Effect of surface scattering on the current-voltage characterístics of thin semiconducting samples

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The current-voltage characteristics (CVC) of classical thin semiconducting films are indicated when the film boundaries are nonideal, under the condition that the thickness $d \ll l$, where l is the momentum mean free path. It is shown that surface scattering can significantly alter the classification of an IVC; in particular it can give rise to negative differential conductivity and the disappearance of the S-shaped portion of the CVC.

1. The problem of how a surface with irregular structure affects the kinetics of current carriers in thin films is one of considerable interest. In recent years, considerable progress has been made in investigating surface scattering, conductivity and high-frequency phenomena in samples of small size.[1] Through the efforts of various workers, a microscopic approach to the interaction of electrons with various boundary imperfections has been developed. Thus, the case of point surface defects with large and small radii was investigated in Refs. 2 and 3; skin effects and magnetic surface levels were studied in Refs. 4 and 5, taking into account nonideal boundaries; the investigation of small and large amplitude roughness was the subject of Refs. 6 and 7. In all models of surface scattering, an important role is played by the magnitude of the projection of the electron momentum perpendicular to the surface, which to a large extent determines the character of the electron reflection. Thus, specular reflection of grazing-incidence electrons is a completely general property, which from a physical point of view is related to the large wavelength associated with the component of motion normal to the surface.[8]

In semiconductors, the characteristic mean free path λ is not strictly related to the crystal parameters, and can vary over quite a broad range. If $\lambda \sim d$, then quantization of the transverse motion occurs. In this case, surface scattering has a considerable effect on the quantum size effects; in particular, the energy levels are shifted and can decay, while the thickness and temperature dependences of the electrical conductivity change.[10] A second effect, which is specific to semiconductors, is heating of the electron gas in a strong external electric field; surface scattering give rise to qualitatively new behavior because of this effect. This phenomenon is also controlled with the main idea of the present work, which may be described as follows. In an increasing electric field the momentum distribution of the current carriers changes so that their mean energy increases. As a consequence of this, the mean free path decreases. It is clear that a decreasing mean free path will strengthen the interaction of the electrons with surface irregularities, and so the current will increase more slowly than in the bulk case. If this situation results in a sufficiently rapid decrease of the conductivity with field, then the current-voltage characteristic (CVC) will exhibit a region where current decreases with increasing voltage; this region is exclusively a consequence of surface scattering and is not a characteristic of a bulk sample. Under these conditions, it becomes possible to obtain thin semiconducting samples with negative differential resistance (NDR) based on materials which are not traditionally considered as candidates for use in generation of UHF radiation. In this case, we will refer to the NDR as "boundary-related." Among the physical models of the surface capable of providing a sharp transition from specular to diffusive scattering, we should mention those with surface band bending.[11] In these models, heating of the electrons can lead to a situation where the majority of them may be capable of surmounting the barrier and scattering off the true surface. A second possibility is scattering from a weakly roughened boundary, the topic is discussed in this article. In the ohmic regime the effect on the mobility of electrons in a semiconductor (in inversion layers) of changing the ratio of the wavelength λ to the mean roughness height was analyzed by the authors of Ref. 12; they found a dependence of the mobility on temperature which was qualitatively different from that of purely diffusive scattering: $\mu \sim T^{-1.5}$ instead of $\mu \sim T^{0.5}$.

In the majority of theoretical papers investigating size effects in a classical hot-electron gas, calculations are usually carried out under the conditions $l \ll L \lesssim d$, where L is the "cooling length." The current state of theoretical understanding of this problem is reflected in Ref. 13, where the influence of thermal boundary conditions, magnetic field and phonon amplification on the CVC of finite semiconductor samples was analyzed. We will be interested in the case $d \ll l$. A detailed discussion of purely diffusive scattering by a film boundary under weakly nonequilibrium conditions is given in Ref. 14. The problem of determining the form of the CVC in the presence of classical size effects has not been discussed up to the present time.

2. Let us consider an adiabatically isolated semiconductor film oriented along the z-axis, and direct the x-axis along the normal to the surface: $-d/2 \leqslant x \leqslant d/2$. We will assume that the Debye radius is the smallest parameter in the problem with dimensions of length, and that all spatial inhomogeneities are absent when the film is in a state of thermal equilibrium. We will take the part of the distribution function $f_0(\varepsilon)$ which is isotropic in momentum space to be Maxwellian with an effective temperature T which depends on the electric field $E \parallel z$. The possibility of introducing an effective temperature in thin semiconductor films was discussed in Ref. 14. Let us assume that T does not depend on the coordinates (we will verify below that in a thin film this is actually the case), and substitute the distribution function $f(\mathbf{p},x) = f_0(\varepsilon) + f_1(\mathbf{p},x)$ in the kinetic equation:

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$$eEv_z\frac{\partial f_0}{\partial \varepsilon}+eE\frac{\partial f_1}{\partial p_z}+v_x\frac{\partial f_1}{\partial x}=\hat{S}t\, f_0-\frac{f_1}{\tau}, \tag{1}$$

where St and τ are the collision operator and momentum relaxation time, while $f_1(\mathbf{p},x)$ is a finite-current correlation which is odd in the variable p_z. Obviously there are no transverse currents by virtue of our assumptions. Separating out that portion of (1) which is odd in p_z and solving the resulting equation we find that

$$f_1=-\frac{eElp_z}{p}\left[1-\Phi(v)\exp-\frac{x}{(\tau v_x)}\right]\frac{df_0}{d\varepsilon}. \tag{2}$$

The function $\Phi(\mathbf{v})$ must be determined from the boundary conditions at $x=\pm d/2$.

Let us first show that it is possible in principle for the CVC of a thin film to be decreasing in some region, using a simple model first proposed by Parrot.[15] In this model, a "specularity parameter" Q is used, which, however, depends on p_x:

$$Q=\begin{cases}1, & |p_x|\leqslant p_0\\ 0, & |p_x|>p_0\end{cases}. \tag{3}$$

From a physical point of view, this model accurately reflects the fact that scattering of grazing-incidence and slow electrons is specular, and that there is a diffusive interaction with the surface for electrons with short mean free paths. Once we have found the unknown function $\Phi(\mathbf{v})$ using the Fuchs boundary condition, it is not hard to obtain an expression for the conductivity σ relative to σ_0, i.e., the conductivity of a bulk sample.

Introducing $\varkappa=p_0^2/2mT$ and neglecting terms of order $(d/1)^2$, we obtain

$$F(\varkappa)\equiv\frac{\sigma}{\sigma_b}=1-e^{-\varkappa}(\varkappa+1)+\frac{3}{2}\varkappa^{3/2}\Gamma\left(\frac{3}{2},\varkappa\right)-\frac{1}{2}\varkappa^{1/2}\Gamma\left(\frac{1}{2},\varkappa\right)+\frac{3}{8}\frac{d}{l}\Gamma(0,\varkappa), \tag{4}$$

where

$$\Gamma(a,\varkappa)=\int_\varkappa^\infty \exp(-t)\,t^{a-1}\,dt. \tag{5}$$

As $\varkappa\to\infty$ only the exponential tail of the electron distribution is scattered diffusively, and

$$F(\varkappa)\approx 1-3\exp(-\varkappa)/4\varkappa. \tag{6}$$

In the high-temperature regime Eq. (4) is correct as long as $\varkappa^{1/2}\gg d/l$ holds. Let us write down the equation of power balance $\sigma_b FE^2=P$, in which σ_b and P (the power delivered to the lattice) have a power-law dependence on $\Theta\equiv T/T_0$, where T_0 is the heat-bath temperature:

$$\sigma_b=\sigma_0\Theta^{-q},\quad P=\nu_0\Theta^{r-1}(\Theta-1). \tag{7}$$

Setting $r=q=0.5$ (this corresponds, e.g., to scattering by optical phonons in nonpolar crystals[13]), let us introduce the dimensionless field $\varepsilon=E(\sigma_0/\nu_0)^{1/2}$ and current $i=j(\sigma_0\nu_0)^{-1/2}$; furthermore, we will assume that $\alpha_0=p_0^2/2mT_0\gg 1$. Then from (4), (7) we obtain

$$i=\left[F\left(\frac{\alpha_0}{\Theta}\right)\frac{\Theta-1}{\Theta}\right]^{1/2},\quad \varepsilon=\left[\frac{\Theta-1}{F(\alpha_0/\Theta)}\right]^{1/2}. \tag{8}$$

In the region $1\ll\Theta\ll\alpha_0\, i\simeq 1$, $\varepsilon\propto\Theta^{1/2}$, Eq. (6) implies that as the temperature continues to increase the current will begin to decrease with increasing field. Numerical calculations using Eqs. (4), (8) show that the current for $d/l\ll 1$ can fall off by 30% of its value $i_{\max}=1$. If we take into account only acoustic scattering, the CVC obtained by the method described above has no NDR portion; nevertheless, in the region of field (or temperature) for which $\varkappa\sim 1$, the differential conductivity decreases markedly, although it remains positive everywhere.

3. It is now well known[8] that any systematic approach to solving kinetic problems in finite samples must include the use of integral boundary conditions which relate the distribution function for incident electrons to the distribution function for electrons reflected from the boundary. For scattering by a weakly roughened surface, Fal'kovskii has shown that the scattering function is proportional to $W(\mathbf{p}_s-\mathbf{p}_{s'})$, i.e., the Fourier transform of the roughness pair correlation function. If the surface is described by the two parameters a, the mean irregularity height and b, the correlation length, where $\lambda\gg b$, then

$$W(\mathbf{p}_s-\mathbf{p}_{s'})\approx\pi a^2b^2=\text{const}$$

and when $d\ll l$ it is not hard to obtain for the current density (in a system of units in which $\hbar=1$)

$$j=\frac{-3e^2Ed}{4\pi^3m(ab)^2}\int\frac{p_z^2}{p_xp^2}\frac{1}{p_x^2+\alpha/p^2}\frac{df_0}{d\varepsilon}d^2p_s\,dp,$$
$$\alpha\approx 3d/2la^2b^2,\quad p=(p_s^2+p_x^2)^{1/2}. \tag{9}$$

From (9) [which is just equal to (4)] we obtain a thickness-independent Joule heating, which justifies the assumption of a uniform temperature. The mean free path in general depends on energy: $l\sim\varepsilon^{1/2-q}$, where q is determined by Eq. (7). Introducing

$$\gamma=\alpha_T^{1/2}/(2mT),\quad \alpha_T=\alpha(\varepsilon=T),$$

using (9), we obtain for the relative conductivity

$$I(\gamma)\equiv\frac{\sigma(\gamma)}{\sigma_b}=\frac{3\gamma^2}{\Gamma(7/2-q)}\int_0^\infty \exp[-(\gamma z)^{4/(5-2q)}]\times\left(\operatorname{arctg} z-\frac{1}{z}+\frac{\operatorname{arctg} z}{z^2}\right)dz, \tag{10}$$

which in various limiting cases is given by the following expressions:

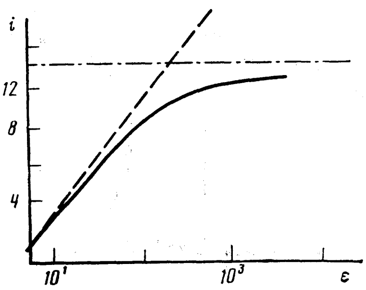

FIG. 1. CVC for a thin film for DA scattering: $\gamma_0=100$. The dashed curve denotes the CVC for bulk sample; the dotted-dashed curve shows the asymptotic value of the current in a thin film.

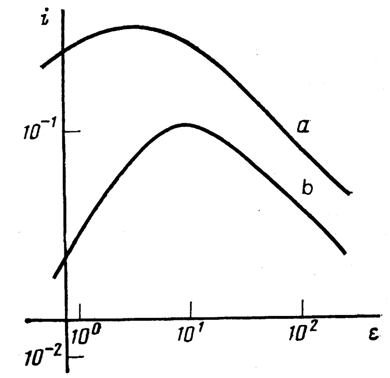

FIG. 2. CVC for a thin film for $r = q = 0.5$; a) $\gamma_0 = 0.1$, b) $\gamma_0 = 0.01$.

$$I(\gamma) \approx 1 - \frac{\Gamma(5-2q)}{5\Gamma(5/2-q)\gamma^2}, \quad \gamma \gg 1, \tag{11}$$

$$I(\gamma) \approx \frac{3\pi}{4} \frac{\Gamma(5/4 - q/2)}{\Gamma(5/2-q)} \gamma, \quad \gamma \ll 1. \tag{12}$$

The parameter γ, which defines the thick-sample and thin-sample limits in (10), has a simple meaning: γ^{-1} determines the number of diffuse collisions within a mean free path for the hot electrons.[6]

Furthermore, from the balance equation it is easy to obtain the CVC in parametric form:

$$i = [\Theta^{r-q-1}(\Theta-1) I(\gamma_0 \Theta^{q/2-5/4})]^{1/2}, \quad \varepsilon = \left[\frac{\Theta^{r+q-1}(\Theta-1)}{I(\gamma_0\Theta^{q/2-5/4})}\right]^{1/2}, \tag{13}$$

where $\gamma_0 = \gamma(T = T_0)$. Using (13), let us investigate a number of specific scattering mechanisms:

(a) $r = 1.5$, $q = 0.5$, i.e., acoustic phonons (deformation-acoustic or DA). For $\gamma_0 \ll 1$, using the asymptotic form (12) in the limit of strong heating $\Theta \gg 1$ we obtain $\Theta = \tilde{\gamma}_0^{1/3} \varepsilon^{2/3}$, where $\tilde{\gamma}_0 = 3\pi\gamma_0/4$. In this case the current saturates; $i = \tilde{\gamma}_0^{1/2}$, whereas in a bulk sample $\Theta = \varepsilon$ and $i = \varepsilon^{1/2}$. The latter dependence can also occur in a thin film for the case $\gamma_0 \gg 1$ (Fig. 1). Then $i = \varepsilon^{1/2}$ for $1 \ll \varepsilon \ll \gamma_0$, while for $\varepsilon \gg \gamma_0^{1/3}$ we again obtain $i = \tilde{\gamma}_0^{1/2}$.

(b) $r = q = 0.5$, i.e., energy relaxation via optical phonons (deformation-optical or DO), and momentum relaxation by acoustic phonons. This case leads to NDR (Fig. 2). In fact, for $\gamma_0 \ll 1$ and $\varepsilon \gg \tilde{\gamma}_0^{-1/2}$ we obtain $\Theta = \tilde{\gamma}_0^{1/2}\varepsilon$, $i = \gamma_0^{1/4}\varepsilon^{-1/2}$. If $\gamma_0 \gg 1$, then saturation of the current precedes the region of decrease for $1 \ll \varepsilon \ll \gamma_0^{1/2}$. Obviously this dependence $i(\varepsilon)$ is also preserved in the case when the only scattering mechanism is via deformation-optical phonons.

(c) If the momentum relaxes via ionized impurities ($q = -1.5$) and $\gamma_0 \gg 0$, then just as in the earlier case of low temperatures, i.e. $\Theta \ll \gamma_0^{1/2}$, the CVC of a thin film duplicates that of a bulk sample; if energy is dissipated in this case because of the DA mechanism, then $i = [\Theta(\Theta - 1)]^{3/2}$, $\Theta = (1 - \varepsilon^2)^{-1}$ and for $\varepsilon \to 1$ the temperature of a bulk sample grows without bound.

A surface without any additional mechanism for volume relaxation can provide a steady state for these systems; for $\Theta \gg \gamma_0^{1/2}$, using (12) and (13) gives us

$$\Theta = (\pi\gamma_0/8)^{1/2}\varepsilon, \quad i = \pi\gamma_0\varepsilon^{1/2}/8, \tag{14}$$

i.e., the current will increase slowly according to a square-root law.

(d) Finally, let us see what happens to an S-shaped CVC when we go to a thin film. Let $q = -1.5$, $r = 0.5$; then the dependence of the temperature on electric field in a bulk sample is shown in Fig. 3a. For $\gamma_0 \ll 1$, from (13) we obtain

$$\Theta = 1 + \gamma^*\varepsilon^2, \quad i = \gamma^*\varepsilon(1+\gamma^*\varepsilon^2)^{-1/2}, \tag{15}$$

where $\gamma^* = \pi\gamma_0/8$. Thus, the S-shape has been eliminated. In the case $\gamma_0 \gg 1$, the initial branch of the S-shaped characteristic appears, after which the current goes over to the dependence given by (15) (Fig. 3c).

4. All the results presented so far are valid to first order in d/l, while we have everywhere assumed the problem was classical. In very thin semiconducting films, with $d \sim 10^{-6}$ cm, quantum effects occur. In reality, the condition for classical behavior $pd \gg 1$ can be weakened. As shown by the authors of Ref. 17 for quasielastic interactions with DA and DO phonons, in the presence of a quantum size effect for specular scattering by a boundary, even in a moderate field, heating suppresses the quantization of the electrons so the CVC for a film and a bulk sample coincide. If this field is smaller than the "switch-on" field for surface scattering, our results can be taken over to the quantized films as well.

In conclusion, we should note that transport phenomena involving hot electrons in semiconductors are presently used in an extremely limited way for the purpose of studying the structures of surfaces. It is clear from the results presented here that the CVC of thin films is quite sensitive to the state of the boundary and can undergo significant qualitative changes as the boundary is changed; this property could find application in the investigation of surface properties of semiconductors.

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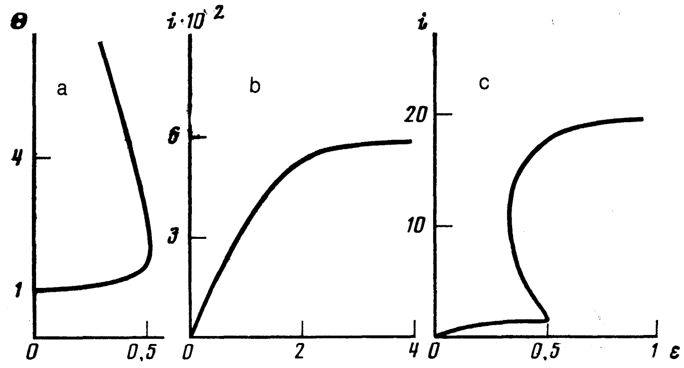

FIG. 3. The case $q = -1.5$, $r = 0.5$; a) temperature dependence on applied field for a bulk sample, b) CVC for a film with $\gamma_0 = 0.01$, c) for $\gamma_0 = 1000$.

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