\sigma})-\eta_{n\sigma}F_1(\eta_{n\sigma})\right]\right\}}{\sum_z\left\{\frac{(\varphi_z^{-2}+1)}{2}\left(\bar{n}_z+\frac{1}{2}\right)^{-1}\sum_{n\sigma}F_1(\eta_{n\sigma})\right\}},$$

$$\alpha_1=\frac{\sum_z\left\{\varphi_z^{-3}\left(\bar{n}_z+\frac{1}{2}\right)^{-2}\sum_{n\sigma}(F_2-\eta_{n\sigma}F_1)\right\}\sum_z\left\{\varphi_z^{-3}\left(\bar{n}_z+\frac{1}{2}\right)^{-2}\sum_{n\sigma}F_1\right\}}{\left[\sum_z\left\{\frac{(\varphi_z^{-2}+1)}{2}\left(\bar{n}_z+\frac{1}{2}\right)^{-1}\sum_{n\sigma}F_1\right\}\right]^2}-$$
$$-\frac{\sum_z\left\{\frac{(\varphi_z^{-2}+1)}{2}\left(\bar{n}_z+\frac{1}{2}\right)^{-1}\sum_{n\sigma}(F_2-\eta_{n\sigma}F_1)\right\}\sum_z\left\{\frac{(\varphi_z^{-2}+1)}{2}\varphi_z^{-4}\left(\bar{n}_z+\frac{1}{2}\right)^{-3}\sum_{n\sigma}F_1\right\}}{\left[\sum_z\left\{\frac{(\varphi_z^{-2}+1)}{2}\left(\bar{n}_z+\frac{1}{2}\right)^{-1}\sum_{n\sigma}F_1\right\}\right]^2}$$

$$-\frac{\sum_s\left\{\frac{(\varphi_s^{-2}+1)}{2}\varphi_s^{-4}\left(\overline{n}_s+\frac{1}{2}\right)^{-3}\sum_{ns}(F_2-\eta_{ns}F_1)\right\}}{\sum_s\left\{\frac{(\varphi_s^{-2}+1)}{2}\left(\overline{n}_s+\frac{1}{2}\right)^{-1}\sum_{ns}F_1\right\}}$$

$$-\frac{\sum_s\left\{\frac{(\varphi_s^{-2}+1)}{2}\left(\overline{n}_s+\frac{1}{2}\right)^{-1}\sum_{ns}(F_2-\eta_{ns}F_1)\right\}\left[\sum_s\left\{\varphi_s^{-3}\left(\overline{n}_s+\frac{1}{2}\right)^{-2}\sum_{ns}F_1\right\}\right]^2}{\left[\sum_s\left\{\frac{(\varphi_s^{-2}+1)}{2}\left(\overline{n}_s+\frac{1}{2}\right)^{-1}\sum_{ns}F_1\right\}\right]^3},$$

$F_r(\eta_{ns})=\int_0^\infty x_s^r\left(-\frac{\partial f_0}{\partial x_s}\right)dx_s$ are the uniparametric Fermi integrals of r index (r=1,2), $x_s=\frac{\varepsilon_s-\varepsilon_{ns}}{k_0T}$, ε_{ns} is the discrete part of energy spectrum (2), $\eta_{ns}=\frac{\xi-\varepsilon_{ns}}{k_0T}$.

For the Hall constant we obtain the analytic expression in the case of arbitrary electron gas degeneration. We can use the following function:

$$F_1(\eta_{ns})=\eta_{ns}+\ln(1+\exp(-\eta_{ns})) \qquad (11)$$

and the results for degenerated and non-degenerated films are obtained.

In the case of degenerated electron gas for the thermopower we have:

$$\alpha_t=-\frac{(\pi k_0)^2T}{3e}\left\{\alpha_0'+\alpha_1'\tilde{v}^2\right\} \qquad (12)$$

where $\alpha_{0,1}'=\alpha_{0,1}(F_1=\xi_F-\varepsilon_{ns},\ F_2-\eta_{ns}F_1=1)$. Here Fermi energy ξ_F is determined as:

$$\xi_F=\frac{\pi d\hbar^2n_s/m_\perp+\sum_s\left\{\varphi_s\sum_{ns}\varepsilon_{ns}\right\}}{\sum_s\left\{\varphi_s\overline{n}_s\right\}} \qquad (13)$$

The analysis of expressions(12) and (13) show us that in this case $\alpha_t\sim1/d$, but because of its dependence on $\overline{n}_s$ the behaviour of thermopower on film thickness has a leap-like character.

In the case of non-degenerated electron gas for α_t is obtained:

$$\alpha_t=-\frac{k_0}{e}\left\{\alpha_0''+\alpha_1''\tilde{v}^2\right\} \qquad (14)$$

where
$\alpha_{0,1}''=\alpha_{0,1}(F_1=\exp(\eta_{ns}),\ F_2-\eta_{ns}F_1=(2-\eta_{ns})\exp(\eta_{ns}))$.
Here the chemical potential ξ is determined as:

$$\xi=k_0T\ln\frac{\pi d\hbar^2n_s}{m_\perp k_0T+\sum_s\left\{\varphi_s\sum_{ns}\exp(-x_{ns})\right\}} \qquad (15)$$

where $x_{ns}=\frac{\varepsilon_{ns}}{k_0T}$.

The analysis of expressions (14) and (15) show us that in this case $\alpha_t\sim\left(\ln d+\frac{1}{d^2}\right)$. Therefore the thermopower in this case also is a nonmonotonous function of film thickness. At the $\overline{n}_s>>1$ limit the result for bulk specimen is obtained that it does not depend on a film thickness.

[1] *V.B. Sandomirsky.* JETF, 1967, v.52, p.158.
[2] *B.A. Tavger.* Physica Status Solidi, 1967, v.22, p.31.
[3] *B.A. Tavger, V.N. Demikhovsky.* UFN, 1968, v.96, p.61.
[4] *B.M. Askerov, B.I. Kuliev, R.F. Eminov.* FNT, 1977, v.3, n.3, p.344.
[5] *B.I. Kuliev, V.M. Gadjiev.* "Fizika" Acad. Sci. Az. Resp., 1996, v.2, n.2, p.22.
[6] *B.I. Kuliev, V.M. Gadjiev.* "Fizika" Acad. Sci. Az. Resp., 1996, v.2, n.4, p.40.
[7] *B.M. Askerov.* The electron transport phenomena in semiconductors. Moscow, "Nauka",1985, §11, p.107.

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n-Ge VƏ n-Si NAZİK TƏBƏQƏLƏRİNDƏ ÖLÇÜYƏ GÖRƏ KVANTLAŞMANIN KİNETİK ƏMSALLARA TƏ'SİRİ

n-Ge və n-Si nazik təbəqələrində səthlərin səmtindən asılı olaraq kinetik əmsallar tədqiq olunur. Akustik və qeyri-polyar optik fononlarda səpilmə mexanizmlərini əhatə edən relaksasiya zamanı üçün ifadələr alınmışdır. Eyni zamanda n-Ge və n-Si nazik təbəqələrin səthində zəif maqnit sahəsində elektron qazının müxtəlif cırlaşma yaxınlaşmalarda Holl əmsalı və termo-EHQ üçün ifadələr alınmışdır.

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ВЛИЯНИЕ РАЗМЕРНОГО КВАНТОВАНИЯ НА КИНЕТИЧЕСКИЕ КОЭФФИЦИЕНТЫ В ПЛЕНКАХ n-Ge И n-Si

Исследуется поведение кинетических коэффициентов в зависимости от ориентации поверхности пленок n-Ge и n-Si. Получены выражения для времени релаксации, охватывающие механизмы рассеяния на акустических и неполярных оптических фононах. Получены также выражения для коэффициента Холла и термо-ЭДС в плоскости пленок n-Ge и n-Si в слабом магнитном поле при различных приближениях вырождения электронного газа.

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