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The effect of nonparabolicity on electron transport in semiconductor thin films

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Abstract. The resistivity of semiconductor thin films of InSb and GaAs at 77 K is investigated in the ultrathin limit with energy band nonparabolicity taken into account. The calculation based on the balance equation theory shows that the resistivity of these samples deviates from the previous result obtained by Arora and Awad for the parabolic limit (1981 *Phys. Rev.* B **23** 5570) which stated that the ratio of film resistivity to bulk resistivity is inversely proportional to d (the thickness of the film). The ratio is larger than unity when the thickness d is less than 100 nm and becomes larger with decreasing thickness of film. The nonparabolicity of the energy band results in the increase of the ratio and the increase of the deviation of the present result from the previous result for the parabolic limit.

1. Introduction

Since the narrow-gap semiconductors are of great technological interest in infrared devices [1], high-speed digital networks [2], optical modulators [3] and other devices, the influence of the energy band nonparabolicity on these materials has been extensively studied in inversion layers [4], heterojunction interfaces [5], quantum wells [6, 7] and superlattices [8, 9]. But few descriptions of the semiconductor thin films are available at this moment. In semiconductor thin films, the electrons are confined in the direction normal to the thin-film surfaces and move freely along the directions parallel to the thin-film surface. When the film is thin enough and the thickness of the thin film is comparable with the carrier mean free path, the so-called quantum-size effect may take place [10]. The wave character of the electron as obtained from the Schrödinger equation should be taken into account.

Years ago, the transport properties of electrons confined to semiconductor thin films and their relation to the bulk properties were studied by using the Boltzmann transport equation [11]. The theoretical results obtained by analysing the electron scattering by acoustic phonons and impurities told us that in the ultrathin limit, the resistivity in both cases is inversely proportional to the thickness of the film ($\hbar = K_B = 1$):

$$\frac{\rho_s}{\rho_b} = \frac{4\sqrt{\pi}\lambda_D}{3d} \tag{1}$$

with

$$\lambda_D = 1/(2m^*T)^{1/2} \tag{2}$$

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where ρ_s and ρ_b are the film resistivity and the bulk resistivity respectively, d is the thickness of the film, T is the lattice temperature, and m^* is the electron effective mass. In the early calculation, however, the energy band nonparabolicity was neglected.

In this paper we shall study the effect of energy band nonparabolicity on electron transport in semiconductor thin films by employing the balance equation theory. The balance equation theory, proposed by Lei and Ting [12] for parabolic band semiconductors, has been extended for studying electron transport in an arbitrary energy band [13]. In this extended theory, an ensemble-averaged inverse effective mass tensor is introduced to describe the effective response of the band electron system to an external electric field and two parameters (the centre-of-mass momentum and the electron temperature) are used to calculate the carrier transport in a uniform electric field. This approach has been successfully employed to study the transport properties in narrow-gap semiconductors [14–16].

In semiconductor thin films, the motion of conduction electrons parallel to the thin film surface may be described by plane waves, and those perpendicular to the film surface will be described by types of standing wave depending on the structure of the potential. For a square-well potential along the z-axis with infinitely high barriers at $z = 0$ and $z = d$, the electron wave function is given by [17]

$$\Psi_{l,\boldsymbol{k}_\parallel}(\boldsymbol{r}, z) = \left(\frac{2}{V}\right)^{1/2} \sin\frac{l\pi z}{d} \exp(\mathrm{i}\boldsymbol{k}_\parallel \cdot \boldsymbol{r}) \tag{3}$$

where the position vector $\boldsymbol{r}$ is given by $\boldsymbol{r} = (x, y)$, and $V = dS$ is the film volume with a surface area S and thickness d. $\boldsymbol{k}_\parallel = (k_x, k_y)$ is the electron wavevector in the x–y plane. The energy of the conduction electrons for the nonparabolic band structure is given by the relation [18]

$$\varepsilon_l(\boldsymbol{k}_\parallel) = \frac{1}{2\alpha}\left\{-1 + \left[1 + 4\alpha\left(\frac{{k_\parallel}^2}{2m^*} + \frac{1}{2m^*}\left(\frac{l\pi}{d}\right)^2\right)\right]^{1/2}\right\} \qquad l = 1, 2, 3, \ldots \tag{4}$$

with the nonparabolic parameter

$$\alpha = \frac{1}{\varepsilon_g}\left(1 - \frac{m^*}{m_0}\right)^2 \tag{5}$$

where ε_g is the energy gap, and m_0 the free-electron mass.

2. Balance equations

We consider a semiconductor thin film under the influence of an applied electric field $\boldsymbol{E}$ along the x-direction. The electrons are made to drift by the electric field and scattered by impurities and phonons. The acceleration and energy balance equations are given as follows:

$$eE\kappa_s + A_s = 0 \tag{6}$$

$$eEv_s - W_s = 0 \tag{7}$$

where

$$v_s = \frac{2}{n_s}\sum_{l,\boldsymbol{k}_\parallel} \frac{\partial\varepsilon_l(\boldsymbol{k}_\parallel)}{\partial k_x} f(\bar{\varepsilon}_l(\boldsymbol{k}_\parallel), T_e) \tag{8}$$

$$\kappa_s = \frac{2}{n_s}\sum_{l,\boldsymbol{k}_\parallel} \frac{\partial^2\varepsilon_l(\boldsymbol{k}_\parallel)}{\partial k_x^2} f(\bar{\varepsilon}_l(\boldsymbol{k}_\parallel), T_e) \tag{9}$$

are the average drift velocity of the system and the component of the ensemble-averaged inverse effective mass tensor in the x-direction (the other components have vanished).

$$f(\bar{\varepsilon}_l(\boldsymbol{k}_\parallel), T_e) = \left\{\exp[(\bar{\varepsilon}_l(\boldsymbol{k}_\parallel) - \mu)/T_e] + 1\right\}^{-1} \tag{10}$$

is the Fermi function at the electron temperature T_e. In these expressions $\bar{\varepsilon}_l(\boldsymbol{k}_\parallel) = \varepsilon_l(\boldsymbol{k}_\parallel - p_d)$ is the relative electron energy with p_d the centre-of-mass momentum along the x-direction. μ is the chemical potential which should be determined by the sheet number of the electrons, $n_s = N/S$ (N is the total number of electrons in the film):

$$n_s = 2\sum_{l,\boldsymbol{k}_\parallel} f(\varepsilon_k(\boldsymbol{k}_\parallel), T_e). \tag{11}$$

A_s ($=A_{is} + A_{ps}$) and W are the frictional accelerations due to impurity and phonon scatterings and the energy loss from the electron system to the phonon system. Expressions for them are respectively given as follows:

$$\begin{aligned} A_{is} = \frac{2n_i}{n_s} \sum_{l,l'} \sum_{\boldsymbol{k}_\parallel,\boldsymbol{q}} &|u(q)|^2 |F_{l,l'}(q_z)|^2 [(v_{l'}(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel))_x - (v_l(\boldsymbol{k}_\parallel))_x] \\ &\times \delta(\varepsilon_{l'}(\boldsymbol{k}_\parallel + q_\parallel) - \varepsilon_l(\boldsymbol{k}_\parallel)) \frac{[f(\bar{\varepsilon}_l(\boldsymbol{k}_\parallel), T_e) - f(\bar{\varepsilon}_{l'}(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel), T_e)]}{|\epsilon(\boldsymbol{q}, \bar{\varepsilon}_l(\boldsymbol{k}_\parallel) - \bar{\varepsilon}_{l'}(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel))|^2} \end{aligned} \tag{12}$$

$$\begin{aligned} A_{ps} = \frac{4\pi}{n_s} \sum_{l,l'} \sum_{\boldsymbol{k}_\parallel,\boldsymbol{q},\lambda} &|M(q,\lambda)|^2 |F_{l,l'}(q_z)|^2 [(v_{l'}(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel))_x - (v_l(\boldsymbol{k}_\parallel))_x] \\ &\times \delta(\varepsilon_{l'}(\boldsymbol{k}_\parallel + q_\parallel) - \varepsilon_l(\boldsymbol{k}_\parallel) + \Omega_{q,\lambda}) \frac{[f(\bar{\varepsilon}_l(\boldsymbol{k}_\parallel), T_e) - f(\bar{\varepsilon}_{l'}(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel), T_e)]}{|\epsilon(\boldsymbol{q}, \bar{\varepsilon}_l(\boldsymbol{k}_\parallel) - \bar{\varepsilon}_{l'}(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel))|^2} \\ &\times \left[n\left(\frac{\Omega_{q,\lambda}}{T}\right) - n\left(\frac{\bar{\varepsilon}_l(\boldsymbol{k}_\parallel) - \bar{\varepsilon}_l(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel)}{T_e}\right)\right] \end{aligned} \tag{13}$$

and

$$\begin{aligned} W_s = \frac{4\pi}{n_s} \sum_{l,l'} \sum_{\boldsymbol{k}_\parallel,\boldsymbol{q},\lambda} &|M(q,\lambda)|^2 |F_{l,l'}(q_z)|^2 \Omega_{q,\lambda} \delta(\varepsilon_{l'}(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel) - \varepsilon_l(\boldsymbol{k}_\parallel) + \Omega_{q,\lambda}) \\ &\times \frac{[f(\bar{\varepsilon}_l(\boldsymbol{k}_\parallel), T_e) - f(\bar{\varepsilon}_{l'}(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel), T_e)]}{|\epsilon(\boldsymbol{q}, \bar{\varepsilon}_l(\boldsymbol{k}_\parallel) - \bar{\varepsilon}_{l'}(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel))|^2} \\ &\times \left[n\left(\frac{\Omega_{q,\lambda}}{T}\right) - n\left(\frac{\bar{\varepsilon}_l(\boldsymbol{k}_\parallel) - \bar{\varepsilon}_l(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel)}{T_e}\right)\right] \end{aligned} \tag{14}$$

where $n(x) = 1/(\mathrm{e}^x - 1)$ is the Bose function, and $|\epsilon(\boldsymbol{q}, \omega)|^2$ is the RPA dielectric function of the system [13]. $(v_l(\boldsymbol{k}_\parallel))_x = \partial\varepsilon_l(\boldsymbol{k}_\parallel)/\partial k_x$ is the component of the velocity vector in the x-direction. $|F_{ll'}(q_z)|^2$ is the form factor due to the confinement of the thin film:

$$\begin{aligned} |F_{l,l'}(q_z)|^2 = &\left|\frac{4\pi^2 q_z \,\mathrm{d}l\, l'}{[(q_z d)^2 - (l - l')^2\pi^2][(q_z d)^2 - (l + l')^2\pi^2]}\right|^2 \\ &\times \begin{cases} 2(1 - \cos(q_z d)) & \text{for even } (l - l') \\ 2(1 + \cos(q_z d)) & \text{for odd } (l - l'). \end{cases} \end{aligned} \tag{15}$$

Also n_i is the impurity density, and $u(q)$ and $M(q, \lambda)$ are the Fourier representations of the electron–impurity and electron–phonon coupling matrix elements of bulk semiconductors.

In the limit of a parabolic band ($\alpha = 0$), the above equations may be reduced to those of the parabolic case [19]. Furthermore, in the bulk limit (d large enough), where spacing between two adjacent levels is very small, the summation over l and l' can be replaced by an integral, and the above equations become the same as those in the bulk nonparabolic case [13].

3. Calculation

In the weak-current limit ($p_d \rightarrow 0$), the solution of the energy balance equation (7) is $T_e = T$ and the linear resistivity can be obtained directly from equation (6):

$$\rho_s = \frac{A_s}{n_b e^2 \kappa_s v_s} \tag{16}$$

where e is the electric charge. n_b is the density of the film and equals N/Sd.

The bulk resistivity is

$$\rho_b = \frac{A_b}{n_b e^2 \kappa_b v_b} \tag{17}$$

where A_b, κ_b and v_b are the frictional acceleration, ensemble-averaged inverse effective mass tensor and drift velocity in the bulk case, respectively, which are given in [13]. Hence the ratio of the film resistivity ρ_s to the bulk resistivity ρ_b is given as

$$\frac{\rho_s}{\rho_b} = \frac{A_s \kappa_b v_b}{A_b \kappa_s v_s}. \tag{18}$$

InSb is a typical narrow-gap semiconductor with energy gap $\varepsilon_g = 0.18$ eV and effective mass $m^*/m_0 = 0.014$, while GaAs is a wide-gap semiconductor with $\varepsilon_g = 1.42$ and $m^*/m_0 = 0.067$. Their nonparabolic parameters are 5.4 and 0.61 respectively. We make use of equation (18) to calculate the ratio ρ_s/ρ_b for InSb film and for GaAs film to show the effect of the nonparabolicity on the electron transport in thin films. The acoustic phonon scattering and ultrathin limit ($l = l' = 1$) are taken into account. The lattice temperature is taken as 77 K. The lattice densities of GaAs film and InSb film are $n_b = 2.0 \times 10^{16}$ cm^{-3} and 2.1×10^{15} cm^{-3} respectively. The other fundamental parameters used in the calculation are taken as the characteristic constants. The thickness of the film ranges from 10 nm to 100 nm.

The ratio of film resistivity to bulk resistivity, ρ_s/ρ_b, for GaAs film is shown in figure 1 as a function of the thickness of film d. The solid line denotes the result from the present balance equation theory (BET) and the dotted line is the result obtained using the Boltzmann transport equation (BTE) by Arora *et al*. For $d = 100$ nm, the ratio of the two results is nearly equal to unity. The quantum-size effect can be neglected if the thickness of the film is large enough. When the thickness becomes small, the ratio of the two results deviates from unity and becomes larger with decreasing thickness. However, the ratio of the present BET results is larger than that of the BTE results because of the nonparabolicity of the energy band. And this effect becomes more significant with decreasing thickness.

The ratio ρ_s/ρ_b for InSb film is plotted in figure 2 as a function of d. Like in figure 1, the solid line is the result from the present BET and the dotted line is the result obtained using the BTE by Arora *et al*. Unlike that for GaAs film, the ratio for InSb film at 100 nm is 2.2. The quantum-size effect still occurs at this thickness. The variation of the resistivity ratio for InSb film with d is similar to that for GaAs film, but the deviation between the present BET results and those obtained using the BTE becomes more substantial with the increase of the nonparabolicity of the energy band. At $d = 10$ nm, the ratio of the present BET results is about four times that of the BTE results for InSb film, whilst the ratio of the present BET results is only two times that of the BTE results for GaAs film.

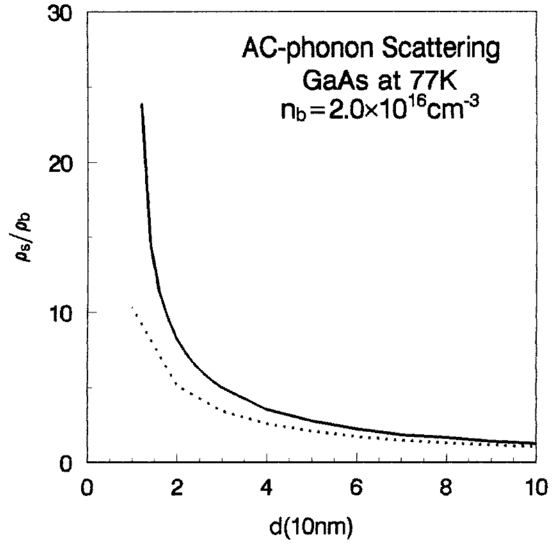

Figure 1. The ratio of the film resistivity to the bulk resistivity, ρ_s/ρ_b, of GaAs at 77 K with $n_b = 2.0 \times 10^{16}$ cm^{-3} is plotted as a function of d. The solid line is the result from the present balance equation theory (BET) and the dotted line is the result obtained using the Boltzmann transport equation (BTE) by Arora *et al.*

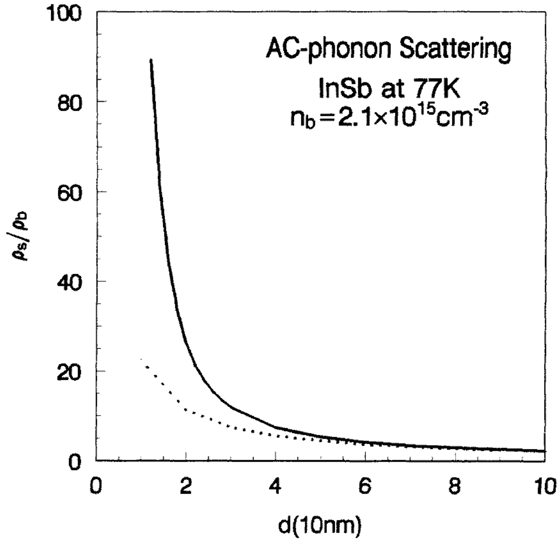

Figure 2. The ratio of the film resistivity to the bulk resistivity, ρ_s/ρ_b, of InSb at 77 K with $n_b = 2.1 \times 10^{15}$ cm^{-3} is plotted as a function of d. The solid line is the result from the present BET and the dotted line is the result obtained using the BTE by Arora *et al.*

4. Conclusion

The balance equations have been employed to study the effect of nonparabolicity of the energy band on transport properties in semiconductor thin films in the ultrathin limit. This limit is not strictly appropriate for the range of thickness studied; however, since it has been employed by Arora *et al*, we still use it to study the electron transport in semiconductor films and compare the present results with the results of Arora *et al* to show the effect of nonparabolicity on electron transport in semiconductor films. By investigating the linear resistivity of wide-gap semiconductor GaAs film and narrow-gap semiconductor InSb film, as it relates to the corresponding bulk resistivity, we find that the ratio of the film resistivity to the bulk resistivity is larger than unity when the thickness of the film is less than 100 nm.

The ratio becomes larger with decreasing thickness of film. The nonparabolicity of the energy band gives rise to an increase of the ratio and an increase of the deviation of the result obtained from the present balance equation theory from that obtained using the Boltzmann transport equation. In short, the effect of nonparabolicity of the energy band should not be neglected in studying the electron properties of semiconductor thin films.

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