Interplay between the Electrical and Thermal Transport of Silicon Nanoscale MOSFETs

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***Abstract*—In this report we introduce our newly developed 3D full-band particle Monte Carlo (MOCA3D) simulator with full electron and phonon dispersion and use it to investigate the electro-thermal behavior of Silicon-on-Insulator n-channel MOSFET.**

I. Introduction

The invention of transistors and integrated circuits has led to the advent of a new era in which humanity has experienced remarkable enhancement and overall productivity in our day-to-day living. From the way in which we communicate to the way we receive healthcare, computer technology has noticeably improved our efficiency. The key to this success has been the advancement in the field of chip design. In 1965, Gordon Moore predicted that the number of transistors in integrated circuit chips doubles every two years. Upholding this trend has led designers to progressively scale transistor size in order to cramp more of them into a single chip. The relentless push for scaling, as dictated by Moores law, has successfully led to packing over a billion transistors into a single chip. Such dense packing has led to performance improvement, increased functionality and overall cost reduction of electronic devices which permeate our everyday life.

However, as all good things come to an end, the march to transistor miniaturization is stumbling over technical and physical barriers. Increased power dissipation is among the top ill-favored consequences of the surge in transistor count per generation. Based on the data reported in [moore], on-chip power density has already exceeded that of a nuclear power at 100 W/cm^2. As a result, thermally conscious blueprints has become in recent years the focal concern of semiconductor roadmaps, at all design phases, as the temperature at the chip level and within a single transistor rises for future electronic devices. Without proper thermal management, inordinate power dissipation can potentially bring an end to integrated circuit functionality.

In this regards, there is substantial interest in designing simulation tools which thoroughly couple accurate electrical and thermal transport models. While there has been several works reported on electron transport (e.g. [1], [2], [3]) and thermal transport models (e.g. [4], [5]), there has been disproportionately less limelight, until recently, in coupling both transport models, especially within the device (electronic) community [6], [7], [8], [9], [10], [11].

In this report we present a 3D full (electron and phonon) band particle Monte Carlo (MC) simulator with 2D quantum correction to investigate the electro-thermal behavior of Tri-gate MOSFET. The self consistent coupling entails feeding the heat generation obtained from our 3D quantum corrected Monte Carlo to a thermal Monte Carlo which dissipates the anharmonic phonon processes. Anharmonic three-phonon decay and the use of full dispersion facilitate a detailed description of heat transfer and the determination of temperature map in nanoscale devices. The temperature map obtained from the heat transport model is fed back to the particle Monte Carlo with temperature dependent scattering table in a self-consistent manner.

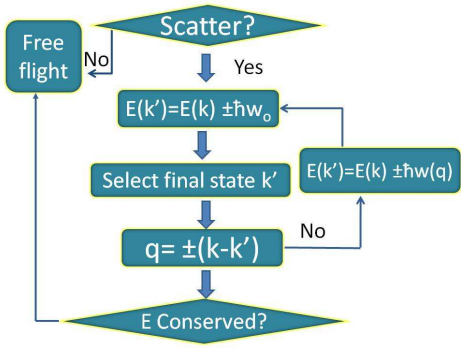

Fig. 1: Flowchart showing the details of the final state selection with the full phonon dispersion. This algorithm is applied at each iteration in order to ensure energy conservation with the phonon dispersion which is tabulated from the adiabatic bond charge algorithm

II. Simulation Model

A. Electrical Transport

The electrical simulation presented in this work were obtained from augmenting the self-consistent three-dimensional ensemble Monte Carlo program (MOCA 3D) developed at the University of Illinois [12], [13]. The numerical bandstructure of silicon is obtained from a local pseudo-potential solution approach [14], and it is used to create tables for the energy dispersion, the carrier group velocity, and the density of states. To insure accuracy of results for phonon events, a full phonon dispersion is included. It is calculated from an adiabatic bond charge model and tabulated for lookup [15]. Fig. 1 shows the details of the final state selection algorithm utilized for the full phonon dispersion. This algorithm is employed at each iteration to ensure energy conservation with the tabulated full-phonon dispersion. The simulator accounts for various scattering mechanisms such as phonon, carrier-carrier, impact ionization, and surface roughness scattering. In addition, the

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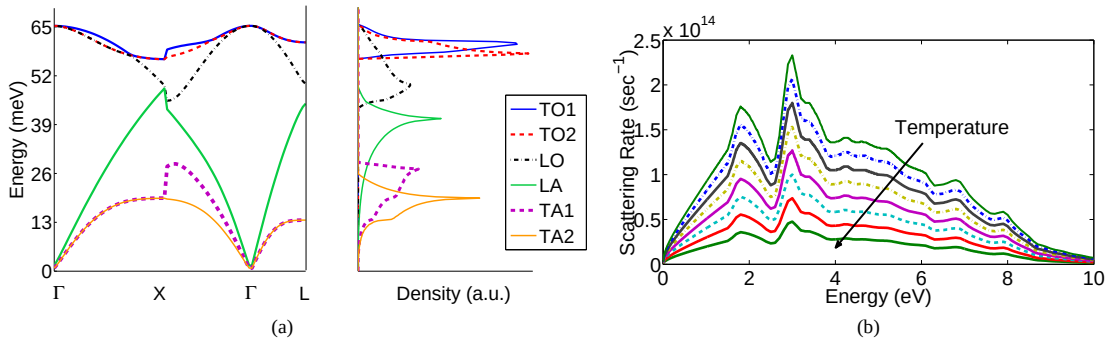


Fig. 2: The coupled electro-thermal simulation uses full phonon dispersion data (top) and temperature dependent scattering rate (bottom)

total scattering rate is adjusted so that at high energies it follows the density of states.

In order to capture 2D confinement inherent in quasi-1D device structures, the 3D Poisson equation is self-consistently coupled with a 2D Schrödinger equation. The details of this approach are thoroughly described in reference [2], in which the 2D Schrödinger equation is solved along the cross section for each slice along the channel. The quantum potential obtained from this approach produces a field which repels electrons from the interface to force the shape of the quantum density.

B. Thermal Transport

We employ the Monte Carlo method to study the anharmonic transport of the phonons generated by the electrical simulation. The process starts by employing the Monte Carlo to select the length of free flight for each phonon in the simulation and to select the momenta of the pair of phonons generated by 3-phonon interactions. The first of these two steps starts when a phonon is generated by the electron scattering. The average life-time of optical phonons is known from previous studies and measurements [9], and can be estimated to be around 2 ps for optical phonons at room temperature. The probability of a particle to stay in its present state is described by the Poisson process so the time of phonon decay can be chosen stochastically by using the Monte Carlo method [16]. This gives the time of phonon decay as:

$$\tau_{decay} = ln(r)\tau_{anh} \tag{1}$$

where τ_{anh} is the lifetime of the phonon due to 3-phonon anharmonic decay, and r is a random number uniformly distributed on the unit interval. Once the time of the decay process is found, then we must search for a final state. This second step is accomplished using the rejection algorithm on the probability distribution for anharmonic decay including the matrix element [17]. The probability distribution for anharmonic decay was obtained by Klemens using time dependent perturbation theory as the product of anharmonic matrix element for the three phonon processes and a time dependent resonance factor:

$$P(q,q') = |\langle q|H'|q'\rangle|^2 \frac{1-\cos(\triangle wt)}{\triangle^2 t} \tag{2}$$

where $\triangle w(q) = w(q) - w(q') - w(q'')$ is the net energy exchange between the initial phonon momentum (q) and the final states (q', q'') and H' is the perturbing hamilitonian due to cubic anharmonicity. The rejection algorithm starts starts by estimating possible pair of final state generated by the anharmonic decay processes– q' is chosen randomly from a uniform distribution in the first Brillouin zone, while the second final state (q'') is determined by ensuring momentum conservation:

$$q'' = q - q' \pm G \tag{3}$$

To determine whether the pair of of final states is accepted, a random number (r_{rej}) uniformly distributed in the unit interval is generated and compared to the probability $P(q,q')$. The pair of final state is rejected if $P(q,q') < r_{rej}$, and a new pair is searched. Finally, once the final state is determined, the phonons are transported until the end of simulation without undergoing any further anharmonic decay.

III. Coupled Electro-thermal Result

In the transistor level, heating is established when immensely energetic electrons, exiting the highly resistive channel, relax by giving off their excess energy to the crystal through electron-phonon interactions. Particularly, the effectual energy relaxation mechanism for energetic electrons is to couple with high frequency optical phonon. Nonetheless, optical phonons have insufficient group velocity imperative for efficient heat transport and hence this process promotes the confinement of thermally nonequilibrium distribution of hot optical phonon at the vicinity of the source-drain region. The excess phonon population eventually diffuse out as the optical modes slowly decay into acoustic phonon mode with higher group velocity. As such, the coupling between electrons and optical phonons, and the subsequent decay of optical phonons towards equilibrium, are found to play a large role in determining the temperature distribution in silicon devices.

Fig. 2 and 3 summarize the electo-thermal coupling process. As shown in the flow diagram in Fig. 3a the self

consistent coupling entails feeding the heat generation obtained from our 3D quantum corrected Monte Carlo to a thermal Monte Carlo which dissipates the anharmonic phonon processes. The Anharmonic three-phonon decay and the use of full dispersion (Fig. 2a) facilitate a detailed description of heat transfer and the determination of temperature map in nanoscale devices. The temperature map obtained from the heat transport model is fed back to the particle Monte Carlo with temperature dependent scattering table (Fig. 2b) in a self-consistent manner until convergence criterion is met.

The device structure presented in this paper is an n-channel gate-all-around MOSFETs with $20nm$ gate length. Devices of cross-section size ranging between 10 and $30nm$ were considered in this study. The source and drain are doped with $N_D = 10^{20} cm^{-3}$ with the S/D junctions ending abruptly at the gate edge. The silicon fin was lightly doped to $N_A = 10^{16} cm^{-3}$. Once the electro-thermal simulation is completed, we are able to generate the temperature map of the device.

In Figure 2 (a), we compare the drain current variation for our 3D Monte Carlo with and without thermal coupling. It is evident that the drain current degrades in the thermally coupled MC due to the influence of temperature dependent scattering rate on carrier transport. Fig. 5 show the temperature distribution profile of gate-all-around structure considering anharmonic phonon decay as we vary the square-crossectional length. Results, demonstrate the proliferation of the peak temperature rise as we reduce the cross-section and that the hot spot radiates more outward into the drain. The reduction of the cross-section in essence traps more carriers in the narrow channel that are unable to diffuse out of the device efficiently due to the low thermal conductivity of the oxide regions.

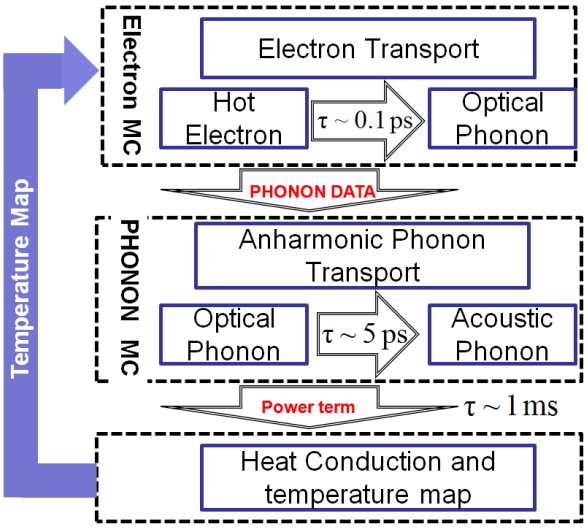


Fig. 3: Flow chart demonstrating the approach we use in thermal Moca to couple both the electrical and phonon transport models.

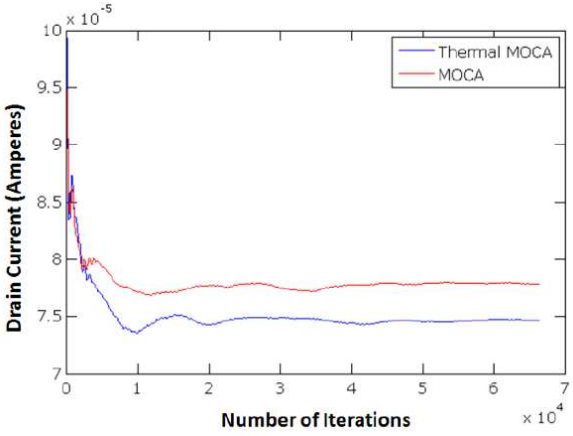
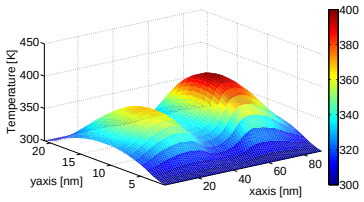
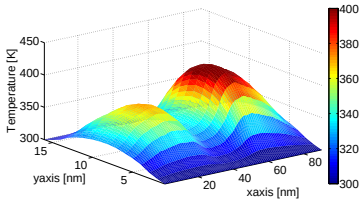


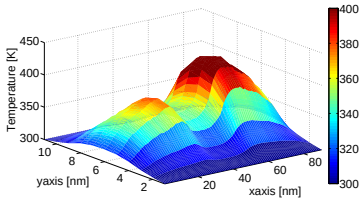
Fig. 4: Convergence of the drain current for the quantum corrected electrical MC vs. the coupled thermal MC.



(a)



(b)



(c)

Fig. 5: Temperature distribution of a GAA structure with square cross-section of a) $5nm$, b) $10nm$ a $20nm$ at an applied bias $V_G = V_D = 0.5$V.The channel region range is from $x = 35$ to $x = 55nm$

IV. Conclusion

A coupled electro-thermal simulator was developed and successfully integrated to our in-house quantum corrected 3D Monte Carlo simulator. A key feature of this tool is the inclusion of full-phonon dispersion and anharmonic phonon

decay processes. The adequacy of the simulator in addressing thermal issues at the nanoscale is confirmed by simulating thermal degradation in gate-all-around mosfet of narrow cross-sections. The current degradation shown here confirm the need to include thermal effects in simulating nanoscale electronic devices.

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