Applying POD-methods onto electron-phonon scattering in the Wigner equation

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***Abstract*— For the computation of the nonballistic electron transport caused by i.e. electron-phonon scattering high performance computing methods are needed. Therefore, a Discontinuous Galerkin (DG) method is used to approximate the Wigner transport equation (WTE). To oppose the resulting high computation times, a Proper Orthogonal Decomposition (POD)-method is introduced and linked with DG.**

INTRODUCTION

Recently a variety of methods to model the electron transport have been developed [1]. Those models mostly neglect the electron-phonon scattering or use relaxation models. Preliminary work to model electron-phonon scattering has already been made by [2], but quantum mechanical effects are neglected. To gain the best sophisticated approach these approximations are examined and results based on a larger amount of phonon modes are discussed. Since the addition of the electron-phonon interaction emerge into high computing times and large memory requirements, Model Order Reduction (MOR) methods like the POD method are introduced to solve these problems and enable an examination of more precisely discretisation schemes [3]. An algorithm can be set up to model the scattering and to include the already mentioned methods.

MODEL

A Wigner-Weyl-transformation of the electron-phonon von Neumann equation results into the Wigner transport equation in the phase space. Through the electron-phonon interaction a hierarchy problem arise. This results in an approximation of the Wigner function based on 4^l phonon states $|n_q>$ with l representing the order of the hierarchy. The hierarchy problem is dissolved through approximations like the random phase approximation (RPA) and the Markov approximation. The DG method is now used in χ-direction. The phase space k regarding the charge carrier and the phase space q of the phonons is discretized which leads to a discrete modal spectrum. For the transient solution a Lawson method of fourth order is applied.

RESULTS

For a test device (Fig. 1) the hierarchy problem is solved for the second order. The expected electron density can be seen in Fig. 2, which is in agreement with results taken by assessing the ballistic transport [4]. Only through the sole consideration of the electron-phonon interaction, the scattering can be seen (Fig. 3). The observed carrier concentration is in agreement with former results in [2] and [5]. From first evaluations (Fig. 4) it can be concluded that the POD method results in a considerable time reduction down to a tenth and can be classified as a promising approach.

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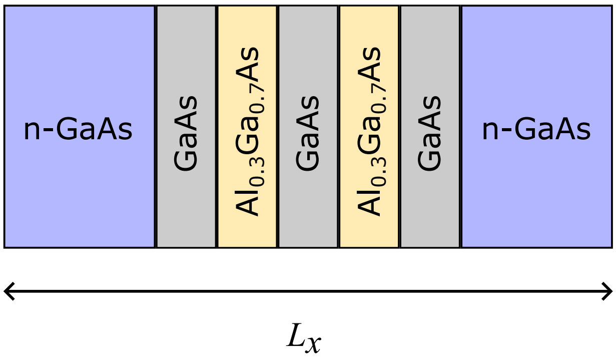

Fig. 1. Schematic GaAs/AlGaAs resonant tunneling diode with a width of L_x = 60 nm. At the edges of the structure the GaAs layer is highly doped. An $Al_{0.3}Ga_{0.7}As$ doublebarrier with 5 nm width is placed in the middle of an undoped GaAs layer with a 5 nm well between the barriers.

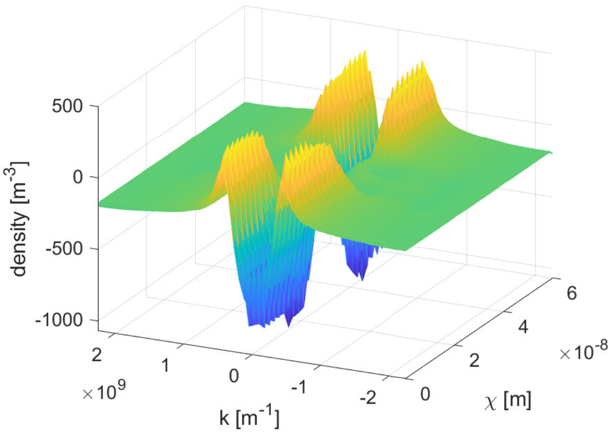

Fig. 3. The density of the scattered electrons is shown as a function dependent on the computation grid. For the q-discretisation N_q = 100 values are used. Two maxima are visible, which represent the creation of electrons at the wavenumber $k+q$ and $k-q$ respectively. The minimum at k=0 depicts the annihilation of an electron through the electron-phonon interaction.

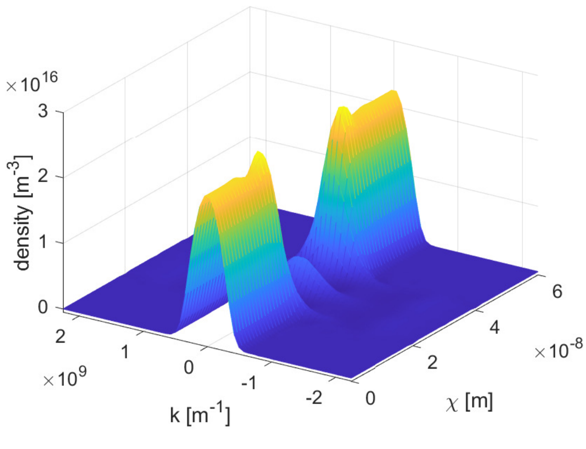

Fig. 2. The electron density within the RTD is shown as a function in dependence of the χ-coordinate and the k-coordinate. N_k = 60 values are considered for the k-discretisation.

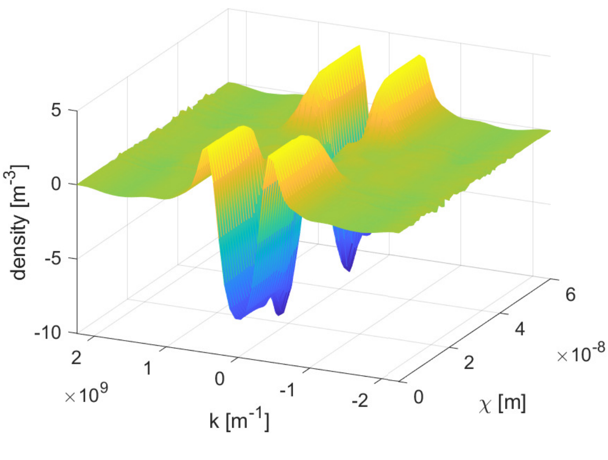

Fig. 4. The density of the scattered electrons is shown as a function of the computation grid. The solution is achieved through the POD method. For the q-discretisation the q phase space is divided into N_q = 11 values. 2750 snapshots are used to create a basis to reduce the order of the matrix of the system. The structure of the scattered electron density is in agreement with the solution gathered in Fig. 3. At the borders of the k-grid instabilities can be seen which shall be resolved through further investigations of the boundary conditions, which have to be adjusted to the expanded phase space $k+q$ and $k-q$.