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AN IMPACT IONIZATION MODEL FOR CURRENT CONTROLLED NEGATIVE RESISTANCE
AND g-r INDUCED NONEQUILIBRIUM PHASE TRANSITIONS

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Résumé. - Nous présentons dans ce papier un modèle simple de génération-recombinaison basé sur un mécanisme d'ionisation des donneurs par impacts à deux étapes. Ce modèle conduit à une caractéristique Courant-Tension de type S et à des transitions de phases hors d'équilibre entre les branches hautes et basses de la résistivité. Nous avons montré qu'une règle de "surfaces égales" est une condition nécessaire pour la formation de filaments ou de couches de courant.

Abstract. - A simple generation-recombination (g-r) model based upon a two-step impact ionization mechanism of donors is presented. It leads to an S-type current-voltage characteristic and to nonequilibrium phase transitions between its high and low resistivity branches. The homogeneous steady state corresponding to the falling branch is shown to be unstable against the formation of high and low current layers and filaments, and an equal area rule for their coexistence is established.

1. Introduction

Current controlled negative differential resistance associated with an S-type current-voltage characteristic and with threshold switching is a wide-spread phenomenon in amorphous¹⁾ and crystalline²⁾ semiconductors, and insulators³⁾ for which thermal as well as electronic mechanisms have been proposed. Here we consider a generation-recombination (g-r) model which is based upon the impact ionization of both ground state and excited donors by hot electrons. It involves an n-type semiconductor with N_D donors, partially compensated by $N_A < N_D$ fully occupied acceptors, at low temperature. Other g-r models with impact ionization of deeply trapped electrons and holes were studied previously⁴⁾.

2. The model

The g-r processes considered are shown schematically in Fig. 1.

Fig. 1: Schematic g-r processes involved in the model.

The rate constants depend upon the electric field E . It is assumed that in the regime of negative differential resistance the field dependence of the impact ionization coefficients dominates that of all other rate constants and of the mobility.

The transport equations are the following:

$$\underline{j} = ne\mu\underline{E} + eD\underline{\nabla}n \quad (1)$$

$$\dot{n} - \frac{1}{e}\underline{\nabla} \cdot \underline{j} = f(n, n_D, n_{D^*}) \quad (2)$$

$$\dot{n}_D = g(n, n_D, n_{D^*}) \quad (3)$$

$$\dot{n}_{D^*} = -f(n, n_D, n_{D^*}) - g(n, n_D, n_{D^*}) \quad (4)$$

$$\underline{\nabla} \cdot \underline{E} = \frac{4\pi e}{\epsilon} (N_D - N_A - n - n_D - n_{D^*}), \quad \underline{\nabla} \times \underline{E} = 0 \quad (5)$$

The g-r rates are given by

$$f(n, n_D, n_{D^*}) = X_1^S n_{D^*} - T_1^S p_D n + X_1 n_D n + X_1^* n_{D^*} n \quad (6)$$

$$g(n, n_D, n_{D^*}) = -X^* n_D + T^* n_{D^*} - X_1 n_D n \quad (7)$$

n	concentration of free electrons
n_D	concentration of electrons in donor ground states
n_{D^*}	concentration of electrons in donor excited states
$p_D = N_D - n_D - n_{D^*}$	concentration of unoccupied donors
N_D	total donor concentration
$N_A < N_D$	compensating acceptor concentration
$\underline{j}$	electron current density
μ	electron mobility
D	diffusion constant

Table I: List of symbols

3. Homogeneous steady states

The homogeneous solutions of (1)-(5) are determined by

$$\dot{n} = f(n, n_D), \quad \dot{n}_D = g(n, n_D) \quad (8)$$

$$\text{and } n_{D*} = N_D - N_A - n - n_D \quad (\text{local neutrality}). \quad (9)$$

Depending upon the values of the rate constants, (8) admits up to three steady states, two of which are stable against small fluctuations

δn , δn_D , while the third is not. The two stable steady states ($n_1 < n_3$) correspond to high (n_1) and low (n_3) resistivity states. The carrier concentrations depend upon the applied static electric field $E_0 = V/L$ via X_1 and X_1^* , where V is the sample voltage, and L the sample length. Thus $j = n(E_0) e \mu E_0$ yields an S-type static current-voltage characteristic, which is plotted in Fig. 2 for the particular field dependence $X_1 = 5 \times 10^{-8} \exp(-6/E_0) \text{ cm}^3 \text{ s}^{-1}$, $X_1^* = 10^{-6} \exp(-1.5/E_0) \text{ cm}^3 \text{ s}^{-1}$.

Fig. 2: Current-voltage characteristics for $N_D = 1.5 \times 10^{15} \text{ cm}^{-3}$, $N_A/N_D = 1/3$, $T_1^S = 10^{-6} \text{ cm}^3 \text{ s}^{-1}$, $T^* = 10^6 \text{ s}^{-1}$. The other parameters are in μs : (a) $X_1^S = 0.5, 1, 2, 10$; $X_1^* = 1$; (b) $X_1^* = 1, 1.1, 1.5, 2$; $X_1^S = 0.5$.

Switching between the high and the low resistivity branches of the current-voltage characteristic can be regarded as a nonequilibrium phase transition of first order between two steady states with overlapping stability range, brought about by variation of E_0 taken as a control parameter. More generally, E_0 is determined from the load line of the external circuit with impedance R and applied voltage U_0 . This includes in particular voltage controlled ($R \rightarrow 0$) and current controlled ($R \rightarrow \infty$) conditions.

By appropriate irradiation the ionisation coefficient X_1^S can be increased, leading to smaller and eventually vanishing bistability

ranges (Fig. 2a). Similarly, with increasing X^* (e.g. increasing temperature, Fig. 2b) or decreasing compensation ratio N_A/N_D the bi-stability vanishes. This agrees well with the qualitative behaviour known from experiments⁵⁾.

4. Inhomogeneous steady states

For small deviations $\delta\phi := (\delta E, \delta n, \delta n_D, \delta n_{D^*})$ from the unstable homogeneous steady state (E_0, n, n_D, n_{D^*}) (1)-(5) can be linearized. With the ansatz $\delta\phi \sim \exp i(\underline{k} \cdot \underline{x} - \omega t)$ for periodic boundary conditions and fixed current we find the dispersion law

$$0 = (i\omega - \Gamma) [(i\omega - \Gamma) (i\omega + \lambda_1)(i\omega + \lambda_2) + (i\mu E_0 \cdot \underline{k} - Dk^2)(-\omega^2 - i\omega\theta + \Delta)] \quad (10)$$

where $\Gamma := \frac{4\pi e n \mu}{\epsilon}$ is the dielectric relaxation frequency,

$\lambda_1 > 0 > \lambda_2$ are the eigenvalues of the linearized rate equations (8), and θ, Δ are positive constants depending upon the rate coefficients, and hence upon E_0 . The spectrum given by (10) contains the damped dielectric relaxation mode $\omega = -i\Gamma$ and three coupled relaxation - recombination - diffusion modes. For transverse perturbations ($\underline{k}, \delta \underline{E} \perp \underline{E}_0$) we obtain in the long wavelength limit an undamped recombination-diffusion mode

$$\omega = i(\lambda_1 - \tilde{D}k^2) \quad (11)$$

with a dressed diffusion constant

$$\tilde{D} = D \frac{\lambda_1^2 + \lambda_1\theta + \Delta}{(\lambda_1 + \Gamma)(\lambda_1 - \lambda_2)} \quad (12)$$

This leads to the bifurcation of a family of inhomogeneous stationary solutions.

To investigate the full nonlinear equations (1)-(5) for a plane geometry, we assume that the concentrations and the field $\underline{E} = E_0 \underline{e}_z + E_\perp \underline{e}_x$ depend upon the coordinate x transverse to the static field $\underline{E}_0$ only, and that the transverse current vanishes. In the steady state (1)-(5) can then be reduced to

$$\frac{d}{d\zeta} n = -n\epsilon \quad \frac{d}{d\zeta} \epsilon = \varrho(n) \quad (13)$$

with the dimensionless coordinate $\zeta = x/L_D$ and transverse field $\epsilon = (eL_DE_\perp) / (kT)$, where $L_D := [(\epsilon D) / (4\pi e \mu (N_D - N_A))]^{1/2}$. The charge density $\varrho(n)$ is found from (3)-(5) by eliminating n_D, n_{D^*} and is a nonlinear function of n . It depends upon E_0 via X_1, X_1^* , and we assume $E_\perp \ll E_0$. A first integral of (13) is

$$\epsilon(n) = \pm \sqrt{-2\phi(n) + \text{const.}} \quad (14)$$

with $\phi(n) := \int (\vartheta(n) / n) dn$.

Eq. (14) includes inhomogeneous oscillatory, solitary and run-away solutions (Fig. 3). The homogeneous steady states (n_1, n_2, n_3) are the extremal points of $\phi(n)$. A solitary solution corresponding to the coexistence of n_1 and n_3 , i.e. to plane low and high current layers, exists if and only if the condition

$$\int_{n_1}^{n_3} \vartheta(n) \frac{dn}{n} = 0 \quad (15)$$

is satisfied. This is analogous to the Maxwell construction obtained for equilibrium and chemical nonequilibrium phase transitions⁶⁾ or the equal area rule known from the Gunn effect⁷⁾ and from other switching models¹⁾.

Fig.3: Phase portrait of the inhomogeneous steady states given by (14) with (15). The parameter varying along the phase trajectories is the transverse coordinate z . The saddle-to-saddle separatrices represent the solitary solutions. The numerical parameters are those of Fig. 2(a), with $x_1^S = 0.5 \mu s$, $E_0 = 8.5 \text{ V/cm}$.

For a cylindrical geometry (13) is replaced by

$$\frac{d}{dr} n = -n\epsilon \quad \frac{d}{dr} \epsilon = -\frac{\epsilon}{r} + \vartheta(n) \quad (13')$$

where r is the dimensionless radial coordinate. The equal area rule (15) has to be modified by a surface term

$$\int_{n_1}^{n_3} \vartheta(n) \frac{dn}{n} \pm \frac{1}{r_0} \int_{n_1}^{n_3} \left(\frac{d}{dr} n \right) \frac{dn}{n^2} = 0 \quad (15')$$

and leads to cylindrical high or low current filaments with mean radius r_0 .

5. Conclusion

The mechanism leading to bistability in the above model can be interpreted as a coupled two-step impact ionization process:

The donor ground levels are depleted by impact ionization (X_1), which results in an enhancement of the excited donor population n_{D^*} , by (7).

Simultaneously, the excited donors are impact ionized, with a rate $X_1^* n_D^* n$ increasing thus stronger than linearly with n . In the bi-stability regime the impact ionization rate is negligible at low n , i.e. in the high resistivity state, where recombination is balanced by the simple generation process X_1^S . Due to the superlinear increase in the impact ionization rate, a second stable steady state is possible at large n , i.e. the low resistivity state.

The model is applicable for materials where the dominant g-r processes are those of Fig. 1. More sophisticated g-r models, e.g. including Auger recombination, yield the same qualitative behaviour for suitable ranges of the rate constants.

There is a close analogy of the above switching transition with phase transitions in equilibrium and in other nonequilibrium systems⁸⁾, such as critical slowing down, soft mode instability of the homogeneous steady state against long wavelength perturbations, bifurcation of inhomogeneous solutions, and phase coexistence when certain equal area rules are satisfied.

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