

# An Advanced Electro-Thermal Simulation Methodology For Nanoscale Device

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**Abstract**—In this work we propose an advanced electro-thermal simulation methodology for nanoscale devices based on a macroscopic model for acoustic and optical phonon energy transfer. This is coupled with the Poisson equation and Current Continuity Equations (CCE) and solved self-consistently. This has been implemented in the GSS ‘atomistic’ simulator GARAND, and the coupled 3D electro-thermal simulation using this methodology is demonstrated on an SOI FinFET example.

**Keywords**—self-heating effects; FinFET; thermal transport; phonon

## I. INTRODUCTION

With the continuous scaling of semiconductor transistors down to the nanoscale regime, further driven by emerging novel architectures such as FinFETs, thermal transport has become one of the major concerns in terms of performance and reliability. Modelling and analysis of self-heating effects in nanoscale devices such as FinFETs has attracted increasingly more interest [1-3]. The schematic of a Silicon-on-insulator (SOI) FinFET is shown in Fig.1.

Recently we have developed a thermal simulation module [4], implemented in the GSS ‘atomistic’ simulator GARAND [5], based on the solution of the coupled Heat Flow, Poisson, and Current Continuity Equations (CCE). We investigated the impact of self-heating on the statistical variability of some FinFET examples [6-7]. In this work, we are going to further investigate an advanced methodology and incorporate it into GARAND for electro-thermal simulation of FinFETs.

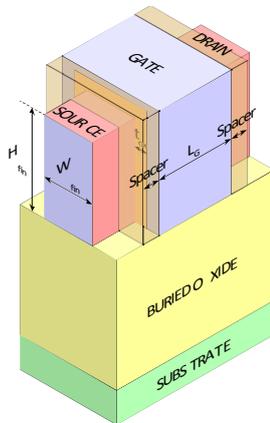


Fig. 1. The schematic view of an SOI FinFET structure.

## II. ADVANCED MODEL AND METHODOLOGY

The advanced electro-thermal simulation methodology for nanoscale devices is based on a macroscopic model [8]. The model for acoustic and optical phonon energy transfer can be written as

$$C_o \frac{\partial T_o}{\partial t} = \frac{3nk}{2} \frac{T_e - T_o}{\tau_{e-o}} + \frac{nm_e v_d^2}{2\tau_{e-o}} - C_o \frac{T_o - T_A}{\tau_{o-A}} \quad (1)$$

$$C_A \frac{\partial T_A}{\partial t} = \nabla(k_T \nabla T_A) + C_o \frac{T_o - T_A}{\tau_{o-A}} + \frac{3nk}{2} \frac{T_e - T_A}{\tau_{e-A}} \quad (2)$$

which involves the temperature of electrons, acoustic phonons and optical phonons  $T_e$ ,  $T_A$  and  $T_o$ , and the relaxation times between them  $\tau_{e-o}$ ,  $\tau_{e-A}$  and  $\tau_{o-A}$  respectively.  $C_o$  and  $C_A$  are heat capacities respectively,  $n$  is the electron density and  $v_d$  is the drift velocity. These can be naturally implemented in Monte Carlo (MC) simulation, however at the cost of long computational time. If focusing on the stationary state, these equations can be simplified. Starting from the energy transfer equations, a new equation in the form of a new heat flow equation can be derived, which includes the terms about  $T_e$  and  $T_A$ .

$$\begin{aligned} \nabla(k_T \nabla T_A) &= -C_o \frac{T_o - T_A}{\tau_{o-A}} - \frac{3nk}{2} \frac{T_e - T_A}{\tau_{e-A}} \\ &= -C_o \left( \frac{3nkT_e + nm_e v_d^2 - 3nkT_A}{2\tau_{e-o} C_o + 3nk\tau_{o-A}} \right) - \frac{3nk}{2} \frac{T_e - T_A}{\tau_{e-A}} \end{aligned} \quad (3)$$

where  $n$  is the electron density,  $v_d$  is the drift velocity, and  $C_o$  is heat capacity. This can be coupled within a Drift-Diffusion framework, which is more computationally efficient. Poisson's equation is:

$$\nabla \cdot \varepsilon \nabla (\psi - \theta) = -q(p - n + N_D^+ - N_A^-) \quad (4)$$

where  $n$  and  $p$  is the electron and hole density,  $N_D^+$  and  $N_A^-$  are ionized donor and acceptor impurity concentrations.  $\theta$  is the band structure parameter for the material:

$$\theta = \chi + \frac{E_g}{2q} + \frac{kT_L}{2q} \ln \left( \frac{N_c}{N_v} \right) \quad (5)$$

where  $\chi$  is the electron affinity of the material,  $E_g$  is the bandgap energy,  $N_c$  and  $N_v$  are the effective conduction and valence band density of states.

The electron current density under the influence of temperature gradient can be written as:

$$J_n = qn\mu_n E_n + k\mu_n T_A \nabla n + k\mu_n n \nabla T_A \quad (6)$$

where  $\mu_n$  is the electron mobility,  $k$  is Boltzmann constant. Note the equation for holes can be formulated in a similar way. The unipolar current continuity equation is:

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot J_n - U_n \quad (7)$$

where  $U_n$  is the net electron recombination rate.

The electrons' temperature  $T_e$  can be pre-calculated by MC simulations and a lookup table of  $T_e$  with respect to  $E$  can be constructed. Then the coupled Poisson, CCE, and energy transfer equations can be solved iteratively. At each iteration,  $T_e$  will be refreshed as well as recalculation of  $T_A$ . Thermal conductivity in the refined fin region will be modelled by a position and temperature-dependent formula. The flow chart of the methodology is illustrated in Fig. 2.

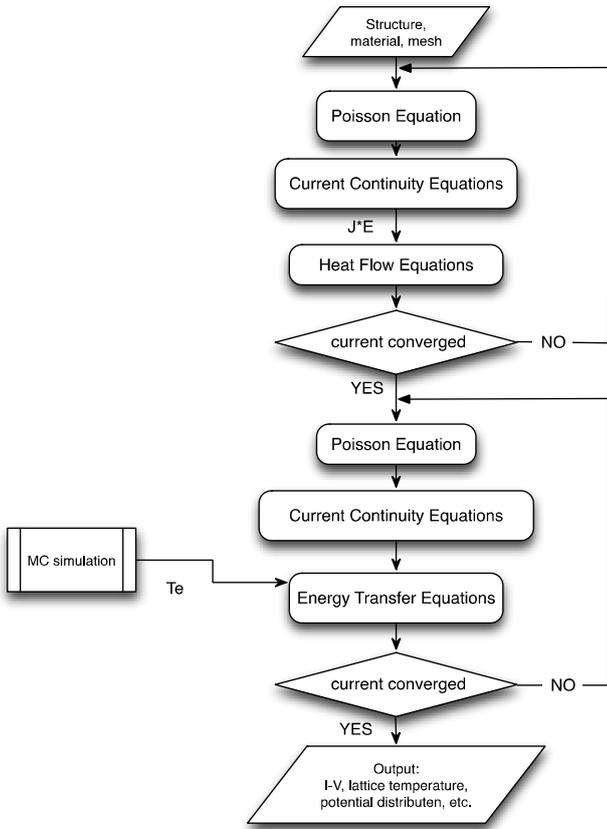


Fig. 2. Flow chart for the advanced electro-thermal simulation methodology

### III. SOI FinFET EXAMPLE

An SOI FinFET is used as a test bed for the advanced methodology. It consists of complex 3D structure and material composition, as shown in Fig. 3.

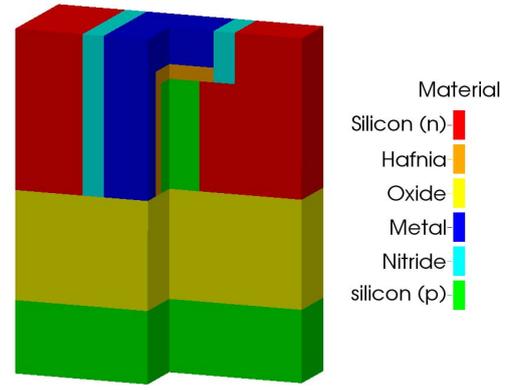
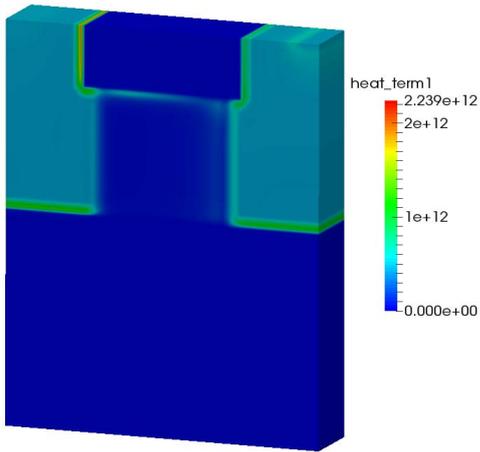


Fig. 3. Materials and structures of the SOI FinFET's electrical simulation domain, showing 3 quarters.

The channel length of this FinFET is 25 nm. The width and height of the Si fin are 12nm and 30nm respectively, while the thickness of the buried oxide (BOX) is 30nm. It has a metal gate and the equivalent oxide thickness (EOT) of the high-k gate dielectric is 0.8nm. Spacers of 6nm are introduced on both sides of the gate. The source and drain regions are highly doped with peak concentration of  $1 \times 10^{20} \text{ cm}^{-3}$  and the channel doping is  $1 \times 10^{15} \text{ cm}^{-3}$ . The supply voltage is 0.9 Volts.

Lattice temperature and potential distributions obtained from coupled Heat Flow, Poisson, and CCE are used as the initial conditions for the advanced electro-thermal simulation. Then this is followed by self-consistent solution of the coupled Poisson, CCE, and energy transfer equations. The resulting heat distribution from this advanced electro-thermal simulation methodology is demonstrated in Fig. 4. As indicated in Eqs. (1)-(3) part of the heat is transferred from  $T_e$  to  $T_o$  and then to  $T_A$ , as illustrated in Fig. 4(a). The heat related to electron velocity is illustrated in Fig. 4(b). Another part of the heat is directly transferred from hot electrons to acoustic phonons, as shown in Fig.4 (c). The distribution of electron temperature  $T_e$  is shown in Fig. 5. A hot area for  $T_e$  with peak temperature above 470K is produced in the channel, mainly because of the high fields. The resulting distribution of lattice temperature  $T_A$  is shown in Fig. 6, and the optical phonon temperature distribution is shown in Fig. 7. As the combined effects of heat generation involving the interaction between electrons, acoustic phonons and optical phonons the lattice temperature tends to spread in the fin region, with peak temperature above 360K. The potential distribution from the coupled electro-thermal simulation is illustrated in Fig. 8. The resulting Id-Vg characteristics are shown in Fig. 9. Compared to the simulation results at room temperature, the self-heating reduces the on-current from 1.24 mA/ $\mu\text{m}$  to 1.13 mA/ $\mu\text{m}$ , which means around 8.9% degradation.



(a) heat transferred from  $T_c$  to  $T_o$  then to  $T_A$

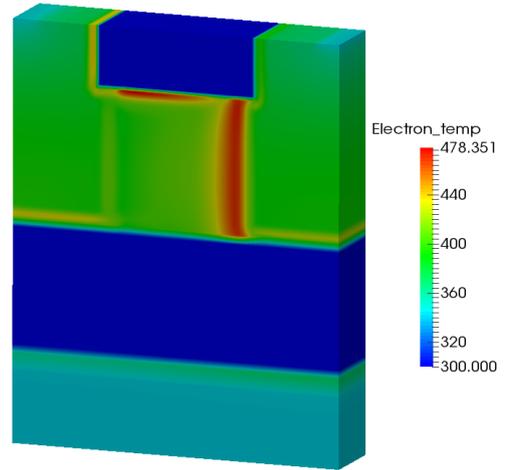
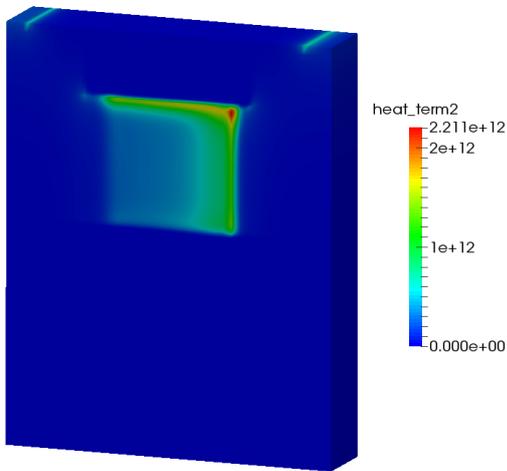


Fig. 5. The electron temperature, showing a cross-section along the channel.



(b) heat related to electron velocity.

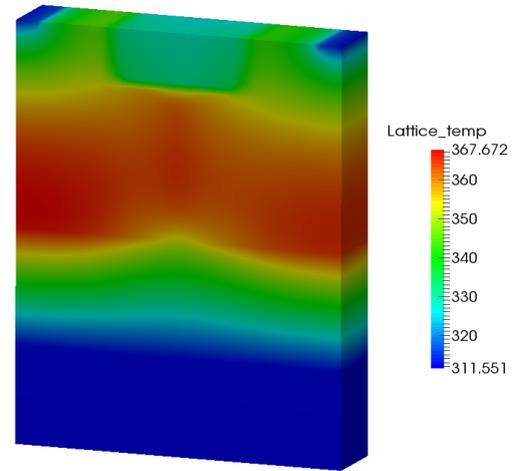
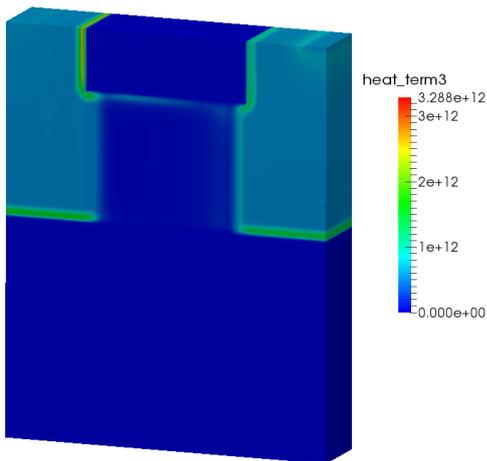


Fig. 6. The lattice temperature distribution, showing a cross-section along the channel.



(c) heat transferred from  $T_c$  to  $T_A$  directly

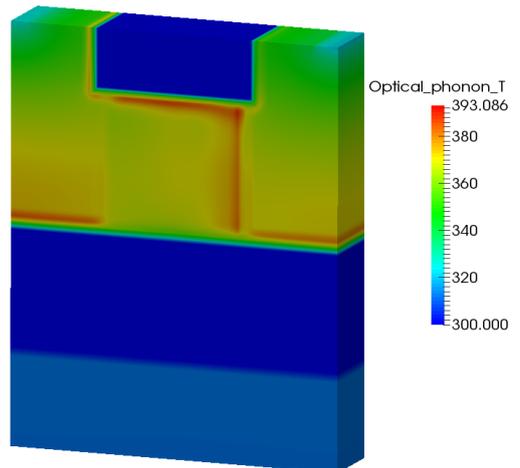


Fig. 7. The optical phonon temperature, showing a cross-section along the channel.

Fig. 4. The heat distribution, showing a cross-section along the channel.

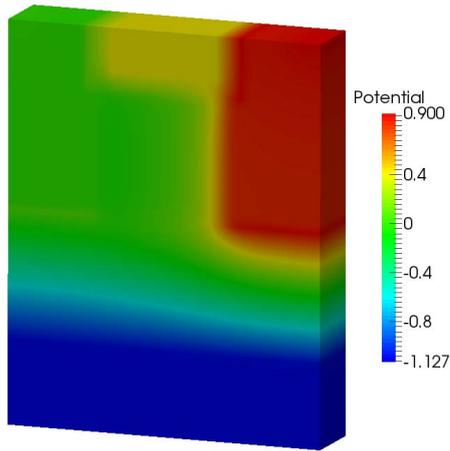


Fig. 8. Potential distribution, showing a cross-section along the channel, at high drain and high gate biases.

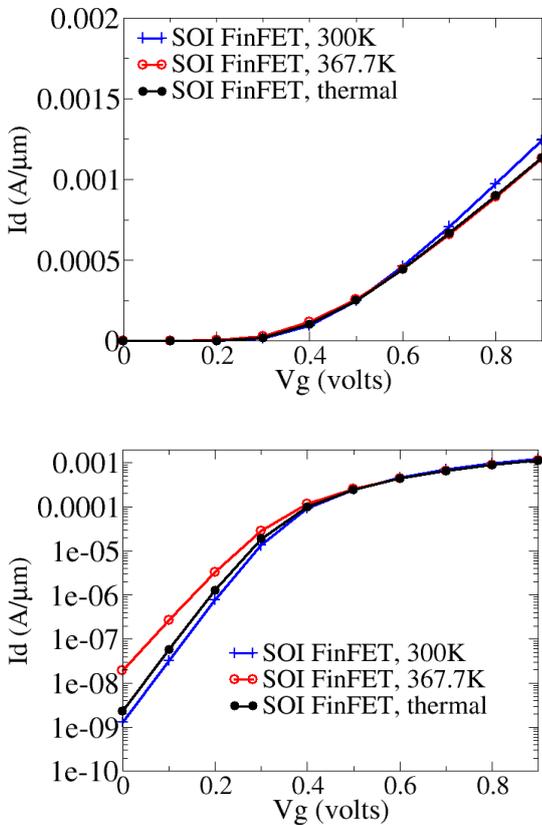


Fig. 9. Id-Vg characteristics at high drain. *Top*: linear scale; *Bottom*: logarithmic scale.

#### IV. CONCLUSIONS

Further to the development of a 3D electro-thermal simulation module, an advanced electro-thermal simulation methodology for nanoscale devices based on a macroscopic model for acoustic and optical phonon energy transfer has been implemented in the GSS 'atomistic' simulator GARAND.

An example SOI FinFET, which consists of complex 3D structure and material composition, is used as a test bed for this advanced methodology. The temperature profiles and the corresponding Id-Vg characteristics of the SOI FinFET have been simulated. The results show complex phonon scattering mechanisms are working inside the device, and as the combined shows, the lattice temperature tends to spread in the fin region. For this FinFET example, the simulation results indicate that the self-heating produces 8.9% degradation for the on-current.

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