Monte Carlo Simulation of Electron Transport in PbTe

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Abstract. A Monte Carlo (MC) technique is employed to investigate stationary electron transport in lead telluride (PbTe). Results for electron mobility as a function of lattice temperature, free carrier concentration, and electric field are compared with experimental data and the few available other Monte Carlo simulation results.

1 Introduction and Monte Carlo Simulation Setup

Material models which incorporate the basic characteristics of the underlying physics in a given semiconductor material are the core of device modeling. While for Silicon and III-V materials such models are well established, models for IV-VI materials are topic of ongoing research. The lead chalcogenides material system is of interest for optoelectronic [1] and electrothermal [2] applications.

The Monte Carlo method is a powerful technique to establish a consistent link between theory and experiments. Our model includes the two lowest valleys of the conduction band (L and W). Several stochastic mechanisms such as acoustic phonon, polar optical phonon, inter-valley phonon, ionized impurity, and optical deformation potential scattering, are considered and their impact is assessed. The particular advantage of the Monte Carlo method is that it provides a transport formulation on microscopic level, limited only by the extent to which the underlying physics of the system is included. Since the PbTe material system is yet not so well explored, several important input parameters are still not that accurately known, especially at higher temperatures. We assess, in an iterative approach, the influence of the input parameters and their interdependencies in order to get a set of parameters which gives agreement with experimental data available for different physical conditions (doping, temperature, field, etc.). Such a calibrated set of models and model parameters delivers valuable data for low-field mobility, velocity saturation, energy relaxation times, etc. These calibrated models can serve as a basis for the development of models for the simulation of PbTe-based electron devices. Device simulation results can in turn be validated against electrical device measurements.

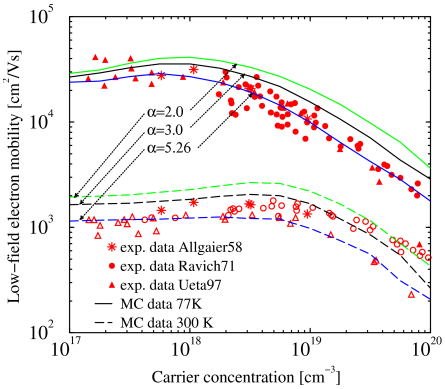

Fig. 1: Low-field electron mobility as a function of carrier concentration in PbTe: Comparison of the MC simulation results and experimental data.

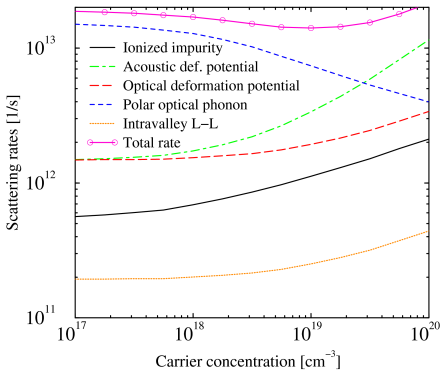

Fig. 2: Illustration of the corresponding scattering rates in our MC simulation of electron mobility in PbTe as a function of carrier concentration at 300 K.

The following calibrated set of model parameters for MC simulation was obtained in this work: energy separation between the lowest conduction bands Δ_{WL} = 0.15 + 0.04 T_0 eV (T_0 stands for the reduced temperature T/300 K); longitudinal and transverse effective electron masses in the L and W valleys $m_{L,l}$ = 0.25 + 0.11 T_0 − 0.011 T_0^2, $m_{L,t}$ = 0.024 + 0.0112 T_0 − 0.0013 T_0^2, $m_{W,l} = m_{W,t}$ = 0.5; non-parabolicity factor α = 3; acoustic deformation potential (ADP) 10 eV; mass density ρ = 8.24 g/cm^3; longitudinal and transverse sound velocities v_{sl} = 3297 − 170 T_0 − 37 T_0^2 m/s, v_{st} = 2016 − 121 T_0 − 45 T_0^2 m/s; optical and static dielectric constants ε_∞ = 428 − 40 T_0 and ε_s = 39 − 6 T_0; optic phonon energy $\hbar\omega_{LO}$ = 13.6 meV; inter-valley phonon energy $\hbar\omega_{ij}$ = 10.5 meV; inter-valley coupling constant 1.6x10^8 eV/cm; optical deformation potential (ODP) coupling constant 10^9 eV/cm;

2 Simulation Results and Discussion

Results for electron mobility as a function of lattice temperature and free carrier concentration were obtained and validated against available measured data [3, 4, 5]. Electron drift velocity versus the electric field was compared with the few available other Monte Carlo simulation results [6] and experimental data (see [6, 7] and the references therein).

Fig. 1 shows the low-field electron mobility in n-PbTe as a function of free carrier concentration at 77K (open symbols − experiment, dashed lines − simulation) and 300K (filled symbols − experiment, solid lines − simulation). The impact of the non-parabolicity factor of the L-valley is demonstrated.

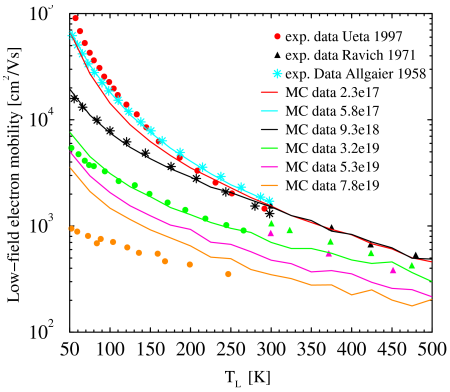

Fig. 3: Low-field electron mobility vs. lattice temperature for different carrier concentrations.

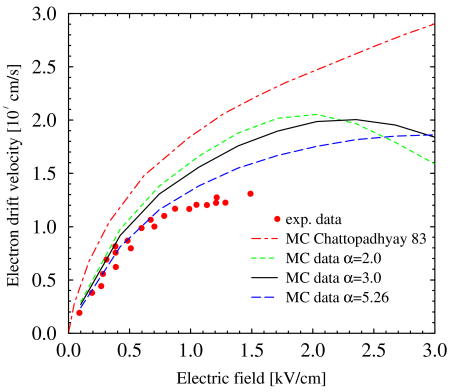

Fig. 4: Drift velocity vs. electric field in PbTe: Comparison to other Monte Carlo simulations at 77 K.

Fig. 2 illustrates the interplay of the different scattering mechanisms for MC simulation at 300K and $\alpha = 3$. As can be also seen from Fig. 3, a very good agreement between measurement and simulation is achieved for wide range of carrier concentrations and lattice temperatures. Note, that using the parameter set from previous MC simulation from [6] the mobility is overestimated at 300 K and underestimated at 77 K. Including ODP scattering and reduced ADP to 15 eV, as proposed in [8] is a step in the right direction. In addition, in our simulation setup we had to secure temperature-dependent sound velocities and set ADP to 10 eV to further decrease the influence of ADP scattering at 77 K; we use temperature-dependent dielectric constants in the polar optical scattering model; we suggest higher ODP coupling coefficient than in [8]. A non-parabolicity factor of $\alpha = 3$ gives better results than the inverse bandgap value. Fig.4 gives the electron drift velocity versus the electric field. The low field data points are in good agreement, at higher fields we suggest either higher electron masses in the W-band or higher inter-valley scattering, etc., rather than higher ADP scattering in the L-band.

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