Accurate Yet Efficient Modelling of Inelastic Hole-Acoustic Phonon Scattering in Monte Carlo Transport Simulations

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Acoustic phonon scattering is known to play an important role in accurately describing hole-transport in semiconductors such as Si and Ge. However, it has always been difficult to treat accurately in Monte Carlo transport simulations due to its complex dispersion relationship, thus it has been often only been treated in a very approximate manner. Here we present an efficient approach for handling inelastic acoustic phonon scattering taking into account the full dispersion relationship. Our methodology makes no assumptions about the carrier distribution function, thus it is suitable for application in modern CMOS device simulations and is able to reproduce accurately the velocity-field characteristics over a wide range of temperatures (see Fig. 1), satisfying simultaneously the requirements of detailed balance.

A frequently employed approximation is the elastic equi-partition approximation. However, this is not well suited for the modelling of hole transport [1], as acoustic phonon scattering is important for the accurate modelling of inter-band scattering between the light and heavy hole bands [2]. One approach in overcoming the elastic approximation takes an average of the acoustic phonon energies and the corresponding momentum transfer [1]. However, the averaging procedure relies on knowledge of the carrier distribution, which is difficult to accurately estimate numerically, in Monte Carlo transport simulations and can vary significantly through in contemporary CMOS devices [3]. The employment of an average momentum transfer <**q**> means the scattering rate no longer has an explicit dependence on **q**. Previous authors [4,5] have noted that this can be an important effect in the warped valance bands of Si and Ge, for an electric-field in the <100> or <111> directions, where acoustic phonon scattering for the heavy-hole is predominately back-scattering. However, for the <110> direction this is not the case, due to the anisotropic nature of the bandstructure (see Fig. 2) and is consistent with the observation that the <110> direction has the highest mobility in Ge as demonstrated in Fig. 3. The methodology we propose here overcomes all of these potential difficulties yet still maintaining computational efficiency. The scattering rate has the following form:

$$\Gamma_{ac}(\mathbf{k}) = \frac{\left(\Delta_{ac}^{\alpha}\right)^2}{4\pi\rho} \int \frac{\mathbf{q}^2}{\omega^{\alpha}(\mathbf{q})\mathbf{k}\mathbf{k}'} d\mathbf{q} \left(N_{ac} + \frac{1}{2} \pm \frac{1}{2} \right) I^2_{\mathbf{k},\mathbf{k}'} \left| \frac{d\mathbf{k}'}{dE(\mathbf{k}')} \right|_{\mathbf{k}=\mathbf{k}'} \delta\left(E(\mathbf{k}') - E(\mathbf{k}) \pm \hbar\omega^{\alpha}(\mathbf{q}) \right)$$

The limits of integration over **q** are carefully chosen to ensure conservation of energy and momentum for the particular acoustic mode, α (one longitudinal and two transverse). These can easily be calculated at the beginning of a simulation and stored for maximum efficiency. The acoustic phonon velocities are obtained by taking an average over all directions, obtained from a solution of the Christoffel equation [6]. Fig. 4 shows the inverse velocities for the different acoustic modes in the *x*-*y* plane for Ge.

Fig. 5 shows the mobility for two different orientations calculated using elastic and inelastic acoustic phonon scattering, showing a difference for the (001) substrate orientation. By considering the occupation of the heavy hole band shown in Fig. 6, this suggests that the decrease in interband transitions plays a significant role in the resulting transport.

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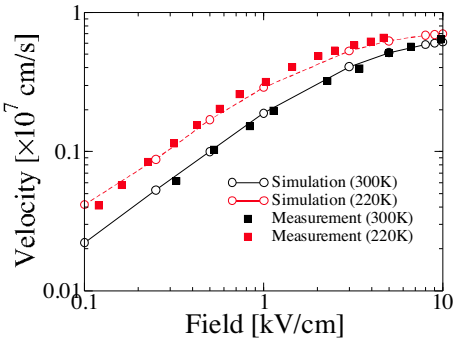

Fig. 1 Velocity field characteristics at 220K and 300K, showing close agreement between simulation and experiment, using a single set of phonon parameters

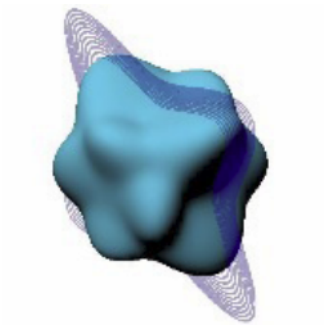

Fig. 2 Energy isosurface for the heavy hole band at .1eV. calculated using 6-band k•p with energy contours out to 2eV.

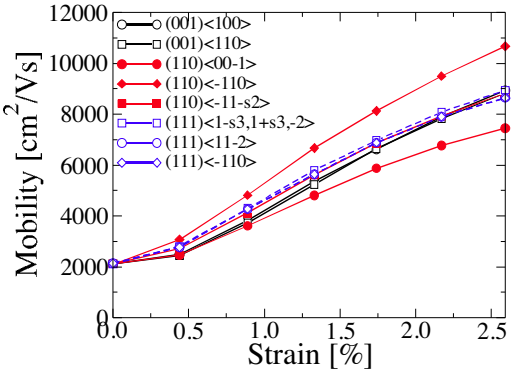

Fig. 3 Mobility in undoped Ge as a function of strain and orientation showing the preferential combination to be <-110>(110).

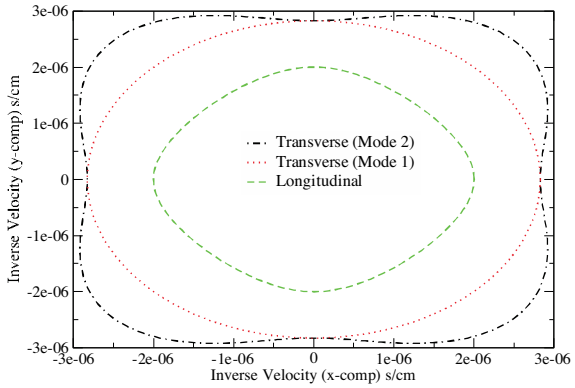

Fig. 4 Inverse velocities for different phonon modes in the x-y plane for relaxed Ge.

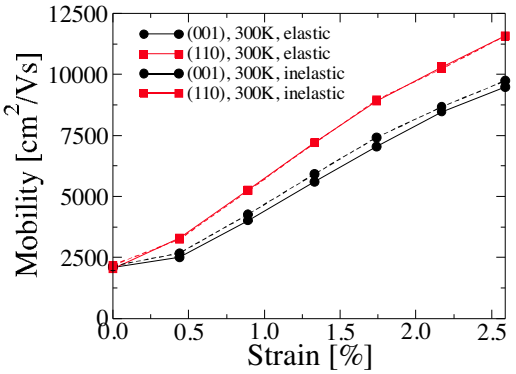

Fig. 5 Mobility as a function of strain in Ge at 300K for the [110] cannel orientation on (001) and (110) surfaces using elastic and inelastic acoustic phonon scattering.

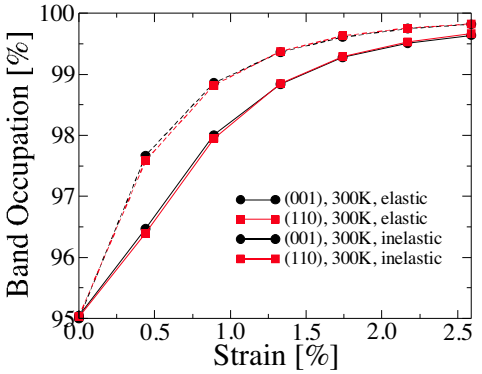

Fig. 6 Occupation of the heavy hole band for the same simulations as in Fig. 5, showing a significant difference based on the approach used for acoustic phonon scattering.