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Full-Band Monte Carlo Simulation of High-Energy Transport and Impact Ionization of Electrons and Holes in Ge, Si, and GaAs

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It is common practice in the calibration of Monte Carlo simulations to extrapolate the low-energy carrier-phonon matrix elements, extracted from mobility data, to high energy and to rely on empiricals impact-ionization rates, such as the Keldysh formula, in order to reproduce the ionization coefficient. This procedure is usually criticized for not providing a unique (and necessarily physically correct) solution to the 'calibration' problem. In this work we report results obtained by following a different strategy. We have computed the rate for impact ionization *ab initio*[1][2] and have employed this rate in full-band Monte Carlo simulations[3] in order to determine the high-energy carrier-phonon deformation potentials. This strategy is motivated by the case of electron transport in Si, for which a satisfactory agreement has been reached recently between theoretical[4][2] and empirically determined[3][5] electron-phonon and impact-ionization scattering rates.[6] These results stress the weak energy-dependence of both the electron-phonon and the Coulomb matrix element and the validity of the *random-k*[7] approximation for the impact ionization process.

We have considered transport and impact ionization of electrons and holes in Ge, Si, and GaAs, the valence bands being treated with nonlocal empirical pseudopotentials and spin-orbit interaction. The impact ionization rates have been computed using three different approximations: 1. the *ab initio* rate, which accounts for energy and momentum conservation and for the dependence of the Coulomb matrix element on both initial and final states, 2. the constant-matrix-element (CME) approximation[8], which employes a constant Coulomb matrix element, and 3. the *random-k* approximation, which relaxes momentum-conservation.

Our main results are, obviously, the carrier-phonon and ionization rates we have determined. Surprisingly, for such cases (Ge, GaAs holes), ionization rates had never before been studied. Additional results are the following:

1. Regarding impact-ionization, the random-k approximation is surprisingly accurate in all cases, with the notable exception of hole-initiated processes in Si. Thus, *Umklapp* processes appear to render the constraint posed by momentum conservation a minor one, compared to energy-conservation and availability of final states. Preliminary results for InAs and $In_{0.53}As_{0.47}As$ indicated that this fortunate situation may not persist in the case of small- and direct-gap materials having high-energy satellite valleys.
2. The electron-phonon deformation potentials required to reproduce the experimental ionization coefficient vs. electric field must be, in general, different in various bands: The matrix elements for intraband processes in the lowest-energy band, fitted to the ohmic mobility and saturated velocity, are unchanged with respect to those previously published[9], but those for all inter-band processes and intraband processes within higher-energy bands are lower (with the exception of electrons in Si).
3. Most notably, a unique choice of the acoustic and optical deformation potentials in the valence bands has enabled us to reproduce remarkably well both the low-field behavior (*i.e.*, the ohmic mobility at 300K) and the ionization coefficient. These deformation potentials are in good agreement with the values calculated from the elastic constants[10] and valence-band deformation potentials d_0[11].

References

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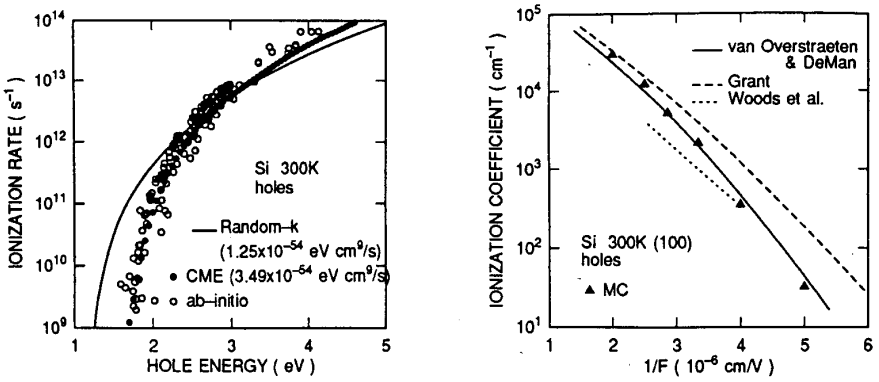

Figure 1: Calculated impact ionization rate (left) and coefficient (right) for holes in Si. Note the failure of the random-k approximation in this case, while the agreement of the *ab initio* results with the constant-matrix-element (CME) indicated the weak dependence of the Coulomb matrix element on energy. Its average value for each approximation (CME and random-k) is also indicated in parentheses. The ionization coefficient, also compared to available experimental data, has been obtained using the *ab initio* ionization rate, averaged over equi-energy shells, and an acoustic deformation potentials Δ_{ac} = 4.6 eV, and an optical deformation potential $(DK)_{op}$ = 6.6 x 10^8 eV/cm. These values yield a low-field mobility of about 500 cm^2/Vs at 300K.

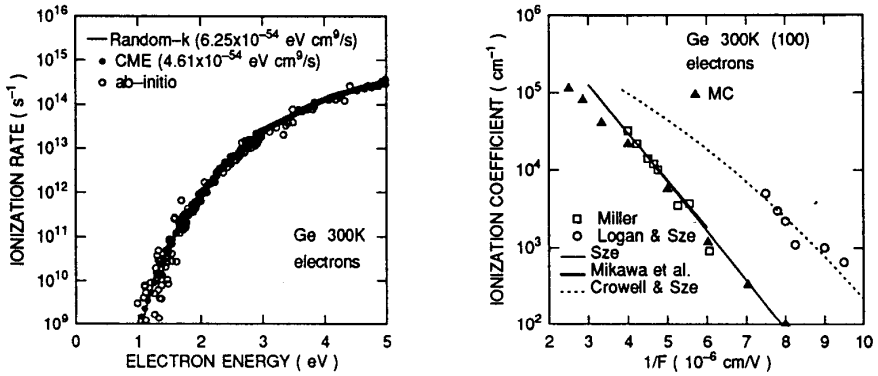

Figure 2: Calculated impact ionization rate (left) and coefficient (right) for electrons in Ge. Note the excellent validity of the random-k approximation in this case. The ionization coefficient, compared to available experimental data, has been obtained using the random-k ionization rate and an acoustic deformation potential deformation potentials Δ_{ac} = 1.5eV, and an optical deformation potential $(DK)_{op}$ = 2.0 x 10^8 eV/cm for intraband transitions within the lowest-lying conduction band, Δ_{ac} = 1.0eV and $(DK)_{op}$ = 1.5 x 10^8 eV/cm in all other cases. These values yield a low-field mobility of about 4500 cm^2/Vs at 300K.

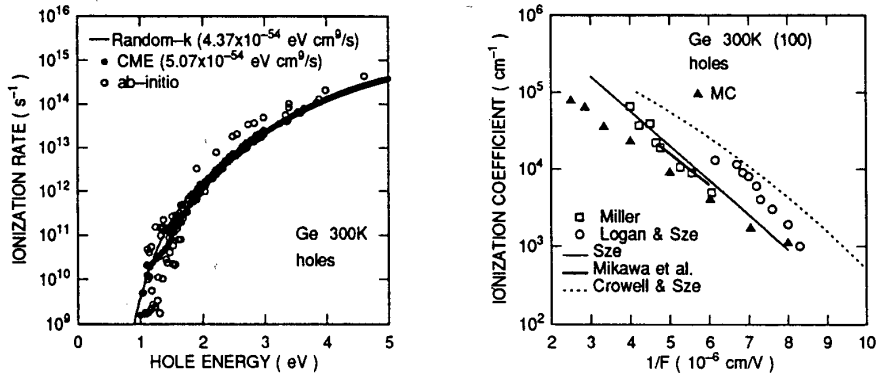

Figure 3: Calculated impact ionization rate (left) and coefficient (right) for holes in Ge. As in the case of electrons, the random-k approximation is very satisfactory. The ionization coefficient, also compared to available experimental data, has been obtained using the random-k ionization rate and an acoustic deformation potential deformation potentials Δ_{ac} = 4.6 eV, and an optical deformation potential $(DK)_{op}$ = 9.0 x 10^8 eV/cm. These values yield a low-field mobility of about 2100 cm^2/V s.