Properties of current-voltage characteristics of semiconductors in the case of resonant scattering of electrons

S. D. Beneslavskiĭ, A. V. Dmitriev, and N. S. Salimov

M. V. Lomonosov State University, Moscow

(Submitted 7 July 1986)
Zh. Eksp. Teor. Fiz. **92**, 305–310 (January 1987)

A study is made of the influence of resonant scattering of carriers by quasilocal levels on the heating of electrons in a semiconductor. It is shown that a strongly nonmonotonic energy dependence of the relaxation time near a resonance may give rise to negative differential conductance (NDC) regions in the current-voltage characteristic. In the case of zero-gap semiconductors the characteristics may exhibit simultaneously both N- and S-shaped NDC regions.

1. INTRODUCTION

Narrow-gap semiconductors frequently have quasilocal electron states of different origin, and the energy levels of these states are superposed on the allowed bands.[1–5] The existence of such energy levels may have a considerable influence on the transport properties of semiconductors. The most thorough experimental[6–9] and theoretical[3,4,10,11] investigations of these effects have been made in weak electric fields. In the interpretation of the experimental results an allowance has been made either for resonant scattering of conduction electrons by centers responsible for quasilocal states or for the possibility of carrier capture by these states, which is reflected in the electron statistics.

The few available experimental results demonstrate the important role played by quasilocal states also in the processes of heating of a carrier gas by an electric field.[12,13] A theory of nonequilibrium processes occurring under these conditions has not been completely developed, but Gel'mont[14] predicted the possibility of an S-shaped current-voltage characteristic for a zero-gap HgTe semiconductor containing acceptors, which give rise to resonance states in the conduction band. An S-shaped characteristic is mainly due to the capture of electrons by acceptors, i.e., it is a concentration effect. The capture by quasilocal states is allowed for also in Ref. 15 where a calculation of the current-voltage characteristic of a zero-gap semiconductor is reported.

Thus the influence of quasilocal states on electron transport properties can be interpreted in two ways, either as resonant scattering or as capture. We shall determine the conditions of validity of the two approaches and study the influence of quasilocal states on the form of the current-voltage characteristic of a semiconductor in the case when such influence gives rise to resonant scattering of carriers. We shall consider a situation in which the particle density is sufficiently high to apply the effective temperature method (i.e., the energy control approximation[16]) and the lattice scattering mechanisms are quasielastic. For simplicity, we shall assume that the electron dispersion law is parabolic and isotropic. We shall consider two kinds of behavior of the carrier density during the heating of carriers: 1) the density of electrons remains constant, which is true of a semiconductor with $\varepsilon_g \neq 0$ in electric fields that do not cause impurity or interband breakdown; 2) the density of electrons increases as a result of heating because of a linear rise of the electron chemical potential with electron temperature. The second situation is typical of zero-gap semiconductors with $m_e^* \ll m_h^*$ (such as HgTe).[13]

2. CONDITIONS OF VALIDITY OF THE TRANSPORT EQUATION IN THE CASE OF RESONANT SCATTERING

From the point of view of kinetics a characteristic feature of resonant scattering is its duration. As in resonant tunneling,[17] the interaction time τ_c (collision duration) of a particle scattered by a center is related to the energy width γ of a resonant state, $\tau_c \propto \gamma^{-1}$, which is governed by the characteristic features of the internal structure of the scatterer and, therefore, τ_c may be considerably longer than the flight or transit time $\tau_f \propto r/v$, where r is the radius of action of the potential of the center and v is the velocity of the incident particle.

One of the main conditions of validity of the Boltzmann transport equation is the requirement that the collision duration be short compared with the mean time between collisions.[18] In the resonant scattering case this means

$$\tau_c \propto \gamma^{-1} \ll 1/(Nv\sigma), \tag{1}$$

where N is the density of the scatterers and σ is the resonant scattering cross section. The condition (1) is most stringent at a resonance, where σ is maximal, and (apart from the dependence on the characteristics of the scatterer) is of the order of p^{-2}, where p is the electron momentum.[19] Then, Eq. (1) becomes

$$N/\gamma \ll \rho(\varepsilon_0), \tag{2}$$

where $\rho(\varepsilon_0)$ is the density of states in a band where the resonance energy is ε_0. Therefore, if the interaction of electrons with centers can be described using the transport equation, it follows from Eq. (2) that the density of states at impurities $\sim N/\gamma$ is small compared with the density of states in a band. Consequently, in this range the influence of quasilocal states on the statistics is weak and the capture of carriers by such states is unimportant. The resonant scattering intensity at energies of the order of ε_0 may be considerably higher than the intensity of other nonresonant mechanisms and it may have a strong influence on the transport processes. This is precisely the situation with which we will be concerned.

When the inequality of Eq. (2) is disobeyed, the trans-

 0038-5646/87/010173-04$04.00

port equation approximation is invalid and the problem has to be solved employing more elaborate methods. At present such methods are not yet available. The published calculations carried out using the Green's function technique[10] do not allow us to go to the range where $N/\gamma \gtrsim \rho(\varepsilon_0)$, particularly under highly nonequilibrium conditions.

However, the transport equation can be used again in the case of a very small width γ of a resonance level, when the duration of interaction of a carrier with a scatterer is so long that an electron can be considered to be captured by a steady state of a trap (attachment). The equation then describes not the resonant scattering, but the processes of the capture of electrons by centers and their release as a result of ionization of the centers by other carriers and phonons. Quasilocal states can then be regarded as localized, i.e., as stable and infinitesimally narrow ($\gamma \to 0$). This picture is valid if the quantum-mechanical "lifetime" of a quasilocal state $\tau_c \propto \gamma^{-1}$ is much longer than the lifetime of an electron at a center governed by the ionization processes. Mikheev and Pomortsev[15] investigated theoretically the heating of carriers in a zero-gap semiconductor in this limit ($\gamma = 0$) allowing for the influence of quasilocal states only on the electron statistics.

3. HEATING OF ELECTRONS UNDER RESONANT SCATTERING CONDITIONS

As described in the Introduction, we shall consider a semiconductor with an isotropic and quadratic energy band and quasielastic scattering of carriers, and we shall use the effective temperature approximation. The reciprocal of the relaxation time of the carrier momentum in the case of resonant scattering ν_p has it usual form:

$$\nu_p(\varepsilon) = \nu_{p0}\gamma^2/[(\varepsilon-\varepsilon_0)^2+\gamma^2],$$

where ν_{p0}, γ, and ε_0 are regarded as parameters. It is assumed that nonresonant scattering is described by relaxation times which depend on the energy in accordance with power laws: $\nu(\varepsilon) = \nu_0(\varepsilon/T_0)^q$ in the case of the momentum relaxation processes and $\tilde{\nu}(\varepsilon) = \tilde{\nu}_0(\varepsilon/T_0)^{r-1}$ in the case of the energy relaxation processes. Here, T_0 is the lattice temperature, and the power exponents q and r, as well as the expressions for ν_0 and $\tilde{\nu}_0$ for different scattering mechanisms are known (see, for example, Ref. 16).

Under these assumptions the electric current flowing in such a semiconductor can be described by

$$j = \int d\varepsilon\, \rho(\varepsilon) \frac{e^2}{3} E v^2(\varepsilon) \tau(\varepsilon) \left(-\frac{\partial f_0}{\partial \varepsilon}\right), \tag{3}$$

where E is the electric field; v is the carrier velocity; $\tau = [\nu_p(\varepsilon)\nu(\varepsilon)]^{-1}$ is the carrier momentum relaxation time; and $f_0 = \{1 + \exp[(\varepsilon - \mu)/T)]\}^{-1}$ is the isotropic part of the distribution function. The quantities μ and T are found from the energy balance and electrical neutrality equations. The former equation is

$$jE - \left(\frac{\partial \varepsilon}{\partial t}\right)_{st} = 0,$$

where

$$\left(\frac{\partial \varepsilon}{\partial t}\right)_{st} = \int d\varepsilon\, \rho(\varepsilon) T_0 \varepsilon \tilde{\nu}(\varepsilon) \left[\frac{\partial f_0}{\partial \varepsilon} + \frac{1}{T_0} f_0(1-f_0)\right]$$

is the energy flux to the lattice.[16] Introducing dimensionless variables

$$\theta = \frac{T}{T_0}, \quad \omega = \frac{\varepsilon}{T_0}, \quad \omega_0 = \frac{\varepsilon_0}{T_0}, \quad \bar{\gamma} = \frac{\gamma}{T_0},$$
$$F = \frac{E}{E_0}, \quad E_0 = \left(\frac{3m_e^* T_0 \nu_0 \tilde{\nu}_0}{2e^2}\right)^{1/2}, \tag{4}$$

we can reduce the energy balance equation to

$$IF - \int d\omega\, \omega^{3/2} \omega^{r-1} (\theta-1) f_0(1-f_0) = 0,$$
$$I = \int d\omega\, \omega^{3/2} f_0(1-f_0) F \left\{\omega^q + \frac{\nu_{p0}}{\nu_0}\left[\frac{(\omega-\omega_0)^2}{\bar{\gamma}^2} + 1\right]^{-1}\right\}^{-1}. \tag{5}$$

The electrical neutrality equation in the case when the carrier density is not affected by heating has the form

$$\int d\omega \omega^{1/2} f_0 = {}^2/_3 \omega_F^{3/2}, \tag{6}$$

where $\omega_F = \varepsilon_F/T_0$, and ε_F is the Fermi energy of electrons.

However, as in the case of gapless semiconductors, as the heating increases the electron density in the conduction band grows because of the transfer of carriers from the valence band. (In this case the contribution to the conduction process made by holes created in the valence band can be ignored because of their large mass and low mobility.) We do not have to solve the exact electrical neutrality equation, but can replace it by the approximate solution taken from the results of Ref. 13:

$$\mu(T) = \varepsilon_F + CT. \tag{7}$$

The quantity C, dependent on the features of the spectrum and on the initial density of carriers, will be regarded as the parameter of the model.

The system of equations (5), (6), or (5)–(7) determines how T and μ depend on E. When such dependences are available, we can readily find the form of the current-voltage characteristic from Eq. (3). Such calculations can be carried out only numerically. However, before giving the results of numerical calculations, we shall consider qualitatively the nature of the solutions.

4. QUALITATIVE ANALYSIS

The width of a resonance level in the conduction band is usually small compared with its energy ε_0 and since we are interested in electrons that undergo resonant scattering, in this region we can ignore the energy dependence of the nonresonant quantities v, ρ, ν, and $\tilde{\nu}$ and assume that they are constant. The width of the level is understood to be the quantity Γ introduced below. It need not be small compared with ε_0, but at this stage for the sake of simplicity we shall assume that $\Gamma \ll \varepsilon_0$. Then the energy balance equation becomes

$$\bar{\sigma}(T) = (T-T_0)/E^2, \tag{8}$$

where the conductivity is described by

$$\bar{\sigma}(T) = \int d\varepsilon\, \bar{\tau}(\varepsilon)(-\partial f_0/\partial \varepsilon), \tag{9}$$

$$\bar{\tau}(\varepsilon) = \nu\tau(\varepsilon) = 1 - (\Gamma^2-\gamma^2)/[(\varepsilon-\varepsilon_0)^2+\Gamma^2], \quad \Gamma = \gamma(1+\nu_{p0}/\nu)^{1/2},$$

and the units used to measure the field E are selected so as to eliminate the constants ν, $\tilde{\nu}$, ρ, and v from the equations.

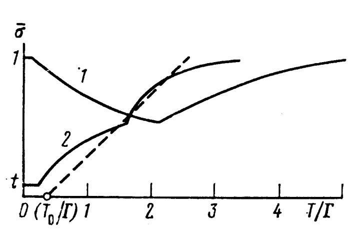

FIG. 1. Temperature dependences of $\bar{\sigma}$ for a constant carrier density ($\mu = \text{const}$): 1) $|\mu - \varepsilon_0| > \Gamma$; 2) $|\mu - \varepsilon_0| < \Gamma$. The dashed curve represents the right-hand side of the energy balance equation (8) corresponding to a particular value of F.

It is clear from the system (9) that scattering has a strong influence on the conductivity only if $|\mu - \varepsilon_0|$, $T \sim \Gamma$, when the region of thermal "smearing" of the Fermi level overlaps considerably the resonant scattering region. Therefore, the special features of the current-voltage characteristics due to the scattering by a quasilocal level can be observed only at low temperatures $T_0 \lesssim \Gamma$ and only at carrier densities such that $|\varepsilon_F - \varepsilon_0| \sim \Gamma$.

We can find the types of the current-voltage characteristic expected in different situations by approximating the functions which describe the thermal smearing and resonant scattering zones in the simplest possible way:

$$-\frac{\partial f_0}{\partial \varepsilon} = \begin{cases} 1/2T, & |\varepsilon-\mu|<T \\ 0, & |\varepsilon-\mu|>T \end{cases},$$

$$\bar{\tau}(\varepsilon) = \begin{cases} t \equiv \nu/(\nu_{p0}+\nu), & |\varepsilon-\varepsilon_0|<\Gamma \\ 1, & |\varepsilon-\varepsilon_0|>\Gamma \end{cases}. \qquad (10)$$

The forms of $\bar{\sigma}(T)$ obtained then for the case $\mu = \varepsilon_F = \text{const}$ are plotted in Fig. 1: they consist of sections of straight lines and hyperbolas (since we are interested in the range $T \sim \Gamma \ll \mu - \varepsilon_0$, we shall ignore the temperature dependence of μ under conditions of constant carrier density).

The most important feature of the current-voltage characteristic which appears because of resonant scattering is the presence of an S-type region of negative differential conductance (NDC) in the case when the Fermi energy lies in the region of a resonance: $|\varepsilon_F - \varepsilon_0| < \Gamma$. The rapid rise of $\bar{\sigma}(T)$ due to the escape of electrons from this zone as a result of heating is responsible for a thermal instability. [It is clear from Fig. 1 that a line representing the right-hand side of Eq. (8) can intersect the dependence $\bar{\sigma}(T)$ represented by curve 2 not only at three points, as shown here, but also at five points in the limit $T_0 \to 0$. This is a consequence of the use of the step function model (10), when the emergence of each edge of the region where $f_0'(\varepsilon) \neq 0$ from the resonant scattering zone is accompanied by an instability. In a real situation, the two dependences merge into one.] As the level ε_F moves away from ε_0 by an amount greater than Γ, the NDC region disappears because of a reduction in the influence of resonant scattering on the electron motion.

The pattern of instabilities is "richer" when μ rises with T sufficiently rapidly while remaining below the resonance level at $T = T_0$. Then, the region where we have $f_0'(\varepsilon) \neq 0$ shifts with increasing temperature across the resonant scattering zone and this happens practically without broadening. If $T_0 \ll T$ then $\bar{\sigma}(T)$ effectively repeats the dependence $\bar{\tau}(\varepsilon)$. The presence of regions of steep fall and rise of $\bar{\sigma}$, when

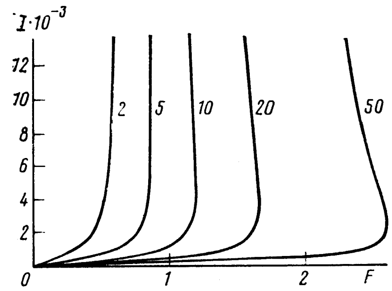

FIG. 2. Family of the current-voltage characteristics calculated for a constant electron density. The dimensionless field F and the current density I are described by Eqs. (4) and (5). The numbers alongside the curves represent the value of the ratio ν_{p0}/ν_0. The other parameters were as follows: $\omega_F = 50$; $\omega_0 = 50$; $\bar{\gamma} = 0.5$; $q = -3/2$; $r = 3/2$.

the Fermi level enters and leaves the resonant scattering zone, is responsible for the simultaneous occurrence of N- and S-type NDC regions in the current-voltage characteristic. It should be pointed out that although for $\mu = \varepsilon_F = \text{const}$ and $|\varepsilon_F - \varepsilon_0| > \Gamma$ the dependence $\bar{\sigma}(T)$ is also nonmonotonic (curve 1 in Fig. 1), this does not give rise to an NDC region, because resonant scattering affects only some of the electrons since the resonant scattering zone now includes the whole of the temperature interval in the vicinity of the Fermi level.

5. RESULTS OF NUMERICAL CALCULATIONS

Calculations were carried out for several cases differing in the nonresonant scattering mechanisms and the values of the parameters of the problem. The calculations confirmed the validity of the qualitative description given in the preceding section. The most typical current-voltage characteristics are shown in Figs. 2 and 3. Figure 2 gives a family of the current-voltage characteristics corresponding to different rates of resonant scattering in the case when the carrier density remains constant, and the nonresonant dissipation of the electron momentum and energy occurs because of collisions with charged impurities and acoustic phonons, respectively. Similar families of curves are obtained also for other combinations of nonresonant scattering mechanisms.

The results of the calculations for the case when the electron density rises as T increases are presented in Fig. 3. A comparison with Fig. 2 shows that because of the stronger dependence of $\bar{\sigma}(T)$ an S-shaped region now appears in the current-voltage characteristic at a much lower relative in-

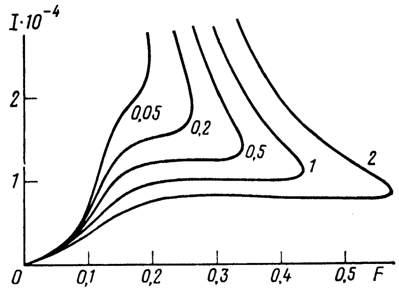

FIG. 3. Family of the current-voltage characteristics calculated for the case when the density of electrons rises as a result of their heating in accordance with Eq. (7). The dimensionless field F and the current density I are described by Eqs. (4) and (5). The numbers alongside the curves represent the ratio ν_{p0}/ν_0. The value of the other parameters were as follows: $\omega_F = 10$; $C = 20$; $\omega_0 = 50$; $\bar{\gamma} = 0.5$; $q = -3/2$; $r = 3/2$.

tensity of resonant scattering than in the variant with a constant carrier density. An increase in the influence of resonant scattering in the initial part of the current-voltage characteristic gives rise to an N-type NDC region.

In the case of the current-voltage characteristics in Figs. 2 and 3 we do not show the upper stable branches of the S-shaped region. These branches represent the mechanisms of electron scattering at higher energies, which may differ from the processes occurring in the vicinity of a resonance level. Determination of the nature of the current-voltage characteristic at high energies is a topic in itself, which is not related to the problem of resonant scattering.

We are grateful to M. I. Kaganov and B. L. Gel'mont for discussing the results.

[1]I. M. Tsidilkovskii (Tsidilkovski), G. I. Kharus (Harus), and N. G. Shelushinia, Adv. Phys. **34**, 43 (1985).

[2]V. I. Kaĭdanov and Yu. I. Ravich, Usp. Fiz. Nauk **145**, 51 (1985) [Sov. Phys. Usp. **28**, 31 (1985)].

[3]B. L. Gel'mont and M. I. D'yakonov, Zh. Eksp. Teor. Fiz. **62**, 713 (1972) [Sov. Phys. JETP **35**, 377 (1972)].

[4]B. L. Gel'mont and A. L. Éfros, Zh. Eksp. Teor. Fiz. **87**, 1423 (1984) [Sov. Phys. JETP **60**, 818 (1984)].

[5]A. Mauger and J. Friedel, Phys. Rev. B **12**, 2412 (1975).

[6]J. Stankiewicz and W. Giriat, Phys. Rev. B **13**, 665 (1976).

[7]V. I. Ivanov-Omskiĭ, B. T. Kolomiets, and V. A. Smirnov, Fiz. Tekh. Poluprovodn. **8**, 620 (1974) [Sov. Phys. Semicond. **8**, 400 (1974)].

[8]C. Verie, F. Raymond, F. Bailly, I. Vacquie, G. Weill, A. Kozacki, and J. Rioux, Proc. Fourteenth Intern. Conf. on Physics of Semiconductors, Edinburgh, 1978, publ. by Institute of Physics, London (1979), p. 241.

[9]I. I. Tal'yanskiĭ, A. V. Matveenko, M. V. Pashkovskiĭ, and E. P. Filimonenko, Ukr. Fiz. Zh. **30**, 782 (1985).

[10]G. Bastard, Phys. Status Solidi B **80**, 641 (1977).

[11]B. L. Gel'mont and A. L. Éfros, Zh. Eksp. Teor. Fiz. **89**, 286 (1985) [Sov. Phys. JETP **62** 161 (1985)].

[12]B. A. Akimov, N. B. Brandt, and V. N. Nikiforov, Fiz. Tverd. Tela (Leningrad) **26**, 1602 (1984) [Sov. Phys. Solid State **26**, 973 (1984)].

[13]S. D. Beneslavskiĭ, V. I. Ivanov-Omskiĭ, B. T. Kolomiets, and V. A. Smirnov, Fiz. Tverd, Tela (Leningrad) **16**, 1620, (1974) [Sov. Phys. Solid State **16**, 1058 (1974)].

[14]B. L. Gel'mont, Fiz. Tekh. Poluprovodn. **6**, 2263 (1972) [Sov. Phys. Semicond. **6**, 1908 (1973)].

[15]V. M. Mikheev and R. V. Pomortsev, Fiz. Tekh. Poluprovodn. **11**, 908 (1977) [Sov. Phys. Semicond. **11** 535 (1977)].

[16]F. G. Bass and Yu. G. Gurevich, Hot Electrons and Strong Electromagnetic Waves in Semiconductor and Gas-Discharge Plasmas [in Russian], Nauka, Moscow (1975), Chap. 1.

[17]B. Ricco and M. Ya. Azbel, Phys. Rev. B **29**, 1970 (1984).

[18]E. M. Lifshitz and L. P. Pitaevskii, *Physical Kinetics*, Pergamon Press, Oxford (1981), §§3, 16.

[19]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory,* 3rd ed., Pergamon Press, Oxford (1977), §145.

Translated by A. Tybulewicz