3D Parallel Full Band Ensemble Monte Carlo Devices Simulation for Nano Scale Devices Application

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A 3D parallel full band ensemble Monte Carlo device simulator is developed for simulation of nano scale semiconductor devices especially for the non planar structures.

In the simulator, the full band structure of Si, Ge and GaAs are calculated by the non-local empirical pseudo-potential approach including spin-orbit interactions [1]. Four conduction bands and three valence bands are considered for Si and Ge. The transition rates for the various scattering processes are calculated based on Fermi's golden rule. The acoustic and optical phonon scattering with both intra- and inter-valley transition are considered. The interaction between phonons and electrons and holes is described in the deformation-potential approach as presented by Jacoboni et al. [2]. Ionized impurity scattering is treated via the screened Coulomb potential in the Brooks-Herring approach [3]. Surface related scattering including remote coulomb scattering, surface roughness scattering and surface phonon scattering are modeled as [4]. The impact ionization is included as a kind of scattering. In order to consider the quantum effect, quantum correction has been included using the effective potential (EP) method [5]. 3D Poisson equation with non uniform hexahedron grid is solved self-consistently after the carriers' free flight and scattering. The MC method and the physical model are well verified and calibrated [6]. Usually the computing resource both of the CPU time and the memory is the big challenge for the 3D MC simulation. Here we parallelize the 3D MC device simulator by utilizing the Trillions [7] software package. By using the Trillions laboratory, the parallel execution issues such as processors communication, grid partitioning and load balancing are handled easily and efficiently.

The physical model and MC method including parallelization will be described in detail. The parallel efficiency will be evaluated. By using the simulator, the performance of various new structures such as Si and Ge GAA MOSFETs, Tri-gates MOSFETs, bulk FinFETs, Silicon-on-Thin-Box MOSFETs are investigated. The impacts of surface related scattering on the new structures in nano scale are evaluated. The results can help in optimize the new development devices especially for the non planar structures.

Reference:

[1] J. R.Chelikowsky and Marvin L. Cohen, Phys. Rev. B 14, 556 1976
[2] Jacoboni C, et al. Rev. Mod. Phys., 645, 55, 1983.
[3] A.T. Pham, et al. ESSDERC, pp. 293-296, 2005.
[4] J.Appl. Phys. 75(1), 1994, p297
[5] R. Thoma, , J.Appl.Phys. 69(4), 1991, p2300-2311
[6] Du G.,IEEE Trans. Electron Devices, vol. 52, p. 2258, 2005.
[7] http://trilinos.sandia.gov/license.html