Forgotten mechanism of nonlinearity in the theory of hot electrons

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It is shown that in general electron-gas heating inevitably results in the change of the carrier concentration in the conduction band. It is proved that this change, as a rule, leads to the kinetic coefficient nonlinearity of the same order as the change of mobility does. The conditions are determined when this change can be neglected. [S0163-1829(99)06235-9]

It is well known that the fundamental reason for nonlinearity of a current-voltage characteristic (CVC) of a homogeneous semiconductor in strong electrical fields is the change of the mean carrier energy (carrier heating). The classical theory of the hot-carrier transport was developed a long time ago and rather explicitly.[1–5] Thus, as a rule, it was considered that the nonlinearity of the CVC is related to the carrier mobility alteration because of the change of carrier mean energy. Some number of works were devoted to nonlinearity caused by impact ionization,[6,7] carrier lifetime change,[8] intervalley redistribution of carriers,[9] or by a nonparabolic form of the carrier dispersion law[10,11] in strong fields. In single-valley semiconductors, by neglecting such processes as an impact ionization and carrier lifetime change in strong fields, it is usually considered[1–5] that only the carriers which already exist are subjected to heating, i.e., during heating the concentration of carriers remains equal to its value at the state of thermodynamic equilibrium. However, as it was shown in Ref. 12, there exists one more mechanism of nonlinearity, connected with the fact that the violation of the energy equilibrium between electrons and holes (the difference between electron and hole temperatures) inevitably results in the violation of the concentration equilibrium between electrons of the conduction band and the valence band. This idea was developed in Ref. 13. However, due to the assumption made that the population of the impurity level does not depend on heating, the results turn out to be incorrect if the heating of electrons and holes is different (electron and holes temperatures are unequal). Besides, the question when this effect takes place was left open.

In general, the discrepancy between electron and hole temperatures should cause the change of the carrier concentrations in both bands and the impurity level population. Hence, the problem is reduced only to what is the magnitude of the contribution of the latter effect to kinetic coefficients in comparison with the change of mobility (relaxation time) at the same temperature discrepancy. Thus, a new origin of strong field nonlinear effects, related to the alteration of the energy-level population in conduction and valence bands due to the difference between electron and hole temperatures in strong electrical fields, is discussed below. It is possible to neglect this phenomenon in the theory of hot electrons only under special conditions indicated below.

Experimental verification of the magnitude of the considered effect is shown in Refs. 14 and 15. Unfortunately, in spite of all these facts, the considered mechanism of nonlinearity in the theory of hot electrons had been actually forgotten and did not obtain further development.

Virtually, the carrier concentration change because of this mechanism is reduced to the carrier recombination rate change, which is owing to the alteration of carrier distribution functions.

Let us consider the elementary model—a homogeneous single-valley semiconductor with one nondegenerate impurity level at an energy ε_t and concentration of impurity N_t. In the given model the kinetics of the carrier concentration change within bands due to heating is determined by the following processes: (1) the capture of electrons from conduction band to the impurity level, (2) the thermal emission of electrons from the impurity level into the conduction band, (3) the capture of holes to the impurity level, and (4) the thermal emission of holes from the impurity level into the valence band. To simplify the calculations we neglect the influence of interband transitions on carrier concentration change at heating.

Let us note that the concentration change is caused by the alteration of the rate of recombination rather than thermal generation. Suppose that only the electron subsystem is subjected to heating. Then, if conditions for carrier concentrations indicated in Ref. 16 are fulfilled, the electron gas can be described by the Fermi distribution function with electron temperature T_e. Subsystems of holes and captured carriers have the lattice temperature T_0.

The capture rate of electrons onto the impurity level can be represented by the following expression:[17]

$$r_n = \alpha_n(T_e) N_t [1 - f_t(T_0)] n(T_e), \tag{1}$$

where f_t is the distribution function of electrons on the impurity level, $N_t[1-f_t(T_0)]$ represents the concentration of free impurity states, $n(T_e)$ is the concentration of electrons, $\alpha_n(T_e)$ is the capture factor of electrons by the trap. Let us emphasize once again that here we do not consider the explicit dependence of the capture factor on the magnitude of the electrical field applied, i.e., we do not take into account such processes as the change of the carrier lifetime in strong fields (see Ref. 8). By definition,

$$\alpha_n(T_e) = \frac{\int_{\varepsilon_c}^{\infty} c_n(\varepsilon)\nu_n(\varepsilon) f_n(\varepsilon, T_e) d\varepsilon}{\int_{\varepsilon_c}^{\infty} \nu_n(\varepsilon) f_n(\varepsilon, T_e) d\varepsilon}. \tag{2}$$

Here $c_n(\varepsilon)$ is a probability of the electron transition from the impurity level into the state with an energy ε, $\nu_n(\varepsilon)$ is a density of states, $f_n(\varepsilon,T_e)$ is the Fermi distribution function with temperature T_e for conduction electrons, ε_c is the energy of an electron at the bottom of the conduction band.

The rate of thermal emission into the conduction band is assumed to be independent of the temperature of electrons in the conduction band (that is correct, at least, for wide-band semiconductors):

$$g_{nT}=\alpha_n(T_0)N_t f_t(T_0)n_1, \tag{3}$$

where $n_1\equiv\nu_{n0}\exp(-\mathcal{I}/T_0)$ is a parameter describing the impurity level, ν_{n0} is the effective density of states in the conduction band, $\mathcal{I}\equiv\varepsilon_c-\varepsilon_t$ is the ionization energy of the impurity level. The parameter n_1 represents concentration of electrons in the conduction band which would take place if the Fermi level would coincide with the impurity level. Obviously, the recombination rate of electrons is equal to $R_n=r_n-g_{nT}$.

Similar equations can be written for the hole subsystem as well,

$$r_p=\alpha_p(T_0)N_t f_t(T_0)p, \tag{4}$$

$$g_{pT}=\alpha_p(T_0)N_t[1-f_t(T_0)]p_1, \quad R_p=r_p-g_{pT}. \tag{5}$$

Here p is a hole concentration and the definition of quantities $\alpha_p(T_0)$ and p_1 is similar to the above-mentioned one for electrons.

In a homogeneous semiconductor in steady state $R_n=R_p=0$, and the condition of the electroneutrality is fulfilled. It is convenient to express such a condition as

$$\delta n+N_t\delta f_t=\delta p, \tag{6}$$

where $\delta n\equiv n-n_0$, $\delta p\equiv p-p_0$, $\delta f_t\equiv f_t-f_t^0$, and n_0, p_0 and f_t^0 are, respectively, electron and hole concentrations and the impurity level population in the absence of heating ($T_e=T_0$).

After solving the set of equations $R_n=R_p=0$ together with the Eq. (6), one obtains the following expressions for the carrier concentration change caused by heating:

$$\delta n=-\left[1+\frac{p_1(n_0+n_1)^2}{n_1(p_0+p_1)^2+N_t n_1 p_1}\right]^{-1}\frac{n_0}{\alpha_n(T_0)}\frac{\partial\alpha_n(T_0)}{\partial T}\delta T, \tag{7}$$

$$\delta p=\delta n\left[1+\frac{N_t p_1}{(p_0+p_1)^2}\right]^{-1}, \quad \delta T\equiv T_e-T_0\ll T_0. \tag{8}$$

Assuming additionally that the gas of carriers is nondegenerate, i.e., the relation $n_0p_0=n_1p_1=n_i^2$ holds, where n_i is the intrinsic carrier concentration (i.e., at $N_t=0$) in the absence of heating, and, besides, bands are parabolic, we will analyze Eqs. (7) and (8) in two limiting cases.

(1) An intrinsic semiconductor with low concentration of shallow traps for electrons. In this case $n_1\gg n_0=p_0=n_i\gg p_1$ and Eqs. (7) and (8) acquire the form,

$$\frac{\delta n}{n_i}=-\frac{\partial\alpha_n(T_0)}{\partial T}\frac{\delta T}{2\alpha_n(T_0)}, \tag{9}$$

$$\delta p\approx\delta n. \tag{10}$$

Thus the magnitude of the carrier concentration change at heating in this case is determined only by the temperature dependence of the electron capture factor α_n. Let us note also that expressions (9) and (10) have the same form as in the case of only interband transition in an intrinsic semiconductor.

(2) An n-type monopolar semiconductor with donor impurity ($n_0\gg n_i\gg p_0$). The relative carrier concentration change in this case is described by the following expressions:

$$\frac{\delta n}{n_0}=-\left[1+1/\left(\frac{n_i^2}{n_0^2}+\frac{N_t}{n_1}\right)\right]^{-1}\frac{\partial\alpha_n(T_0)}{\partial T}\frac{\delta T}{\alpha_n(T_0)}, \tag{11}$$

$$\delta p=\delta n\left[1+\frac{n_0^2}{n_i^2}\frac{N_t}{n_1}\right]^{-1}. \tag{12}$$

It is easy to verify that in this case the carrier concentration change at heating is determined not only by the temperature dependence of the electron capture factor α_n, but also depends on concentration of impurity and on the temperature T_0. In the range of high temperatures [$T_0\gg\mathcal{I}/\ln(\nu_{n0}/N_t)$, i.e., $N_t\ll n_1$] the functional dependence of $|\delta n/n_0|$ on N_t has a deep minimum at $N_t\approx\sqrt[3]{n_i^2n_1}$, being equal to

$$\left|\frac{\delta n}{n_0}\right|_{\min}=\left(\frac{2n_i}{n_1}\right)^{2/3}\frac{\partial\alpha_n(T_0)}{\partial T}\frac{\delta T}{\alpha_n(T_0)}\sim\exp\left(-\frac{\varepsilon_g-2\mathcal{I}}{3T}\right)\ll 1, \tag{13}$$

where ε_g is the band-gap width. Thus, near the indicated concentration the additional contribution to the conductivity change is negligibly small and heating effects are described by existing theories.[1–5]

At low temperatures or, what is equivalent, heavy doping ($N_t\gg n_1$), we come back to expression (9). Let's note, that in this case [in contrast to Eq. (10)] $\delta p\ll\delta n$.

In the monopolar case, as well as for an intrinsic semiconductor, the deviation from the conventional theories is determined by the temperature dependence of the electron capture factor α_n. For simplicity we will analyze model dependence for two cases: attracting and repulsive potentials of impurity centers.

In the case of the electron capture by an attracting potential $\alpha_n(T)\sim T^{-m}$, and m varies within the limits from $m\simeq 1$ up to $m\simeq 5$ depending on the nature of the semiconductors and impurities.[18,19] Then

$$\frac{\delta T}{\alpha_n(T_0)}\frac{\partial\alpha_n(T_0)}{\partial T}=-m\frac{\delta T}{T_0}. \tag{14}$$

In the case of electron capture by a repulsive potential of impurity (for example, ions of gold or copper in germanium) the temperature dependence of the capture factor is satisfactorily described by the expression[20]

$$\alpha_n(T)\sim\exp\left[-\left(\frac{T^*}{T}\right)^{1/3}\right], \tag{15}$$

where T^* is a parameter depending on the specific kind of the semiconductor and the impurity in it.

Hence,

$$\frac{\delta T}{\alpha_n(T_0)}\frac{\partial \alpha_n(T_0)}{\partial T}=\frac{1}{3}\left(\frac{T^*}{T_0}\right)^{1/3}\frac{\delta T}{T_0}. \tag{16}$$

As long as T^* usually lies in the range from 10^4 to 10^9 K,[20,21] in the case of a repulsive potential the contribution to the conductivity change in the heating field can be even more pronounced.

Thus, the electron concentration change caused by carrier heating alters kinetic coefficients as much as the mobility (relaxation time) change does. It should be mentioned that there exist only two specific, not very interesting, situations, namely (1) the electron Fermi level lies far enough both from the middle of the gap and from the impurity level, and (2) the electron capture factor weakly depends on the temperature, when the traditional theory of hot electrons is correct.

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