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Kinetic approach to field emission from semiconductors by computer simulation using particles

V E Gherm, N V Mileshkina and E A Semykina
Institute of Physics, Leningrad State University, 198904 Uljanovskaya 1, Leningrad, Petrodvorets, USSR

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Abstract. Direct statistical simulation of non-stationary non-equilibrium electronic phenomena in one-dimensional semiconductor structures is carried out to estimate their influence on the field emission from semiconductors in different working modes of needle cathodes. A macroparticles method is used with self-consistent electric field conditions, taking into account the three-dimensional character of the electron scattering. Computation results are given for n-type $A_{III}B_{V}$ semiconductors.

1. Introduction

The analytical theory of field emission of electrons from semiconductors derived by Stratton [1, 2] is based on the 'zero current' approximation which suggests that electron escape through the crystal surface is compensated by the transport of electrons from the bulk to the near-surface region of a semiconductor. Penetration of the external field into the semiconductor results in band bending with respect to the Fermi-level at the surface, whereas the Fermi-level itself remains constant up to the surface. In n-type semiconductors emission occurs from the degenerate conduction band and the near-surface distribution of electrons is defined by the Fermi–Dirac function.

The penetration of the external electric field into the crystal, resulting in deviation from thermodynamic equilibrium of electron energy distribution in the conduction band, was treated by Elinson [3]. A set of differential equations for the current, energy flow densities, electron temperature and concentration was solved numerically for the case of a steady-state field emission from a wide band-gap n-type semiconductor with a low electron affinity.

Electron field emission from semiconductors is governed by the external electric field $\boldsymbol{E}$, crystal volume parameters and, in particular, by space-charge region (SCR). The SCR thickness is comparable to the electron momentum and energy relaxation lengths, therefore the present paper makes use of the kinetic approach employed in [4] with application to the submicron semiconductor structures, for treatment of the non-equilibrium processes involved in the field emission. We treat evolution of the electron processes in a self-consistent electric field with allowance for the three-dimensional character of the electron scattering by phonons and impurity atoms in the momentum space. Transition processes and attainment of a steady-state field emission current are analysed.

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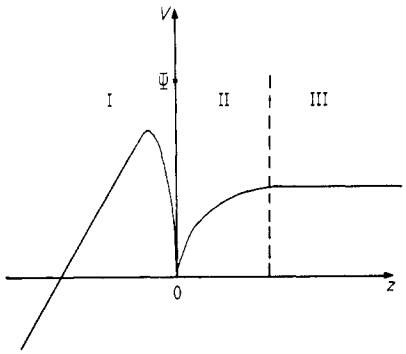

Figure 1. Energy diagram of semiconductor field emitter: I, vacuum; II, the near-surface region of a semiconductor, the computation region; III, the bulk of a semiconductor.

A particle method, developed in [5] for the simulation of the kinetic electron processes in the submicron Schottky gate field transistors is exploited for the numerical solution of the set of kinetic Boltzmann equations. A real electron gas is substituted in this method by a model particle gas, characterised by the same $\tilde{e}/\tilde{m}$ ratio as in a real electron gas e/m (e: electron charge; $\tilde{e}$: particle charge; m: electron mass; $\tilde{m}$: particle mass); in the case of a non-parabolic dispersion law for electrons $\varepsilon(\boldsymbol{p})$ we have

$$e\partial^2\varepsilon/\partial\boldsymbol{p}^2 = \tilde{e}\partial^2\tilde{\varepsilon}/\partial\tilde{\boldsymbol{p}}^2$$

($\tilde{\varepsilon}$: energy of the particle with the momentum $\tilde{\boldsymbol{p}}$), which provides identity of both real and model gases.

One might hope to trace the evolution of the distribution function by calculating the particle trajectories, recalculating the self-consistent electric field for every time interval and performing the particle-scattering procedure (transitions in the momentum space) in conformity with the known probabilities.

The processes of electron scattering by lattice vibrations and impurity atoms are simulated in the present paper by particle scattering using a Monte-Carlo procedure, just as in [5].

A flow of the field emission current is provided by the boundary conditions proposed by us for the case of the field emission and presented below. These conditions define the electron transport from the volume of the semiconductor to the SCR and electron escape from the surface to vacuum.

Initial conditions (electron distribution function $f(t, p, z)$ and potential energy profile $\theta(z)$) are chosen in a form allowing treatment of transition processes involved in field emission.

2. Formulation of a problem

Electron field emission is a result of the electron tunnelling through the potential barrier at the semiconductor–vacuum interface under the application of a strong electric field, E_s, to the semiconductor crystal. With allowance for the image-charge forces, the barrier shape is approximated by:

$$\Phi(z) = \Psi - eE_s z + (\kappa + 1)/(\kappa - 1)(e^2/4z) \qquad z < 0$$

(region I in figure 1) (Ψ: electron affinity; κ: dielectric constant). The tunnelling probability is determined by the transparency coefficient $D(p_z)$, where p_z is the electron momentum component, perpendicular to the surface.

The distribution function of electrons in the conduction band for the case of the non-equilibrium field emission in the SCR (region II in figure 1) is obtained from a solution of a set of Boltzmann kinetic equations in a self-consistent electric field:

$$\partial f_i(t, \boldsymbol{p}, z)/\partial t + (\partial \varepsilon_i/\partial p_z)(\partial f_i(t, \boldsymbol{p}, z)/\partial z) - e\boldsymbol{E}(\partial f_i(t, \boldsymbol{p}, z)/\partial \boldsymbol{p}) = S_i \tag{1}$$

$$\operatorname{div} \boldsymbol{E} = -\frac{4\pi e}{\kappa}\left(\sum_i \int f_i \, \mathrm{d}\boldsymbol{p} - \mathcal{N}_\mathrm{D}\right) \tag{2}$$

where $\boldsymbol{E}$ is the self-consistent electric field strength, $f_i(t, \boldsymbol{p}, z)$ is the electron distribution function for the valley i, $i = (\Gamma, \mathrm{L}, \mathrm{X})$. Here '$i$' denotes electron energy minima which correspond to the Γ, L, X points. $\mathcal{N}_\mathrm{D}$ is the ionised donor concentration. A model developed by Kein [6] is used as a dispersion law:

$$\varepsilon_i(1 + \alpha_i \varepsilon_i) = \boldsymbol{p}^2/2m_i$$

where m_i is the electron effective mass at the bottom of the i-valley; α_i is the non-parabolicity parameter.

An explicit form of the collision integrals, S, is determined by the probabilities of electron transitions between different electron states. The electron–electron interaction is considered to be negligibly small; the effects due to possible electron gas degeneration at the surface (i.e. SCR) are also neglected. In the collision integrals the following processes are taken into account: (1) intra-valley scattering by the ionised impurities, acoustical phonons and optical phonons; (2) inter-valley transitions with absorption and emission of an inter-valley phonon (transitions with absorption and emission of a phonon are assumed to be different).

Boundary conditions for the set of the differential equations (1)–(2) (the left- and right-hand boundaries of region II in figure 1) are defined taking into account the following considerations.

(i) The right-hand boundary of region II is chosen so far from the surface that the electron concentration is equal to the concentration in the bulk of the sample. Therefore the electron distribution function on the right-hand boundary of the region under investigation is equal to the function in the bulk and its spatial gradient is equal to zero. So the distribution function on the boundary is defined from the solution of a set of Boltzmann kinetic equations (1) in which the second term must be put equal to zero.

(ii) For the left-hand boundary of region II, at $z = 0$, $\boldsymbol{E} = \boldsymbol{E}_\mathrm{s}/\kappa$. The electron escape into the vacuum is defined by the transparency coefficient $D(p_z)$, which is calculated from the Schrödinger equation. For the electron distribution function at $z = 0$ we have:

$$f_i(p_z) = (1 - D(p_z))f_i(-p_z).$$

Initial conditions for the solution of the set of equations (1)–(2) are specified from the spatial distribution of the electric field potential, which is obtained from solution of a self-consistent problem assuming thermodynamic equilibrium between the electron gas and the lattice

$$\mathrm{d}^2\Phi(z)/\mathrm{d}z^2 = -(4\pi e^2 \mathcal{N}_\mathrm{D}/\kappa)(\mathrm{e}^{-\Phi(z)/kT} - 1)$$

$$\mathrm{d}\Phi(z)/\mathrm{d}z|_{z=0} = eE_s/\kappa \qquad \Phi(z) \to 0 \qquad \text{under} \qquad z \to \infty$$

and the local Maxwell distribution function

$$f(\boldsymbol{p}, z) = \mathcal{N}_\mathrm{D} \exp(-\Phi(z)/kT) f_0(\boldsymbol{p})$$

where $f_0(\boldsymbol{p})$ is the Maxwell distribution function, k is the Boltzmann constant and T is temperature.

3. Numerical simulation of a problem

According to the particle method, the electron gas is represented in a one-dimensional coordinate space as an ensemble of flat sheets, infinite in two dimensions, with the homogeneously distributed charge and mass, their dynamics being identical to that of real electrons [7].

On passing from the real electron gas to the model one, we have

$$e\int f_i \,\mathrm{d}\boldsymbol{p} = \tilde{e}\int \tilde{f}_i \,\mathrm{d}\tilde{\boldsymbol{p}}$$

where

$$\tilde{f}_i(t,\tilde{\boldsymbol{p}},z) = \sum_{j=1}^{\mathcal{N}_i} \delta(z - z_j(t))\delta(\tilde{\boldsymbol{p}} - \tilde{\boldsymbol{p}}_j(t))$$

is a discrete distribution function for the i-type macroparticles, $\mathcal{N}_i$ is a number of particles of the i-type, $z(t)$ and $\tilde{\boldsymbol{p}}(t)$ and coordinate and momentum of the j-particle of the i-type at a moment of time t. Under this condition the electric field potential is invariant with respect to such a transition. To ensure invariance of the Debye screening length, r_D, and the plasma frequency as one passes to the model gas, the following relations should be fulfilled:

$$\partial\varepsilon_i/\partial\boldsymbol{p} = \partial\tilde{\varepsilon}_i/\partial\tilde{\boldsymbol{p}} \qquad \tilde{e}\boldsymbol{p} = e\tilde{\boldsymbol{p}}.$$

We seek a solution for the set of the microscopic kinetic equations for the discrete distribution functions

$$\partial\tilde{f}_i(t,\tilde{\boldsymbol{p}},z)/\partial t + (\partial\tilde{\varepsilon}_i/\partial\tilde{p}z)(\partial\tilde{f}_i(t,\tilde{\boldsymbol{p}},z))/\partial z - \tilde{e}\boldsymbol{E}(\partial\tilde{f}_i(t,\tilde{\boldsymbol{p}},z))/\partial\tilde{\boldsymbol{p}} = \tilde{S}_i \tag{3}$$

$$\operatorname{div}\boldsymbol{E} = -\frac{4\pi\tilde{e}}{K}\sum_i \int \tilde{f}_i \,\mathrm{d}\tilde{\boldsymbol{p}} + \frac{4\pi e}{K}\mathcal{N}_D \tag{4}$$

where $\tilde{S}_i$ is the collision integral for the i-type macroparticle.

The collison integrals in the kinetic equation (3) provide 'mixing' of the particle distribution in the momentum space, which is described by the relations

$$\tilde{S}_i = \sum_{i',l}(-\tilde{S}^{(1),l}_{i,i'}[\tilde{f}_i] + \tilde{S}^{(2),l}_{i,i'}[\tilde{f}_{i'}]) \tag{5}$$

where $\tilde{S}^{(1),l}_{i,i'}[\tilde{f}_i]$ and $\tilde{S}^{(2),l}_{i,i'}[\tilde{f}_{i'}]$ describe, respectively, the depopulation and population of the state with momentum $\tilde{\boldsymbol{p}}$ as a result of scattering of the macroparticles of the $i(i')$-type by means of an l-mechanism with transformation into the $i'(i)$-type. Then

$$\tilde{S}^{(1),l}_{i,i'}[\tilde{f}_i] = \tilde{\lambda}^l_{i,i'}(\tilde{\boldsymbol{p}})\tilde{f}_i(\tilde{\boldsymbol{p}})$$

$$\tilde{S}^{(2),l}_{i,i'}[\tilde{f}_{i'}] = \int \tilde{f}_{i'}(\tilde{\boldsymbol{p}}')\tilde{W}^l_{i',i}(\tilde{p}',\tilde{p},\cos\theta)\delta(\tilde{\varepsilon}_{i'}(\tilde{\boldsymbol{p}}') - \tilde{\varepsilon}_i(\tilde{\boldsymbol{p}}) + \tilde{\Delta}^l_{i,i'})\,\mathrm{d}\tilde{\boldsymbol{p}}'$$

$$\tilde{\lambda}^l_{i,i'}(\tilde{\boldsymbol{p}}) = \int \tilde{\omega}^l_{i,i'}(\tilde{p},\cos\theta)\,\mathrm{d}\cos\theta\,\mathrm{d}\varphi$$

where φ is the azimuth, $\tilde{\omega}^l_{i,i'}(\tilde{p},\cos\theta)$ is the angular dependence of the macroparticle scattering probability, $\tilde{W}^l_{i',i}(\tilde{p}',\tilde{p},\cos\theta)$ is the probability of macroparticle transition from the i'-type valley to the i-type valley as a result of the scattering by means of the l-mechanism and $\tilde{\Delta}^l_{i,i'}$ is the energy difference between the final and the initial states of

the scattered particle, which is equal to the corresponding phonon energy. It should be noted that integrals in (5) are not evaluated, but the matrix elements $\tilde{\omega}^l_{i,i'}$ and $\tilde{W}^l_{i,i'}$ in the form presented in [5] are used for the calculation of transition probabilities.

The Monte-Carlo procedure is performed as follows: macroparticles of the i-type ($i = \Gamma, L, X$) change their momenta $\tilde{\boldsymbol{p}}$ as a result of scattering throughout by one of the ten possible mechanisms, characterised by the probability $\tilde{\lambda}^l_{i,i'}(\tilde{p})$. This process is described by $\tilde{S}^{(1),l}_{i,i'}[\tilde{f}_i]$ in (5). In the spherical coordinate system with the polar axis along $\tilde{\boldsymbol{p}}$, the angles of the macroparticle scattering θ and φ are incidentally obtained in conformity with the probability $\tilde{\omega}^l_{i,i'}(\tilde{p}, \cos\theta)$. A new particle is added to the particle ensemble instead, with the momentum that is found by the described procedure above. This process corresponds to $\tilde{S}^{(2),l}_{i,i'}[\tilde{f}_{i'}]$ in (5).

In intervals between scattering, the particles obey classical mechanics laws for a self-consistent electric field, defined from the equation (4). With allowance for a dispersion law, the equations of motion are of the form:

$$\mathrm{d}z_j(t)/\mathrm{d}t = \tilde{p}_{zj}(t)/\tilde{m}_i(1 + 2\tilde{\alpha}_i\tilde{\varepsilon}_j(t)) \qquad \mathrm{d}\tilde{p}_{zj}/\mathrm{d}t = F_z(z_j(t))$$

$$\tilde{\varepsilon}_j(t)(1 + \tilde{\alpha}_i\tilde{\varepsilon}_j(t)) = (\tilde{\boldsymbol{p}}_j(t))^2/2\tilde{m}_i$$

where $\boldsymbol{F}(z_j(t)) = -e\boldsymbol{E}(z_j(t))$ is the field strength, and $\tilde{m}_i = m_i\tilde{e}/e$ and $\tilde{\alpha}_i = \alpha_i e/\tilde{e}$ are the mass and non-parabolicity parameters of the i-type macroparticle.

For a numerical solution of these equations, a second-order of accuracy in a time finite-difference scheme is used:

$$z_j(t + \tau/2) = z_j(t) + \tau\tilde{p}_{zj}(t)/2\tilde{m}_i(1 + 2\tilde{\alpha}_i\tilde{\varepsilon}_j(t))$$

$$\tilde{p}_{zj}(t + \tau) = \tilde{p}_{zj}(t) + \tau F_z(z_j(t + \tau/2)) \tag{6}$$

$$z_j(t + \tau) = z_j(t + \tau/2) + \tau\tilde{p}_{zj}(t + \tau)/2\tilde{m}_i(1 + 2\tilde{\alpha}_i\tilde{\varepsilon}_j(t + \tau)).$$

We note that, in view of the possibly large electric field and particle concentration gradients in the SCR for numerical solution of equation (4), an irregular net is used in the coordinate space, which is the more dense the closer it comes to the semiconductor–vacuum interface (region II, figure 1). This enables an increase in computation accuracy without a concomitant increase in the number of gridpoints.

The penetration of the electron through the potential barrier at the surface is simulated by means of a probability procedure as follows: a macroparticle incident on the interface ($z = 0$) with momentum $\tilde{\boldsymbol{p}}$ is backscattered with probability $(1 - D(p_z))$; and with probability $D(p_z)$ it is removed from the ensemble of the calculated macroparticles.

The electron injection to the region being calculated (II in figure 1) from the volume region (III in figure 1) is simulated by the 'periodic' boundary conditions: when a particle on its way to the surface crosses the border between the outermost and neighbouring cells of the coordinate net and leaves the outermost cell, a new particle of the same type and momentum is generated in the outermost cell. Here the particle momentum distribution function in the outermost cell corresponds to the solution of a set of Boltzmann equation (3), under the assumption that there is no distribution function gradient.

A practical realisation of the macroparticle method suggests that the convergence of the method should be proved by proceeding from the results of the numerical simulation. The solution should not change with increasing number of particles or with variation of the parameters of the model.

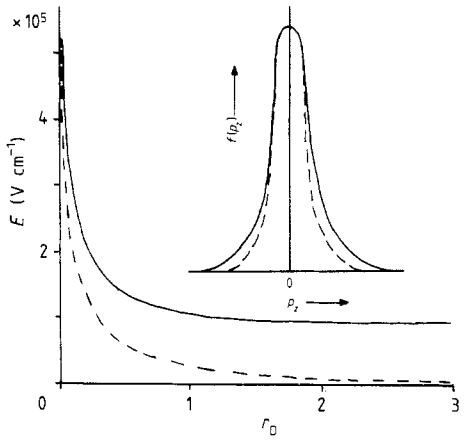

Figure 2. Electric field profile and distribution function of the electrons in the SCR: dashed curve, 'zero-current' approximation; solid curve, under current flow.

The processes involved in electron field emission from the semiconductor to the vacuum are simulated by means of evolution of the discrete distribution functions in time. Let us introduce the time net $t_n = n\Delta t$, where n is the number of steps and Δt is the time interval. The free path time τ_1 is defined for every macroparticle. When $\tau_1 \geqslant \Delta t$; the coordinates and the momentum components at the moment of time $t_{n+1} = (n+1)\Delta t$ are obtained from the equations of motion (6). When $\tau_1 < \Delta t$, the coordinates and the momentum components at the moment of time $t_n + \tau_1$ are defined from the solution of (6), then the particle is scattered by the procedure described above. For the next step the electron path time is τ_2. If $t_n + \tau_1 + \tau_2 \geqslant t_{n+1}$, a particle described by (6) is shifted on the time scale by the time interval $\Delta t - \tau_1$; otherwise it shifts by the time interval τ_2 with subsequent scattering. The procedure is repeated until the particle reaches the moment t_{n+1} on the time scale. After the time shift of all the particles by Δt up to the moment t_{n+1}, the volume charge distribution is defined by their discrete distribution functions; afterwards, equation (4) is solved and the self-consistent electric field at a moment of time t_{n+1} is found. After that the procedure is repeated.

In the present paper the calculation is performed for the n-type GaAs-emitter with the parameters taken from [8]. Typical values for the parameters used are: particle number, up to 10000; number of gridpoints in the spatial net, of the order to 100; number of steps before attainment of the stationary emission process, from 1000 to 10000 depending on concentration (10^{13}–10^{17} cm^{-3}); and applied field (10^7–5×10^7 V cm^{-1}).

4. Results and discussion

The analysis of our results shows that the 'zero current approximation' used by Stratton [1, 2], may become inappropriate for the field emission processes.

The electron distribution function close in to the surface barrier potential for the case of an absolutely impermeable barrier (a so-called 'zero current' case) is presented in figure 2, dashed curve. As may be inferred from the full curve, the electron escape into the vacuum changes the distribution function with respect to the case when the emission is absent.

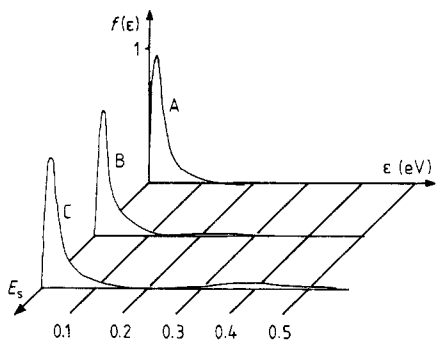

Figure 3. Electron energy distribution functions in the SCR for external field strengths, E_s: A, $E = 3 \times 10^7$ V cm^{-1}; B, $E = 3.5 \times 10^7$ V cm^{-1}; C, $E = 4 \times 10^7$ V cm^{-1}.

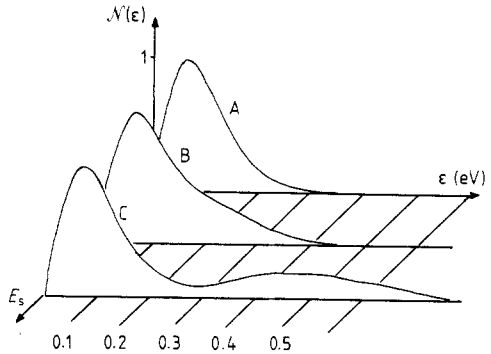

Figure 4. Energy distributions of the emitted electrons for external field strengths E_s: A, $E = 3 \times 10^7$ V cm^{-1}; B, $E = 3.5 \times 10^7$ V cm^{-1}; C, $E = 4 \times 10^7$ V cm^{-1}.

The results of our computation indicate that the electron-gas heating already occurs at low fields, sufficient for electron tunnelling through the barrier. Figure 3 shows the energy distribution of the electrons in the SCR. As follows from our numerical results, increasing the electric field strength results in a broadening of the electron distribution function. We can propose a possible mechanism leading to the broadening of the electron distribution function.

Due to the increase in the tunnelling probability with the electric field rise the electron escape from the near-surface region is not compensated by the electron transport from the semiconductor volume. The charge, accommodated in the near-surface region, decreases, and is not sufficient to screen the external field, which penetrates the bulk and brings about heating of the electron gas.

Thus, the distribution function for electrons, drawn from the bulk into the SCR, is materially non-equilibrium: the width of the energy distribution in strong fields may be as great as several tens of kT (figure 3).

If the energy relaxation length is comparable to (or exceeds) the SCR thickness, which is of the order of the Debye radius, energetic electrons, arriving from the bulk, are not completely thermalised. The electron distribution function at the barrier is a superposition of distribution function for the nearly thermalised electrons and 'quasiballistic' particles (which have as a result of scattering lost only a part of their energy, acquired in the field) penetrating the bulk. The distribution function of the near-surface electrons for different external fields is given in figure 3.

Figure 4 shows the energy distributions of the emitting electrons at the same conditions. At low values of the external electric fields, the main contribution to the emission current is due to thermalised electrons from the bottom of the conduction band. With increasing field strength, another process also contributes to the current, namely, transport of quasiballistic electrons with increased kinetic energy. The emission regime is defined by relation between the electron free path and lifetime in the near-surface potential well with respect to emission.

Thus, the kinetic approach derived for the simulation of the semiconductor emitter operation indicates strong influence of the electric field on the electron distribution function and emission regime. In the theory, given by Stratton [1, 2] the field affected

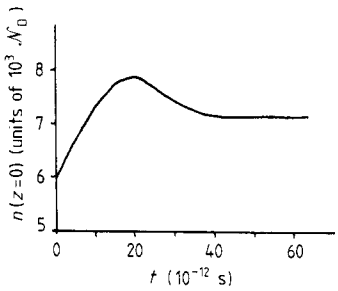

Figure 5. Time dependence of the near-surface electron concentration.

the near-surface band bending without changing the electron distribution function; whereas, according to our calculations, a field increase results in emission regime and energy spectrum changes.

Time evolution of the near-surface electron concentration in the transient process of attainment of a new stationary state under abrupt increase of the external field from 3×10^7 V cm^{-1} to 3.5×10^7 V cm^{-1} is shown in figure 5. We note that time durations of the transient processes are of the order of several tens of picoseconds; therefore semiconductor materials can be used as high-speed emitters. We also note that the advantage of the direct particle approach used in the present paper makes possible direct observations of the transient processes of field emission current steady-state attainment.

The results of the numerical simulation presented in this paper demonstrate that the non-equilibrium electron processes must be taken into account for field emission investigations of semiconductors.

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