Numerical Methods for the Deterministic Solution of the Boltzmann Transport Equation in Semiconductors and Insulators

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The subject of this research is the development of a numerical method for the deterministic solution of the Boltzmann Transport Equation in silicon devices. The main motivation for it is the necessity to reach a trade-off between minimizing CPU-time consumption in the simulation of two or three-dimensional devices, and the necessity of knowing the carrier-distribution function at high energies.
In the past years this method has been enriched with several scattering mechanisms, which are relevant for the correct modeling of electron transport in silicon, and with the silicon full-band structure in terms of density of states and group velocity for both the conduction and the valence band. After the full-band structure has been implemented, the most relevant scattering models have been adapted to it for both electrons and holes. The results reproduce with good accuracy the available experimental data. Furthermore the temperature dependence has been studied in order to correctly reproduce the main transport properties for a wide range of temperatures. As far as silicon dioxide is concerned, a first-order investigation of the transport and energy-loss processes has been worked out as well, still in the frame of the spherical-harmonics solution of the Boltzmann Transport Equation. The relevant scattering mechanisms have been modeled: both the polar and non-polar electron-phonon scattering mechanisms have been considered. The scattering rates for each contribution have been analyzed in comparison with Monte Carlo data. The investigation showed a good agreement with experiments for the calculation of mobility and mean energy in the low-field regime and for different temperatures. A more accurate description of the bands at higher energies has been carried out by tackling the calculation of the full-band structure of SiO_2. As the amorphous SiO_2 shows a number of electronic and optical properties in common with some silica polymorphs, a selected set of crystals have been analyzed. *Ab initio* calculations of the full-band structure have been worked out by means of two different techniques: Hartree-Fock (HF) and Density-Functional Theory (DFT). Accurate calculations of both valence and conduction band structures, of the corresponding densities of states (DOS), have been carried out.
Then, the analysis of the interface between the silicon and silicon dioxide has been tackled with, in the two-dimensional case, in order to fully simulate MOSFET devices. **Presented by Massimo Rudan**