Monte Carlo Simulation of Electron Transport in PbTe

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A Monte Carlo (MC) technique is employed to investigate stationary electron transport in lead telluride (PbTe). Our model is validated by comparing its results with measured data from the literature. While for Silicon and III-V materials similar models are well established, for IV-VI materials the model development is still a topic of ongoing research. The lead chalcogenides material system, in particular, is of interest for lasers and detectors operating in the mid-infrared [1] and for 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, and ionized impurity scattering, are considered and their impact is assessed. The particular advantage of the MC method is that it provides a transport formulation on a 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. Results for electron mobility as a function of lattice temperature and free carrier concentration were obtained and compared to measured data [3,4]. The electron drift velocity versus electric field was compared with the few available other Monte Carlo simulation results [5,6] and with experimental data (see [5] and the reference therein).

As a particular example, Figure 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 (alpha) of the L-valley is demonstrated.

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