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Computer simulation of kinetic processes near a semiconductor surface at a high electric field using the particle method

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Abstract. The feasibility of computer simulation of electronic relaxation at a semiconductor–vacuum interface under a strong electric field is demonstrated. A kinetic description of conduction band electrons in a space-charge region layer with a self-consistent electric field under electron–impurity and electron–phonon scattering is developed by the particle method and Monte Carlo procedure. Results for the transient electronic process in a semiconductor field emitter are given.

1. Introduction

This work deals with the investigation of the electron transport through the space-charge region (SCR) of the semiconductor field emitter under conditions of field emission. Electron field emission from semiconductors arises because the electron tunnels through the potential barrier at the crystal–vacuum interface and it is governed by the electric field strength as well as by the crystal volume parameters.

Electron field emission from semiconductors has been described in [1]. Electron field emission from GaAs crytals has been observed since 1969 [2] and subsequently some experimental work has been devoted to the investigation of field emission from GaAs crystals [3–5].

The theory of field emission from semiconductors developed by Stratton [6, 7] is based on the 'zero-current' approximation which implies thermodynamic equilibrium of the electron energy distribution. This approximation is valid when the emission current is not very strong. The current–voltage characteristic of the field emitter in the logarithmic coordinates of the current against inverse voltage is a straight line. The value of the tunnelling current density depends on the type of crystal, the concentration of ionized donors (or acceptors) and the radius of the emitter tip. The maximum value of current density may be variated from 10^{-2} Å cm^{-2} up to 1 Å cm^{-2}. When the electric field rises, the current–voltage characteristic diverges from the straight line. In our opinion, a deviation from thermodynamic equilibrium arises and Stratton's theory becomes invalid. To describe the case of strong emission current it is necessary to consider the non-equilibrium electron transport through the SCR.

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The SCR thickness under the conditions of interest is comparable with the relaxation lengths of the electron momentum and energy. This provides the possibility that substantially non-equilibrium processes occur. Therefore the kinetic approach must be used for adequate description of the process under investigation.

Computer simulation of the transitional processes in semiconductors by means of the kinetic model gives correct results when the particle method is used. The main idea of the particle method is the replacement of a very large number of real electrons by a countable set of the model macroparticles. These particles move according to the laws of classical mechanics in a self-consistent electric field. The three-dimensional character of electron scattering in momentum space and the details of the energy band structure are also taken into account.

According to this method the dynamical properties of a system of model particles are similar to the properties of conduction band electrons [8]. This equivalence is provided by the identity of e/m ratio and dispersion law of both real and model particles. Therefore it is possible to investigate the real electron system by observing the behaviour of the model system of macroparticles.

The particles move in the SCR which is bounded by the crystal surface and by the volume of the crystal. The escape of particles through the potential barrier into vacuum and their injection from the volume of the crystal are described by special boundary conditions proposed by us for the case of field emission. On the basis of these boundary conditions the simulation procedure is developed, which provides the possibility of investigating the non-equilibrium phenomena taking place under the heavy current.

The kinetic approach to field emission from semiconductors was put forward in our previous paper [9], where the particle method was used for the numerical simulation of the transitional processes in the SCR of a semiconductor field emitter under various conditions. It was shown that non-equilibrium processes must be taken into account in field emission investigations.

In the present paper the main attention is paid to the details of the distribution function of electrons in the substantially non-equilibrium regime. In addition, the modification of the particle method for the case of motion in the surface potential well is described; this allows us to develop a faster algorithm than that of the ordinary method.

The choice of a GaAs field emitter as the object of the study is explained by its application in fast-response microelectronic devices.

2. Formulation of the problem

Let us consider the one-dimensional model of the near-surface region of a semiconductor under a strong electric field. The energy diagram of semiconductor field emitter is represented in figure 1, where the potential profile of the bottom of the conduction band is shown. The sample is placed at $z > 0$. To the left of the semiconductor–vacuum interface a potential barrier exists. Its shape can be approximated with allowance for the image-charge forces by the expression

$$\phi(z) = \psi - eE_s z + (\kappa + 1)/(\kappa - 1)(e^2/4z) \tag{1}$$

where ψ is the electron affinity, κ the dielectric constant, E_s the applied electric field strength and e the electron charge.

The kinetic description implies that the electron system is described by means of the distribution functions. Since the GaAs conduction band has three valleys, there are

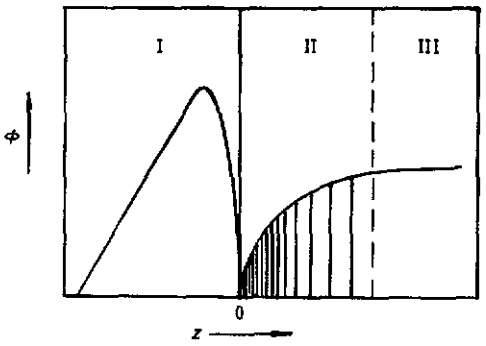

Figure 1. Energy diagram of a semiconductor field emitter: I, vacuum; II, semiconductor surface region (region of calculation); III, semiconductor bulk.

three types of electron which correspond to the Γ, L and X points of the electron energy minima. Each type of electron is described by the corresponding distribution function f_i, $i \equiv \Gamma, L, X$. The distribution functions are governed by the system of Boltzmann kinetic equations

$$\partial f_i(t,p,z)/\partial t + (\partial \varepsilon_i/\partial p_z)[\partial f_i(t,p,z)/\partial z] - eE[\partial f_i(t,p,z)/\partial p_z] = S_i \qquad i \equiv \Gamma, L, X \tag{2}$$

where E is the self-consistent electric field strength which is found from the equation

$$\frac{\partial E}{\partial z} = \frac{-4\pi e}{\chi}\left(\sum_i \int f_i(t,p,z)\,dp - N_D\right) \tag{3}$$

where S_i are the collision integrals and N_D is the ionized donor concentration. A model developed by Kein [10] is used as a dispersion law:

$$\varepsilon_i(1 + \alpha_i \varepsilon_i) = p^2/2m_i \tag{4}$$

where m_i is the electron effective mass at the bottom of the i valley, α_i is the non-parabolic parameter, and ε_i and p are the electron energy and momentum, respectively. The collision integrals S_i are the linear functional of the distribution functions. They can be written in the form

$$S_i = \sum_{i',l} (-S^{(1),l}[f_i] + S^{(2),l}[f_{i'}]) \tag{5}$$

where $S^{(1),l}[f_i]$ and $S^{(2),l}[f_{i'}]$ describe the depopulation and population, respectively, of the electron state with momentum p as a result of scattering of the electrons of the i (i') type by means of an l scattering mechanism with their transformation into the i' (i) type. Then

$$\begin{aligned} S^{(1),l}[f_i] &= \lambda_{i,i'}(p) f_i(p) \\ S^{(2),l}[f_{i'}] &= \int f_{i'}(p) W_{i',i}(p', p, \cos\theta)\delta[\varepsilon_{i'}(p') - \varepsilon_i(p) + \Delta_{i,i'}]\,dp' \\ \lambda^l_{i,i'}(p) &= \int W^l_{i,i'}(p, p', \cos\theta)\delta[\varepsilon_i(p) - \varepsilon_{i'}(p') - \Delta_{i,i'}]\,dp' \\ &= \int \omega_{i,i'}(p, \cos\theta)\,d(\cos\theta)\,d\varphi \end{aligned} \tag{6}$$

where $W^{l}_{i,i'}(p, p', \cos\theta)$ is the probability of electron transition from the i'-type valley to the i-type valley as a result of the scattering by means of the l mechanism, $\omega^{l}_{i,i'}(p, \cos\theta)$ is the angular dependence of the scattering probability of electron with momentum equal to p, $\Delta^{l}_{i,i'}$ is the energy difference between the final and the initial states of the scattered electron equal to the corresponding phonon energy, and φ is the azimuth.

In the collision integrals the following processes are taken into account: intra-valley scattering by the ionized impurities, acoustical phonons and optical phonons, 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) [8].

To complete the formulation of the problem, it is necessary to specify boundary conditions for the distribution functions and for the electric field potential. The region being investigated is bounded from the left-hand side by the semiconductor–vacuum interface at $z = 0$. The electron escape through the potential barrier into the vacuum is determined by the transparency coefficient $D(p_z)$ calculated from the Schrödinger equation.

For the distribution functions of electrons with momenta $p_z > 0$ at $z = 0$ we have

$$f_i(p_x, p_y, p_z, t) = [1 - D(p_z)] f_i(p_x, p_y, -p_z, t). \tag{7}$$

The electric field strength at $z = 0$ is determined by the condition of the electric induction vector normal component continuity:

$$E(0) = E_s/\kappa. \tag{8}$$

The right-hand boundary of the region under investigation is chosen to be far enough from the surface that the electron concentration is equal to that in the volume of the sample. Therefore the electron distribution functions on the boundary are equal to those in the volume and their spatial gradients are equal to zero. So the distribution functions of the electrons with momenta $p_z < 0$ on the right-hand boundary are determined from the set of Boltzmann kinetic equations in which the terms including the spatial gradients are omitted:

$$\partial f_i/\partial t - eE\,\partial f_i/\partial p = S_i \qquad i \equiv \Gamma, L, X. \tag{9}$$

The initial state of the system to be investigated is the state of thermodynamic equilibrium between the electron gas and the lattice. So the spatial distribution of the electric field potential $\phi(z)$ (which is connected with the electric field strength $E(z)$ by the relation $d\phi/dz = eE$) is obtained from solution of a self-consistent problem:

$$\begin{aligned} &d^2\phi(z)/dz^2 = -(4\pi e^2 N_D/\kappa)\{\exp[-\phi(z)/kT] - 1\} \\ &d\phi(z)/dz_{z=0} = eE_s/\kappa \qquad \phi(z) \to 0 \qquad z \to \infty. \end{aligned} \tag{10}$$

The initial electron distribution function is taken in the form of the local Maxwellian distribution function

$$f(p, z) = N_D \exp[-\phi(z)/kT] f_0(p) \tag{11}$$

where $f_0(p)$ is the Maxwellian distribution function, k is the Boltzmann constant and T is temperature.

3. The numerical simulation procedure

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 with those of real electrons [8]. These particles move in the self-consistent electric field which is determined taking into account the distribution of charged particles in the region. The interaction of particles with the lattice is described by considering the scattering processes. The macroparticle method includes a standard Monte Carlo procedure; it is one of the variants of the many-particle Monte Carlo method. The simulation of the particle scattering on the impurities and the lattice oscillations and defining of the particle energy and momentum after the scattering act is performed by means of the ordinary Monte Carlo technique [11].

In intervals between scatterings the particles obey classical mechanics laws. With allowance for a dispersion law (4) the equations of motion are of the form

$$\begin{aligned} &dz_j(t)/dt = p_z(t)/m_i[1 + 2\alpha_i\varepsilon_j(t)] \\ &dp_z(t)/dt = -eE[z_j(t)] \\ &\varepsilon_j(t)[1 + \alpha_i\varepsilon_j(t)] = [p_j(t)]^2/2m_i \end{aligned} \tag{12}$$

where p_z and ε are momentum and energy of a macroparticle, m_i and α_i are the mass and non-parabolicity parameters of the i-type macroparticle, and j is the macroparticle number. To describe the spatial distributions of the electric field, particle concentration and other characteristics the empirically chosen spatial grid is introduced, refining the mesh spacings in the near-surface region where high gradients of carrier concentration electrostatic potential are expected. The ordinary simulation procedure of the time evolution of a system is as follows [9].

The time step τ which is the time interval between two consequent moments of electric field correction is introduced. During τ the electric field is assumed to be unchangeable. Let us suppose that the coordinates and momenta of every macroparticle as well as the electric field distribution are known at the time t. For each macroparticle the following procedure is performed. A free-flight time τ_1 is selected stochastically in accordance with given scattering probabilities:

$$\tau_1 = -\Gamma^{-1} \ln \xi \tag{13}$$

where ξ is a random number in $[0, 1]$ and Γ is the total scattering probability (the probability that a macroparticle suffers a scattering during the time dt) including a fictitious 'self-scattering' which does not change a particle momentum as if no scattering at all takes place. The introduction of self-scattering simplifies the procedure of free-flight time selection and significantly reduces the computer time [10]. Generally it is sufficient that Γ is not less than the maximum value of the total real scattering probability.

When the τ_1 obtained is greater than τ, the coordinate and momentum of a macroparticle at the time $t + \tau$ are obtained by numerically solving the equations of motion (12) and the time step for this macroparticle is completed. In the opposite case, when the τ_1 obtained is less than τ, the coordinate and momentum of a macroparticle are calculated from (12) at the time $t + \tau_1$; then the scattering event is simulated. The type of scattering is selected according to the relative weight of the various processes included in the model and a new momentum is selected in accordance with a given angular dependence of the differential cross-section of the particular scattering mechanism

($\omega_{i,i}(p, \cos\theta)$ in (6)). Then the new free-flight time τ_2 is randomly chosen as described above and compared with the remaining part of the time step equal to $\tau - \tau_1$. If $\tau_2 > \tau - \tau_1$, a particle is shifted in accordance with (12) in the time scale by the time interval $\tau - \tau_1$; otherwise it is shifted by the time interval τ_2 with subsequent scattering. The procedure is repeated until the particle reaches the moment $t + \tau$.

When the procedure described is completed for every macroparticle, update of the electric field distribution must take place.

To perform the new distribution of electric field the electric charge distribution is obtained from the known distribution of macroparticle coordinates. When this is done the electric field strength is found from the equation

$$dE/dz = -(4\pi e/\kappa)n(z) + (4\pi e/\kappa)N_D \tag{14}$$

where $en(z)$ is the electric charge distribution.

The penetration of electrons through the potential barrier to the surface is simulated by means of a probability procedure as follows: a macroparticle incident on the barrier with momentum p is back-scattered with probability $1 - D(p_z)$ and with probability $D(p_z)$ it is removed from the ensemble of the calculated macroparticles.

The injection of particles into the region being calculated from the volume of the sample is simulated by specifying the 'periodic' boundary conditions in the furthest-right computational cell of the space mesh; when a particle on its way to the surface leaves the outermost cell, a new particle of the same type and momentum is generated on the opposite border of the cell. Here the particle distribution function in the outermost cell corresponds to the solution of a set of Boltzmann equations (9) under the assumption that there is no distribution function space gradient. It should be stressed that such an approach to the simulation of particle injection takes into account the fact that the particle gas is heated by the electric field penetrating into the volume of the sample.

To provide accuracy of computations it is necessary to choose the time step τ to satisfy certain conditions. Firstly, the temporal variation in the electric field during the time step τ must satisfy the condition

$$\tau < T_p \tag{15}$$

where T_p is the period of plasma oscillations. Secondly, the spatial variation in the electric field through the spatial segment passed by particle during the time step τ must be small too:

$$\tau < h/v \tag{16}$$

where v is the macroparticle velocity and h is the distance along which the field changes considerably; it can be estimated as a step of the spatial grid. When large field gradients exist inside the region, it is necessary to specify a very small spatial step h. In such a case the condition (16) may be stronger than (15). The time step τ is reduced as it is proportional to h and the simulation time increases.

So the ordinary macroparticle method in the presence of large field gradients becomes very time consuming. It should be noted, however, that the motion of particles in the near-surface potential well has an oscillatory character. Taking this fact into account it becomes possible to construct a more effective algorithm.

If the free-flight time is greater than the time interval between two consequent particle reflections from the walls of the potential well, there is no need to repeat the calculation for each oscillation. A more successful method is as follows. When the first oscillation is calculated, it becomes possible to estimate the amount of oscillations by

dividing the free-flight time by the period of oscillation. Then the time equal to the number of oscillations multiplied by the period is subtracted from the remaining time of the free flight and the ordinary procedure completes the time step. The probability of tunnelling must be modified:

$$P(N) = 1 - (1 - D)^N \tag{17}$$

where N is the number of oscillations.

The simulation procedure according to the algorithm described above is much more effective than the ordinary method in the case of a narrow potential well.

During the simulation process it is possible to observe the time evolution of a system as well as the average values of physical quantities of interest, such as the drift velocity and the mean energy, by calculating the ensemble average over all particles of the system. In particular, the distribution function is proportional to the number of particles $n(p, z, t)\ \Delta p\ \Delta z$ that at time t are found to be in a coordinate–momentum cell of fixed volume Δz around z and Δp around p. When a stable state is investigated, we can obtain the time average of a physical quantity.

In the present paper the simulation is performed for an n-type GaAs emitter at the temperature $T = 300$ K. Parameters for the GaAs band structure and scattering mechanisms were taken from [12]. Typical values of the computational model parameters used are as follows: particle number, up to 10 000; number of grid points in the spatial grid, of the order of 100.

4. Results and discussion

The main purpose of the paper is the investigation of non-equilibrium processes under the conditions of a large electric field and a large electron concentration gradient. The series of simulations has been performed with different values of electric field strengths E_s, from 3.5×10^7 to 4.0×10^7 V cm^{-1}. As can be seen from the results of simulations, such a range of electric field variations corresponds to a variation in the emitter operation regime from complete equilibrium to strong non-equilibrium. So, when $E_s = 3.5 \times 10^7$ V cm^{-1} the charge transfer process through the SCR is equilibrium. The outer electric field almost does not penetrate to the bulk of the sample and the heating of the electron gas does not take place. All the electrons are in the Γ valley and their energy distribution function has an equilibrium form. The emission process in this case is fully described by Stratton's [6, 7] equilibrium theory. The escape of electrons from the SCR due to tunnelling is fully compensated by their influx from the bulk.

The electric field increase leads to a surface potential barrier thickness decrease and hence to an increase in the transparency coefficient D. The tunnelling current increases. To compensate the electron escape from the SCR the bulk current has to increase. However, the field dependence of the electron drift velocity through the GaAs sample has a saturation region [12]. Therefore, after the saturation current is achieved, the influx of electrons from the bulk cannot compensate their disappearance. It leads to reduction in the SCR full charge and to violation of the outer field shielding conditions. The electric field penetrates deeply into the semiconductor volume and heats the electron gas. A saturation region appears in the current–voltage curve. This is explained by the drift velocity saturation in the semiconductor bulk.

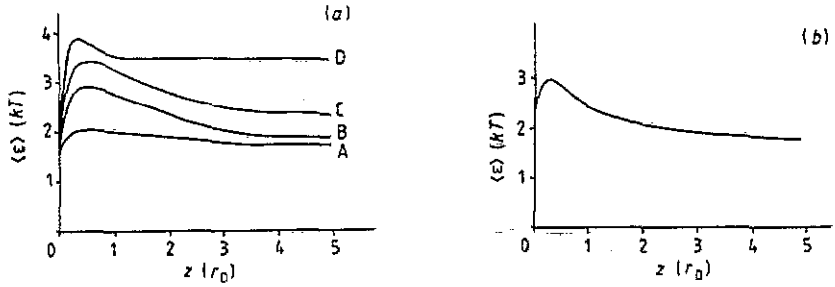

Figure 2. The spatial distribution of the electron's mean kinetic energy for different external electric field strengths: (*a*) Γ valley, curve A 3.5×10^7 V cm^{-1}; curve B, 3.7×10^7 V cm^{-1}; curve C, 3.8×10^7 V cm^{-1}; curve D, 3.9×10^7 V cm^{-1}; (*b*) L valley, 3.9×10^7 V cm^{-1}.

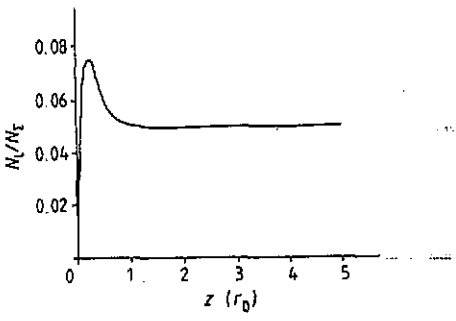

Figure 3. The relative occupation N_L/N_Σ of the L valley.

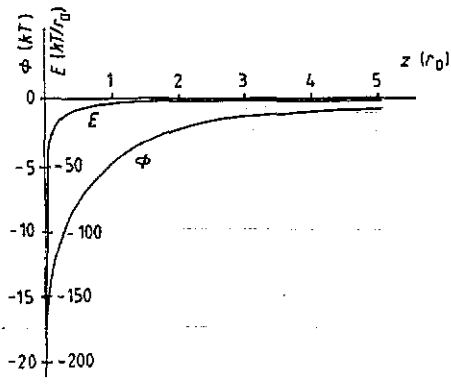

Figure 4. The potential profile $\phi(z)$ in the SCR at a field strength E_s of 3.9×10^7 V cm^{-1} and the electric field profile $E(z)$ in the SCR.

In figures 2(*a*) and 2(*b*) the spatial distributions of the mean electron kinetic energy for different strengths of external electric field are represented for the Γ valley and for the L valley, respectively. Figure 2(*a*) shows that a small change in the external electric field value leads to substantial heating of the electron gas followed by the operation regime change from quasi-equilibrium to non-equilibrium.

As can be seen from the electron temperature distributions the electron's mean kinetic energy in the volume differs from its equilibrium value and rises towards the surface. The maximum of the electron's mean kinetic energy is located at a distance of (0.3–0.5)r_D (where r_D is the Debye radius) from the surface. The relative occupancy of the L valley also has a maximum and its location coincides with the location of the electron's maximum temperature (Figure 3). The features noted may be explained by the existence of two slightly interacting electron subsystems in the near-surface region:

(1) a subsystem almost in equilibrium described by a Maxwell distribution function with temperature equal to the lattice temperature;

(2) a strongly non-equilibrium subsystem formed by electrons coming from the volume.

The interaction between these occurs by exchange of electrons as a result of electron scattering. The interaction weakness is provided by the small size of the SCR compared

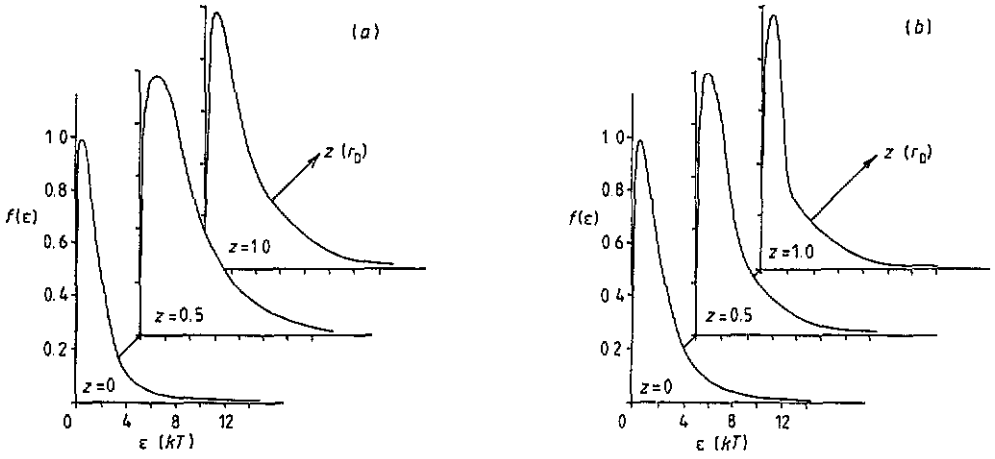

Figure 5. The electron's energy distribution function at different distances from the surface: (*a*) Γ valley; (*b*) L valley.

with the electron energy relaxation length (if $N_D = 10^{17}\,cm^{-3}$, then $r_D \simeq 10^{-6}\,cm$ and $l_\varepsilon \simeq 10^{-5}\,cm$).

The electron density distribution of the equilibrium subsystem is strongly non-uniform and has a sharp maximum on the surface; therefore the mean values near the surface are close to their equilibrium values. Far from the surface where the electron concentrations of the two subsystems are comparable the mean values are determined by taking into account the existence of both electron groups.

In figure 4 the potential profile and the spatial distribution of the electric field in the SCR at an external field strength E_s of $3.9 \times 10^7\,V\,cm^{-1}$ are plotted. It corresponds to the strong penetration of the external electric field into the sample volume.

The electron's energy distribution functions at different distances from the surface for the Γ valley and L valley are shown in figures 5(*a*) and 5(*b*), respectively. The distribution function width at a distance $0.5r_D$ is greater than at other distances; this corresponds to the location of the electron's mean maximum kinetic energy.

In conclusion we note that mathematical modelling of semiconductor devices on the basis of a kinetic description is a powerful tool for investigating physical processes. It permits us to investigate such detailed characteristics as the valley distribution of electrons, the spatial dependences of temperatures, the concentrations and other values which cannot be measured directly.

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