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TRANSPORT PROPERTIES OF HIGHLY EXCITED SEMICONDUCTORS

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It is shown that under specific stationary excitation conditions in surface excited semiconductors spatial regions of "inverse diffusion" may be created, in which the particle-hole current flows in the direction of increasing density. The cross-over to normal diffusion is directly related to experimental observations.

The investigation of highly excited semiconductors has by now led to a satisfactory understanding of the stationary optical response which in turn has given a wealth of information on the underlying thermodynamics of the created electron-hole plasma (EHP).[1] Most model studies start from a homogeneous state. However, the necessarily inhomogeneous excitation will in general lead to an inhomogeneous state, which should therefore exhibit internal macroscopic currents. The investigation of such currents is the subject of transport theory.

We want to show in this contribution that the combination of conventional transport theory with conventional solid state theory and optics can lead to quite unexpected results - which nevertheless are easily interpreted and in agreement with pertinent experiments.

The model set-up for the investigation of one-dimensional energy transport consists in placing an infinite (semiconductor-) slab between two heat reservoirs at different temperatures $T_1 > T_2$. The resulting temperature gradient ∇T gives rise to a heat current j_u^o. We now may ask ourselves: what happens if we replace the heat reservoir T_1 by a monochromatic laser field of frequency $h\omega > E_g$ (E_g is the electronic energy gap of the semiconductor) impinging perpendicularly on the surface at x=0 with an energy current density $\vec{j}_\varepsilon^{\,Las} = j_\varepsilon \hat{x}$.

Let us treat the effect of this laser field simply by the constraints

$$j_n(x=0) = (1-R)j_\varepsilon/h\omega, \quad (1)$$

$$j_{u,ph}(x=0) = 0, \quad (2)$$

$$j_u(x) = \beta(x)\left(\frac{\partial u}{\partial n}\right)_T j_n(x). \quad (3)$$

with R = reflectivity, $u=u_e+u_h$ = density of the internal energy (we neglect exchange-correlation contributions here)

Here $j_{u,ph}$ is the current of internal energy within the phonon subsystem, j_n is the electron-hole particle current and j_u the corresponding energy current. Mind that the EHP is treated within the quasi-thermodynamic approximation, i.e. electrons e and holes h are supposed to be distributed according to individual Fermi distributions $f_{e,h}$ which obey the local conditions $n_e = n_h = n$ for the number density and $T_e = T_h$ for the temperature. The dimensionless factor β is a "loading parameter": $\beta \gtrsim 1$ is the region of isothermal transport (see below), while large β correspond to excess energy transport. This description allows to prescribe initial values for j_n and j_u from which ∇T, ∇n within the EHP and ∇T_{ph} within the phonon system (i.e. finally temperature and eh-density profiles) should follow. In this sense the present set-up is just conjugate to the conventional conditions discussed at the beginning.

A systematic approach to the Boltzmann-equation governing the electron-hole and phonon subsystems is provided by the Chapman-Enskog scheme.[2] Restricting ourselves to the dominant scattering mechanisms e-ph, h-ph we find in first order:

$$f_{e,h} = f^o_{e,h} + \Phi^{(1)}_{e,h}(\nabla n, \nabla T) \text{ and } f_{ph} = f^o_{ph} + \Phi^{(1)}_{ph}(\nabla T_{ph}). \quad (4)$$

where f^o_i are the zero order results. In this approximation the equations for the currents are given by

$$\left.\begin{aligned} j_n &= L_{11}\nabla n + L_{12}\nabla T, \\ j_u &= L_{21}\nabla n + L_{22}\nabla T, \end{aligned}\right\} \quad (5)$$

$$j_{u,ph} = L_{22,ph}\nabla T_{ph}, \quad (6)$$

while the collision invariants read under stationary conditions

$$\mathrm{div}\ j_n(x) = \sigma_n^d + \sigma_n^A \tag{7}$$

$$\mathrm{div}\ j_u(x) = \sigma_u^d + \sigma_u^A + \sigma_u^{ph} \tag{8}$$

with $\sigma_n^d < 0$: source term for direct recombination, $\sigma_n^A < 0$: source term for Auger recombination, and $\sigma_u^{ph} < 0$: lattice cooling. The last equation determines the evolution of $\beta(x)$.

The transport coefficients for the EHP follow from a thermodynamic-phenomenological approach (compare Ref. 3)

$$L_{11} = - D_1 \tag{9}$$

$$L_{12} = - \alpha_T n D_1/T \tag{10}$$

$$L_{21} = - d_{21}\left(\frac{\partial u}{\partial n}\right)_T D_1 \neq L_{12} \tag{11}$$

$$L_{22} = \frac{d_{21}d_{32}}{T}\left[T\left(\frac{\partial u}{\partial T}\right)_n + \left(1-\frac{1}{d_{32}}\right)\frac{\left(\frac{\partial u}{\partial n}\right)_T^2}{\left(\frac{\partial \mu}{\partial n}\right)_T}\right]D_1 . \tag{12}$$

Here D_1 is the isothermal diffusivity, α_T the so-called thermal diffusion factor, μ the chemical potential of the EHP. The ratios d_{21}, d_{23}, found by comparison with the relaxation-time approximation for equ. (4), sensitively depend on the degeneracy of the EHP and on the scattering model: Assuming for the scattering time

$$\tau_k = A|k|^{2s} \tag{13}$$

we find (for $m_e = m_h$; for unequal masses proper averages are used)

$$\alpha_T = \frac{3}{2}(d_{21}-1) = \begin{cases} 0 & \text{for quantum limit (q)} \\ s+1 & \text{for classical limit (c)} \end{cases} \tag{14}$$

$$d_{21} = \begin{cases} 1 & \text{for q} \\ 1/3(2s+5) & \text{for c} \end{cases} \tag{15a}$$

$$d_{32} = \begin{cases} 1 & \text{for q} \\ 1/5(2s+7) & \text{for c} \end{cases} . \tag{15b}$$

In general, equs. (14) and (15) can be expressed in terms of Fermiintegrals, i.e. are functions of the plasma degeneracy only. In the following we will consider s=-1/2, i.e. accoustic-phonon-scattering.

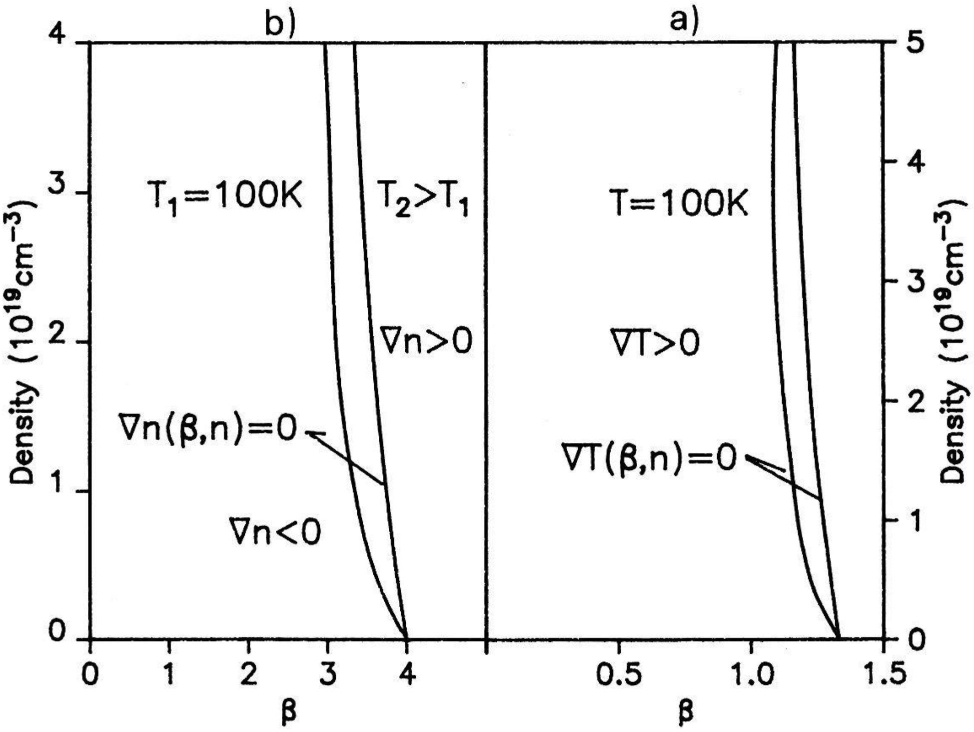

Fig. 1 a) Sign of ∇T and b) ∇n as function of n and β. See text.

For given β equ. (5) can now be solved for the gradients of the temperature and the density:

$$\nabla T \sim [d_{21} - \beta] j_n \tag{16}$$

$$\nabla n \sim [-T(\frac{\partial u}{\partial T})_n + \frac{(\frac{\partial u}{\partial n})_T^2}{(\frac{\partial \mu}{\partial n})_T} \delta(\beta)] j_n \tag{17}$$

$$\delta(\beta) = -(1- \frac{1}{d_{32}}) + \frac{\beta}{d_{32}}(1- \frac{1}{d_{21}}) \ . \tag{18}$$

The sign of $\nabla T(\beta,T,n)$ for given n is shown in Fig. 1a. We see that large β-values require large negative temperature gradients, which are necessary to push the energy through the sample. The isothermal regime is between $\beta = 1$ and $\beta = 4/3$. The sign of $\nabla n(\beta,T,n)$ is shown in Fig. 1b. If there were no thermal diffusion (i.e. no cross-effects) the negative temperature gradient would influence only the heat current. With $\alpha_T > 0$, however, ∇T also induces a large j_n, which must be counterbalanced by a positive ∇n to reconcile the constraints j_n, j_u. In consequence, large β lead to spatial regions of reverse diffusion. Note also that if the system were forced into equilibrium with the lattice at any point in space (~isothermal conditions) this new effect would be excluded.

Let us focus now on the transition from reverse to normal diffusion. In the classical limit this happens at $\beta = 4$ (quantum limit: $\beta = 0$). If we start at high β - values we have to cross over to the region of normal diffusion. This crossing is obviously characterized by a maximum density $n_{max}(\beta,T)$, for which an interesting correlation with the temperature is found:

$$\frac{n_{max}}{T^{3/2}} = f(m,\beta) \; . \qquad (19)$$

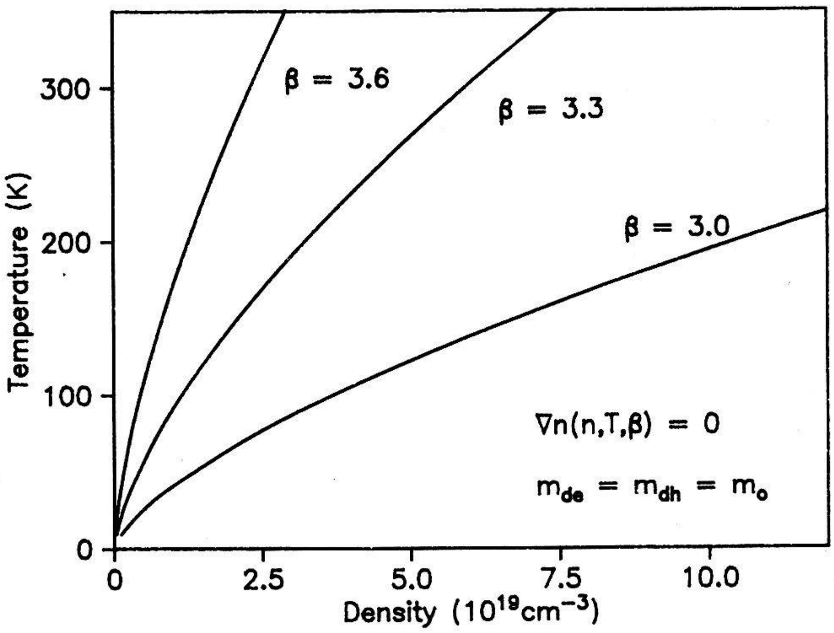

Fig.2 Dependence of the spatial density maximum on density and temperature for different values of the coupling parameter β.

The dependence of n_{max} on T and β is illustrated in Fig. 2 for a model semiconductor with $m_e = m_h = m_o$. In Fig. 3 we compare the theoretical result equ. (19) for $\beta = 3$ with a broad set of experimental data. Here the reduced densities have been plotted versus the respective reduced density of states masses $m_d^{3/2}$. Fig. 3 convincingly demonstrates the postulated correlation of eletron-hole plasma density and bandstructure. This correlation has for a long time obscured the interpretation of many experiments[4] in this field. We remark, that up to now there is no alternative explanation for this bandstructure dependence of the plasma densities.

Preliminary results have been reported in Ref. 5. These correspond to $d_{21} = 2$, $d_{32} = 1$, and $\beta = 1$, in which case the reduced heat current

$$j_q = j_u - \left(\frac{\partial u}{\partial n}\right)_T j_n \qquad (20)$$

is zero. The present study, which pays particular attention to the scattering model, shows that for moderate degeneracies reverse diffusion occurs at higher β values than previously expected.

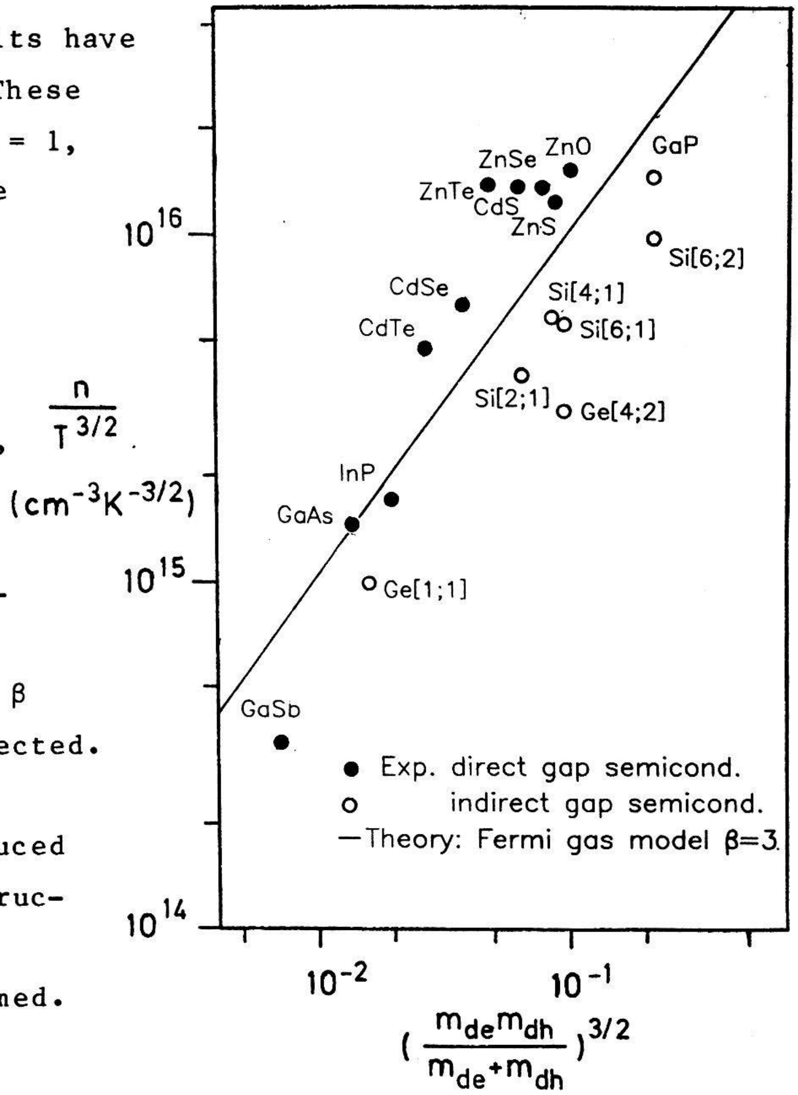

Fig. 3 Relationship of reduced plasma densities on bandstructure. For the theory equal masses of e and h are assumed.

Extensions of the present theory comprise: the detailed study of the balance equations leading to explicit density and temperature profiles, inclusion of exchange-correlation contributions, the study of transport properties near thermodynamically unstable points as well as applications to laser annealing and exciton drift.

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