Results to implement non-equilibrium phonon distributors into a conventional Monte Carlo electron transport simulation are report. A new code for a simulation of the simplified model of low-temperature steady-state acoustic phonon-electron transport in GaAs has been developed and applied. This model has been extended to a fully time-dependent (transient) calculation of optical phonon interactions with near ballistic electrons in n-GaAs in the overshoot regime at room temperature (1) by modifying standard Monte Carlo codes to accommodate the numerical procedures required for nonequilibrium phonon calculations and by applying these to real device phenomena such as picosecond response in n-GaAs to a high field pulse.
The physical model used in the preceding as well as in the present research project consists of electrons in isotropic and parabolic $\Gamma$- and $L$-conduction band minima with the standard electron-phonon coupling, polar optical, incompressible and equivalent intervalley, acoustic deformation potential, optical deformation potential (C-valley), piezoelectric (not contained in the Monte Carlo model), and impurity scattering. The model assumes spatial homogeneity, neglecting in particular the very small LO-phonon diffusion, but should nevertheless allow its extrapolation to a coarse-grained and therefore locally homogenous description of space-dependent situations.

The results of "Submicron Phononics I" could be summarized as follows:

(1A) Neglecting the upper $L$-valleys, a non-equilibrium-phonon-induced collective breakdown occurs within the typical field and time range of the overshoot effects in the actual many-valley bandstructure. The breakdown is caused by an LO phonon avalanche through a "phonon-Cerenkov" mechanism (i.e., the carrier drift velocity exceeds the phase velocity of the phonons) and requires a sufficiently high carrier concentration. As the mathematical resonance condition in the absence of the BDM distribution of the carriers, the model dependence of this prediction is obvious, but a Cerenkov-like phonon amplification should be expected, whenever the actual carrier distribution is of BDM form.

(1B) For the realistic many-valley bandstructure it turns out that the loss of fast-drifting $\Gamma$-electrons through transfer into the "hot" LO-valley suffices to stop the above mentioned single-valley breakdown and to ensure the establishment of an asymptotic steady state at arbitrary fields. Carrier drag by the initially amplified forward phonons gives rise to the above steady state drift velocity $v$. For higher fields $v$ is reduced, because the reduced cooling efficiency of the "hot" LO phonons leads to a higher $\Gamma$-valley temperature and therefore to a higher population of the $\Gamma$-valleys of lower mobility. Both the drag and the heating-induced corrections amount to more than 20% at the highest investigated carrier concentrations (several $10^{17}$/cm$^2$).

In these calculations the integration of the time-dependent Boltzmann equation for the phonon distribution functions was performed in parallel to the number-, energy- and momentum balance for the the BDM electrons in the $\Gamma$- and $L$-valleys for the momentary phonon distribution, implying an instantaneous adaption of the carriers to any change in the phonon population. However, besides the well-known BDM requirement of an extremely fast internal carrier thermalization, such a complete concealment of the carriers by the LO phonons would be justified only if the energy and momentum relaxation rates of the carrier system as a whole were much larger than the rate of change of the LO-phonon distribution. This condition is well fulfilled for the dominant polar-optical-LO phonon coupling, and was therefore sufficient for the investigation of the drift velocity and the corresponding stabilisation of the carrier-photon system. But the model did not allow a detailed estimate of the initial transients and especially of the overshoot phenomena, where the comparable time scales for the $\Gamma$- $L$-valley transfers and the LO-phonon buildup require a treatment of the time evolution of both carriers and phonons on the same footing.

So two questions remained:

(1C) Would a rapid initial phonon heating and the ensuing rise of the mean energy of the $\Gamma$-electrons lead to an accelerated $\Gamma$ $L$ transfer and thereby to a reduction of the overshoot through the earlier breakdown of the mean carrier velocity.

(1D) Would this earlier onset of the transfer very soon reduce the number of fast-drifting $\Gamma$-electrons below their threshold value for strong LO-phonon amplification; in this case the phonon avalanches would be automatically quenched in its initial stages and the non-equilibrium-phonon effects kept low.

The present research project was set up to clear these points within the model-free and highly effective Monte Carlo approach.

2. Scope and Objectives of "Submicron Phononics II"

The scope of the project was

(2A) to implement non-equilibrium phonon distributions into a conventional Monte Carlo electron transport simulation.

...
The objective of the project was:

(28) to use the new code for a simulation of the simplified model of low-temperature steady-state acoustic phonon-electron transport in GaAs

(29) to extend this model to a fully time-dependent (transient) calculation of optical phonon interactions with near ballistic electrons in n-GaAs in the one-band regime at room temperature (1) by modifying standard Monte Carlo code to accommodate the numerical procedures required for nonequilibrium phonon calculations, (2) by applying these to real device phenomena such as-picocurrent response in n-GaAs to a high field pulse

(30) to collaborate with Professor Hess (University of Illinois) to ensure that the computer algorithms are included in his Monte Carlo codes.

1. Results

(3 4) regarding item (28)

In collaboration with M. Ringer (Univ. Graz) and with P. Borodun, C. Jacoboni, P. Legli, and L. Reggiani from the University of Modena (Italy) a very general Monte Carlo code has been developed, which includes a full Monte Carlo treatment of the phonon distribution and provides the first model-independent transport theory of nonequilibrium carrier-phonon systems. The code provides for conventional one-particle simulation of steady-state transport as well as for ensemble simulation of time-dependent transport, displaying the important carrier parameters (such as density, mean drift velocities and source, and eventual changes of screening parameters), the scattering statistics of carriers and phonons, and the phonon distribution as function of the magnitude and oriention of the phonon wavevector. The program, of the conventional sequential type, is written in FORTRAN, and was run on the VAX 785 of the University of Graz (its general flow chart is shown below).

(35) regarding item (28):

Instead of the originally planned simulation of nonequilibrium electron-phonon systems in GaAs the most interesting case of low-temperature minima transport of holes in p-GaAs has been studied. Using the purely electronic one-particle Monte Carlo code of the Modena group, with analytical nonequilibrium phonon distributions (from "Stabilization Phononics") whose carrier parameters were obtained from the conventional carrier simulation in an investive way, indications of a nonequilibrium - i.e. a photon-induced current activation - but confirmed by more complete RD model calculations (References 1 and 2 below).

(37) regarding item (29)

To test the full Photon Monte Carlo, but to confirm the very time-consuming astrophysical scattering dynamics for the strongly peaked phonon distributions in high d.c. field transport, the simpler case of isotropic phonon amplification during the energy relaxation of laser-pulse excited carriers in GaAs was successfully simulated (References 3 and 4). The leading investigation in these studies was P. Legli. These results confirmed earlier hot-electron calculations of the Graz group, showing the decisive role of LO phonon amplification for the slowing down of the thermalization of highly excited electron-hole plasma (Reference 4).

Finally the main objective of the present project was achieved by the application of the code (34) to the transient high-field response of n-GaAs. It confirmed the physical picture of the earlier DHR results (Sections 1A and 1B above) about the effectiveness of the intervalley transfers to prevent the development of a nonequilibrium phonon-induced instability and to ensure the approach to a steady state for fields of up to several kV/cm. Moreover, it was demonstrated that the initial LO phonon amplification is also sufficiently quenched to prevent the destruction or reduction of the velocity overshoot, corroborating the hypothesis (10) and thereby ruling out the hypothesis (17) of our introductory discussion. These results are summarized in Figures 1 to 3 below (from Reference 5).

(39) regarding item (22)

The VAX compatibility of our code should guarantee a straightforward implementation of our program.