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Electro-Thermal Models of Vertical Field Effect Transistors

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Arizona State University

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Final Report

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1.0 SUMMARY

In this document, we offer the final report of the Air Force Office of Scientific Research (AFOSR) award #FA9550-16-1-0406. An overview of the project is discussed, and the progress of the research activity is assessed, as related to the program milestones.

It should be noted, however, that it became necessary to modify the milestones and proposed research activity due to changes of collaborating personnel.

Within this project, effort has been undertaken to extend two separate types of electro-thermal models. First, a particle-particle approach which models the phonon dynamics directly, and secondly, a model where the stochastic dynamics of charge carriers (electrons and holes) is tightly coupled with an elliptic solver for a set of energy balance equations representing the mechanisms of heat generation and transport within a device and its surroundings. The latter constitutes a particle-flux approach, since electrical charge is modeled as particles while heat is modeled with a system of differential equations solving for the thermal energy flux.

2

3.0 METHODS, ASSUMPTIONS, AND PROCEDURES

The methods and procedures discussed in this section outline the development of a dedicated theoretical and computational framework that was required for the planned electrothermal simulations, the results of which are seen in section 4. First, a method that would allow us to retain the speed advantages of the CMC approach while still implementing temperature-dependent scattering rates at runtime was needed in order to perform high-quality, fast Monte Carlo (MC) electrothermal device simulations. This has been realized through the implementation of a rejection algorithm briefly discussed in section 3.1.

Section 3.2 outlines the completion of a phonons-as-particles framework which has been used in the synchronous simulation of electrons and phonons simultaneously. On the other hand, a phonons-as-flux model developed from the energy balance equation (EBE) derived from the moments of the Boltzmann transport equation (BTE) itself is outlined in section 3.3. Two separate approaches for including temperature-dependent thermal conductivities within a finite difference framework, the Kirchhoff transformation and the iterative method, are detailed in sections 3.4 and 3.5, respectively.

Finally, sections 3.6-3.8 detail the numerical details of the computational grid, boundary, and interface conditions. In particular, the inclusion of convective boundary conditions is a principle advantage of the iterative method as compared to the Kirchhoff transformation.

3.1 Rejection Algorithm for Scattering

The capabilities of the original CMC algorithm [1] have been extended through the use of a rejection algorithm. This approach retains the simulation speed advantages of the CMC scheme while allowing the adaptation of the scattering rates to the real time local conditions. Figure 2 shows the rejection algorithm flow chart in the most general case. Within the simulation framework presented here, after the CMC triggers an event with probability $g(x) = P_{CMC}$, a new scattering probability $f(x) = P_{loc}$ is computed from the values of local parameters. The rejection probability $P_{rej} = P_{loc}/P_{CMC}$ is then used in a stochastic procedure to decide whether the scattering event is accepted or rejected. This process is depicted in Figure 1.

The scattering probability after the rejection is

$$P_{k \rightarrow k'} = P_{CMC} \left(\frac{P_{loc}}{P_{CMC}} \right) = P_{loc} \quad (1)$$

where k is the initial state, and k' the final state.

3.2 Phonon Scattering Rate

Perturbation theory is used to implement both phonon-phonon and phonon-defect interactions. The anharmonic decay and recombination scattering rate based on the Klemens model [2] is given by

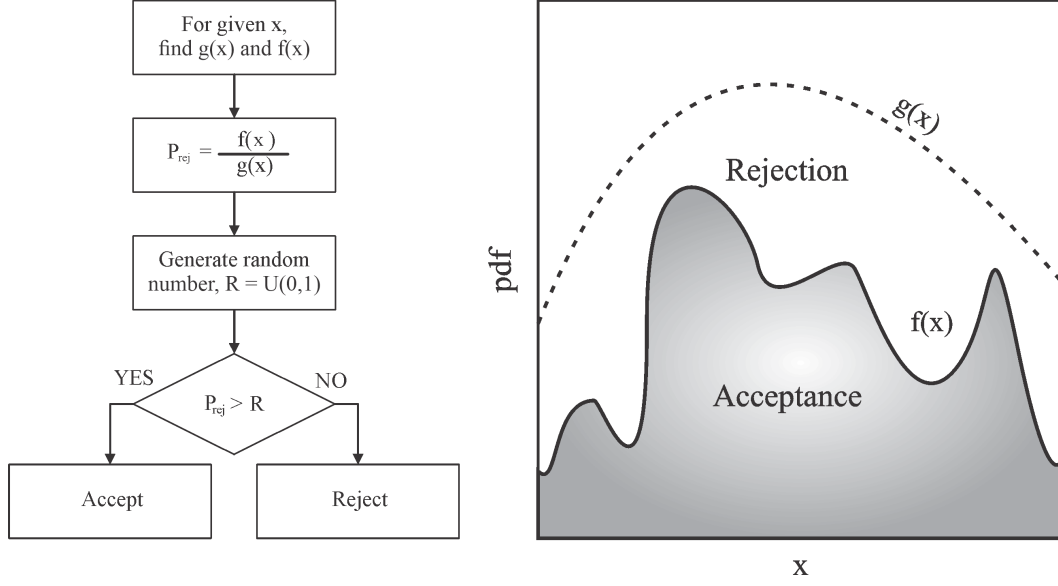


Figure 1. Flowchart For The Rejection Algorithm (Left) And Illustration Of The Rejection Method Obtaining The Correct Local Scattering Rate (Right)

$$P_{k \rightarrow k', k''} = \frac{2\hbar}{M^3} \frac{c^2(\mathbf{k}, \mathbf{k}', \mathbf{k}'')}{\omega \omega' \omega''} \delta(\omega \omega' \omega'') \delta(\mathbf{k}, \mathbf{k}', \mathbf{k}'') F_{loc} \quad (2)$$

where $F_{loc} = F(n'_{loc}, n''_{loc})$ is a local population-dependent factor, n'_{loc} and n''_{loc} are the populations at $\mathbf{k}'$ and $\mathbf{k}''$, respectively, M is the average mass, $c^2(\mathbf{k}, \mathbf{k}', \mathbf{k}'')$ is the anharmonic coefficient obtained from the perturbation Hamiltonian, and ω , ω' , and ω'' are the angular frequencies corresponding to the states $\mathbf{k}$, $\mathbf{k}'$, and $\mathbf{k}''$.

The phonon-defect scattering probability used is based on the work of Srivistava [3] and given by

$$P_{k \rightarrow k', k''} = \frac{V_W \Gamma}{6} \omega \omega' (\mathbf{e}_{\mathbf{q}}^* \cdot \mathbf{e}_{\mathbf{q}'})^2 \delta(\omega - \omega') (n'_{loc} + 1) \quad (3)$$

where $\mathbf{e}$ is the polarization vector, V_W is the Wigner-Seitz cell volume, and Γ is an expression that depends on the phonon-defect type.

Computing the local scattering probability, P_{loc} , requires estimating the local phonon populations, n'_{loc} and n''_{loc} , which F_{loc} from Equation (2) depends upon. This task requires defining a sampling volume of the particle position in both real space, V_{loc} , and momentum space, Ω_{loc} , and subsequently counting the number of simulated phonons in the volume, $\eta(\Omega_{loc}, V_{loc})$. Finally, the phonon population is obtained using the approximation

$$n_{loc} \approx \frac{\eta(\Omega_{loc}, V_{loc})}{N_{states}} = \eta(\Omega_{loc}, V_{loc}) \frac{8\pi^3}{\Omega_{loc} V_{loc}} \quad (4)$$

where N_{states} is the total number of states in the volume.

3.3 Energy Balance Equation

The particle-flux based approach that has been developed under the scope of this work is based on solving the EBE for phonons, which is derived directly from the second moment of the phonon BTE. The EBE approach, as compared to using the heat transport equation, is better suited to self-consistent coupling with the electron dynamics and allows for improved accuracy by supplying a separate solution for each phonon mode (or group of modes, e.g., the group of all acoustic modes). The phonon BTE is written as

$$\frac{\partial f}{\partial t} = -\mathbf{v} \cdot \nabla_{\mathbf{r}} f + \left. \frac{\partial f}{\partial t} \right|_{coll}. \quad (5)$$

The n th moment of the phonon BTE is obtained by multiplying Equation (5) by some function of $\mathbf{k}$, $\phi(\mathbf{k})$, and dividing by a volume of reciprocal space:

$$n_{\phi} = -\frac{1}{\Omega} \sum_{\mathbf{k}} \phi(\mathbf{k}^n) \frac{\partial f}{\partial t} - \frac{1}{\Omega} \sum_{\mathbf{k}} \phi(\mathbf{k}^n) \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \frac{1}{\Omega} \sum_{\mathbf{k}} \phi(\mathbf{k}^n) \left. \frac{\partial f}{\partial t} \right|_{coll}. \quad (6)$$

The $n = 2$ moment is found by letting $\phi(\mathbf{k}) = E(k)$, where $E(\mathbf{k}) \propto k^2$, which yields

$$\frac{1}{\Omega} \sum_{\mathbf{k}} E(\mathbf{k}) \frac{\partial f}{\partial t} + \frac{1}{\Omega} \sum_{\mathbf{k}} E(\mathbf{k}) \mathbf{v} \cdot \nabla_{\mathbf{r}} f = \frac{1}{\Omega} \sum_{\mathbf{k}} \left. \frac{\partial f}{\partial t} \right|_{coll}. \quad (7)$$

The first term here is the rate of change of the ensemble energy density in the volume Ω , and can be written as $\partial W / \partial t$ where W is the total ensemble energy density in the volume Ω , having units of $[\text{J}/\text{m}^3]$. The second term is an energy flux, $\mathbf{F}_W$, and can be approximated using Fourier's law as $\mathbf{F}_W = -\kappa \nabla T$. Finally, the collision term on the right-hand side can be split into two distinct processes which contribute to changes in the phonon energy density through changes in the phonon populations themselves: 1) the increase (or decrease) in the phonon energy density due to an electron-phonon scattering event where phonons are emitted or absorbed, and 2) the change due to phonon-phonon interactions causing the recombination of acoustic phonons to a high energy optical phonon or the decay of optical phonons to low energy acoustic phonons. In other words, they denote the heat generation rates, for the particular phonon mode due to interaction with electrons, $\partial W / \partial t|_{e-p}$, and with other phonons, $\partial W / \partial t|_{p-p}$, respectively.

Using these substitutions in Equation (7), we can write the time-dependent EBE for phonons as

$$\frac{\partial W}{\partial t} = -\nabla \cdot (-\kappa \nabla T) + \left. \frac{\partial W}{\partial t} \right|_{e-p} + \left. \frac{\partial W}{\partial t} \right|_{p-p}, \quad (8)$$

and, finally, under steady-state conditions the time derivative on the left-hand side is zero. If μ is used to denote the group of modes in each equation, and P_{μ} to represent the sum of the electron-phonon and phonon-phonon contributions, then Equation (8) becomes

$$\nabla \cdot (\kappa_\mu(\mathbf{r}, T) \nabla T) = - \left(\frac{\partial W_\mu}{\partial t} \Big|_{e-p} + \frac{\partial W_\mu}{\partial t} \Big|_{p-p} \right) = -P_\mu, \quad (9)$$

where one equation in the form of Equation (9) is obtained for each phonon mode, or group of modes, being considered.

It should be noted that ballistic heat transfer effects are not explicitly included in our model as a consequence of using Fourier's law to approximate the heat flux. This is because Fourier's law is diffusive in nature, implying the presence of scattering. However, it has been suggested that ballistic heat transfer effects can in fact be captured either through a choice of boundary conditions [4] or by solving a generalized form of Fourier's law derived using the Peierls-Boltzmann Equation [5].

Equation (9) is subject to the conditions that both the temperature (in the absence of a nonideal interface) and the heat flux in the normal direction are continuous across a boundary [6], Σ . That is,

$$T \text{ continuous across } \Sigma \quad (10)$$

$$\kappa_1(T) \hat{n} \cdot \nabla T|_\Sigma = \kappa_2(T) \hat{n} \cdot \nabla T|_\Sigma, \quad (11)$$

which must also be satisfied in the derivation of the computational grid as discussed in Sec. 3.6.

Equations of the form of Equation (9) can be solved directly with a finite element analysis (FEA) approach, while such an equation is non-trivial to solve using finite difference methods. Although, in principle, a MC device simulator could include a field solver using finite element methods, the process of particle tracking would become more complicated when using non-rectangular grids, as is often the case in FEA simulation.

Furthermore, an efficient finite-difference solver for the Poisson equation, a linear elliptical partial differential equation (PDE), is present in any MC electrical device simulator. Hence, manipulating Equation (9) into the form of a linear elliptical PDE would allow for a more straightforward implementation including temperature-dependent effects within the finite difference framework. Simply put, if we are able to pull $\kappa_\mu(\mathbf{r}, T)$ outside of the divergence operator on the left-hand side of Equation (9), we can then work with a Poisson-like linear equation of the form:

$$\kappa_\mu \nabla^2 T = -P_\mu, \quad (12)$$

The main issue in performing this manipulation is the dependence of $\kappa_\mu(\mathbf{r}, T)$ on both position and temperature. For the former, we assume that the thermal conductivity is piecewise constant. In other words, the thermal conductivity is constant within any particular cell, C , but allowed to vary when moving from one cell to another. This is perfectly analogous to the approach used for the dielectric constant in the solution of Poissons equation. Hence, we will express this restricted position dependency with the cell index C rather than via a full functional dependence on the position vector $\mathbf{r}$. For the latter case of the temperature dependence, two separate approaches have been taken to perform this manipulation: 1) the Kirchhoff transformation, and 2) an iterative approach which overcomes many of the restrictions imposed by the use of the Kirchhoff transformation.

As for the functional form used for the temperature dependence of the thermal conductivity itself, it has been found that a simple power law provides a good fit to experimental measurements for a large number of materials [6–11]

$$\kappa_{\mu,C}(T) = \kappa_{ref} \left(\frac{T}{T_{ref}} \right)^\alpha, \quad (13)$$

where κ_{ref} is the independently known thermal conductivity at the reference temperature T_{ref} , often taken as 300K.

3.4 Kirchhoff Transformation

The Kirchhoff transformation is defined as [6, 12, 13]

$$\Theta_{\mu,C}(T) = T_{ref} + \frac{1}{\kappa_{\mu,C}(T_{ref})} \int_{T_{ref}}^T \kappa_{\mu,C}(\tau) d\tau, \quad (14)$$

where Θ denotes a new “apparent” temperature which implicitly includes the temperature dependence of the thermal conductivity. T_{ref} is a chosen reference temperature, often 300K, at which the thermal conductivity value, $\kappa_{\mu,C}(T_{ref})$, is independently known.

Using the apparent temperature, Θ , we can now linearize the EBE in the form of a Poisson-like equation as

$$\nabla^2 \Theta_{\mu,C} = -\frac{P_\mu(\mathbf{r})}{\kappa_{\mu,C}(T_{ref})}. \quad (15)$$

However, a few significant restrictions are imposed by the Kirchhoff transformation. First, Equation (15) requires that both the temperature and its derivative in the normal direction, *i.e.*, the heat flux, are continuous across a boundary [6]. For the temperature continuity condition, say from the left (L) side of an interface to the right (R), from Equation (14)

$$\Theta_L - \Theta_R = \frac{1}{\kappa_L(T_{ref})} \int_{T_{ref}}^{T_L} \kappa_L(\tau) d\tau - \frac{1}{\kappa_R(T_{ref})} \int_{T_{ref}}^{T_R} \kappa_R(\tau) d\tau. \quad (16)$$

In order for the apparent temperature to be continuous across a boundary, $\Theta_L - \Theta_R = 0$, the two materials must have the same functional form for the thermal conductivity. If we use the power law fit discussed previously, this means that the two relationships can differ only by the multiplying constant κ_{ref} , while the exponent α must be the same for both materials.

Secondly, functions representing Dirichlet and simple Neumann boundary conditions, corresponding to a constant temperature or heat flux, respectively, are linear under the Kirchhoff transformation. In contrast, convective boundary conditions become nonlinear under the Kirchhoff transformation [12, 13]. Convective boundary conditions describe thermal contacts that have an inherent thermal resistance, R_{TH} , or a finite heat transfer coefficient, H , where $H = 1/R_{th}$.

Clearly, as $R_{th} \rightarrow 0$, $H \rightarrow \infty$ and the perfect thermal contact of a Dirichlet boundary condition is recovered. In addition, convective conditions can also occur at material interfaces, which often introduce a resistance to the heat passing from one material to the other.

$$-\kappa \nabla \mathbf{T} = H (\mathbf{T}_L - \mathbf{T}_R), \quad (17)$$

Since the Kirchhoff transformation is nonlinear for any nonlinear functional form of the thermal conductivity, it is generally not true that $H(\Theta_L - \Theta_R) = H(T_L - T_R)$.

To overcome the discussed restrictions related to the Kirchhoff transformation, a classical iterative approach to solving the EBE has also been implemented. This takes advantage of the fact that the thermal conductivity is allowed to vary, in a piece-wise constant way, from one cell to another to incorporate the temperature-dependent values, and a sequence of constant-conductivity problems is solved where the thermal conductivity in each cell is updated with each new solution according to the local temperature. In other words, we solve a system of the form:

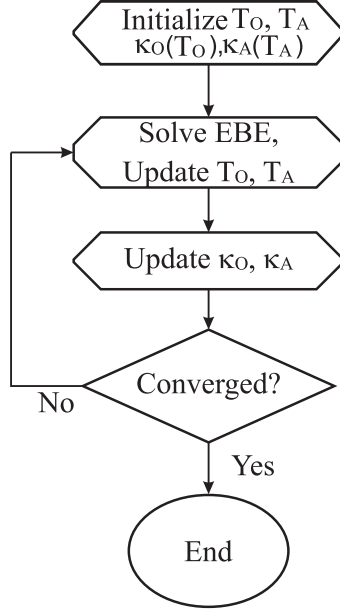


Figure 2. Flowchart for the Self-Consistent Thermal Solution Using the Iterative Method

This is significant for devices such as a HEMT which is studied in a later section, where material interfaces are used to create a 2-dimensional electron gas (2DEG) conduction channel, as well as in layouts attempting to use a high thermal conductivity material to transport heat away from the active device, where the interface can have an associated thermal resistance.

It should be noted, however, that the thermal conductivity is likely to assume different values in every computational cell in Equation (18), and so classical multigrid methods are likely to become very inefficient. One possible approach to mitigate this if multigrid methods are desired is to attempt to average the thermal conductivity, assuming the values fall within a reasonable range, between cell which are merged together, however this could be dubious. Fortunately, in an electrothermal simulation the solution to Poisson's equation, where the iterative method is not used, is required orders of magnitude more times than that of the phonon EBE.

3.6 Computational Difference Scheme

For a given cell inside the computational domain, labeled c , the northern, eastern, western, and southern neighbors are labeled as n , e , w , and s , respectively. The distances δ_x and δ_y are the x and y dimensions of cell c . The distances δ_n , δ_s , δ_w , and δ_e are the respective distances from the center of cell c to the center of the northern, southern, western, and eastern neighbor cells, respectively. These distances cannot be assumed to be equivalent the δ_x and δ_y for inhomogenous grids. Lastly, the $\delta_{xw,xe}$, $\delta_{yn,ys}$ are the distances from the center of the neighbor cell to the nearest boundary of cell c , which are needed to perform interpolations from cell-to-cell.

The Laplacian operator in Equation (12) can be approximated by the difference relation

$$\nabla^2 T_c \approx a_n T_n + a_e T_e + a_s T_s + a_w T_w + a_c T_c + O(\Delta_x \Delta_y)^m, \quad (19)$$

where the final term is an error term dependent upon the chosen grid sizing. For uniformly spaced grids $m = 3$, while for inhomogenous grids $m < 3$ [14].

In the most general case, considering an inhomogenous grid with a piece-wise constant thermal conductivity, the coefficients in Equation (19) are given by

$$\begin{aligned}
a_w &= \left[\frac{2}{\delta_w (\delta_e + \delta_w)} \right] \left[1 + \frac{\delta_{xw}}{\delta_x/2} \right] \left[\frac{\kappa_w \delta_x/2}{\kappa_c \delta_{xw} + \kappa_w \delta_x/2} \right] \\
a_e &= \left[\frac{2}{\delta_e (\delta_e + \delta_w)} \right] \left[1 + \frac{\delta_{xe}}{\delta_x/2} \right] \left[\frac{\kappa_e \delta_x/2}{\kappa_c \delta_{xe} + \kappa_e \delta_x/2} \right] \\
a_n &= \left[\frac{2}{\delta_n (\delta_n + \delta_s)} \right] \left[1 + \frac{\delta_{yn}}{\delta_y/2} \right] \left[\frac{\kappa_n \delta_y/2}{\kappa_c \delta_{yn} + \kappa_n \delta_y/2} \right] \\
a_s &= \left[\frac{2}{\delta_s (\delta_n + \delta_s)} \right] \left[1 + \frac{\delta_{ys}}{\delta_y/2} \right] \left[\frac{\kappa_s \delta_y/2}{\kappa_c \delta_{ys} + \kappa_s \delta_y/2} \right] \\
a_c &= -\frac{2}{\delta_e \delta_w} - \frac{2}{\delta_n \delta_s} + p_w + p_e + p_s + p_n,
\end{aligned} \tag{20}$$

where the values of the p_i terms in the center coefficient are further given by

$$\begin{aligned}
p_w &= \left[\left(1 + \frac{\delta_{xw}}{\delta_x/2} \right) \left(\frac{\kappa_c \delta_{xw}}{\kappa_c \delta_{xw} + \kappa_w \delta_x/2} \right) - \frac{\delta_{xw}}{\delta_x/2} \right] \\
p_e &= \left[\left(1 + \frac{\delta_{xe}}{\delta_x/2} \right) \left(\frac{\kappa_c \delta_{xe}}{\kappa_c \delta_{xe} + \kappa_e \delta_x/2} \right) - \frac{\delta_{xe}}{\delta_x/2} \right] \\
p_s &= \left[\left(1 + \frac{\delta_{ys}}{\delta_y/2} \right) \left(\frac{\kappa_c \delta_{ys}}{\kappa_c \delta_{ys} + \kappa_s \delta_y/2} \right) - \frac{\delta_{ys}}{\delta_y/2} \right] \\
p_n &= \left[\left(1 + \frac{\delta_{yn}}{\delta_y/2} \right) \left(\frac{\kappa_c \delta_{yn}}{\kappa_c \delta_{yn} + \kappa_n \delta_y/2} \right) - \frac{\delta_{yn}}{\delta_y/2} \right].
\end{aligned} \tag{21}$$

In the case of the Kirchhoff transformation, the temperature dependence of the thermal conductivity is absorbed into the temperature variable Θ , and so the κ values in the above coefficients are simply those at the reference temperature. Hence, the Laplace operator, and all of the associated coefficients, only need be set up once at the beginning of the simulation and stored as they will be constant throughout the simulation. On the other hand, in the iterative approach the various values of κ in Equation. (20) and (21) are updated only after each new temperature solution is found.

3.7 Boundary Conditions

Two kinds of boundary conditions are considered in this work with the context of device simulation in mind. These are the Dirichlet boundary condition [15, 16] of a prescribed constant temperature (Equation (22)), and the convective (or Robin) boundary condition [15, 16] which is related to a prescribed non-zero Neumann condition on the heat flux (Equation (24)).

The Dirichlet condition on the temperature of the boundary cells, T_b , is expressed as:

$$T_b = T. \quad (22)$$

To implement the Dirichlet condition on the cell c , the coefficients of Equation (20) reduce in the normal way such that

$$\begin{aligned} a_w &= 0 \\ a_e &= 0 \\ a_n &= 0 \\ a_s &= 0 \\ a_c &= 1. \end{aligned} \quad (23)$$

This reduces Equation (19) to $T_c = T_b$ and has the effect of fixing the temperature in the Dirichlet cells where the forcing function is set to the prescribed value T_b .

The convective boundary condition is based on Newton's law of cooling [13, 15, 16], and given by

$$-\kappa \nabla T = H(T_b - T_\infty), \quad (24)$$

where T_b is again the interior temperature at the boundary cell, T_∞ is the ambient temperature specified outside of the boundary, which is assumed to be constant, and H is a heat transfer coefficient. In particular, the heat transfer coefficient is expressed in $\frac{W}{m^2 K}$ and is the inverse of an associated thermal resistance, R_{TH} . The problem modeled by Equation (9) with the convective boundary condition of Equation (24) is well-posed as long as the ratio of thermal conductivity and heat transfer coefficient is positive, $\frac{\kappa}{h} > 0$ [15], which represents any physically realistic case, as either a negative thermal conductivity or a negative heat transport coefficient is nonsensical from a physical perspective.

3.8 Interface Conditions

To implement the material interface condition, we follow the work of Hickson *et al.* [17]. However, here we are interested in solving the steady-state problem rather than the time-dependent problem studied in [17]. Furthermore, here we use a first order accurate expression for the interface coefficients as the second order expressions are much more cumbersome [17], and, since we generally work with non-homogeneous grids, we expect only first order accuracy in the Laplacian. Considering only the 1-D case on the x-axis, Figure 3 depicts the cells nearest an interface with an associated heat transfer coefficient H . The temperatures at the edge of each side of the boundary are given by T_L and T_R , while the temperatures at the central cell points are denoted $T_{i\pm n}$.

The second derivatives on each side of the interface are written as follows [14]:

$$\frac{\partial T_{i-1}}{\partial x^2} \approx \frac{\Delta_{xw} T_L - (\Delta_{xL} + \Delta_{xw}) T_{i-1}}{\Delta_{xL} \Delta_{xw} (\Delta_{xL} + \Delta_{xw})}, \quad (25)$$

$$\frac{\partial T_{i+1}}{\partial x^2} \approx \frac{\Delta_{xe} T_R - (\Delta_{xR} + \Delta_{xe}) T_{i+1}}{\Delta_{xL} \Delta_{xe} (\Delta_{xL} + \Delta_{xe})}, \quad (26)$$

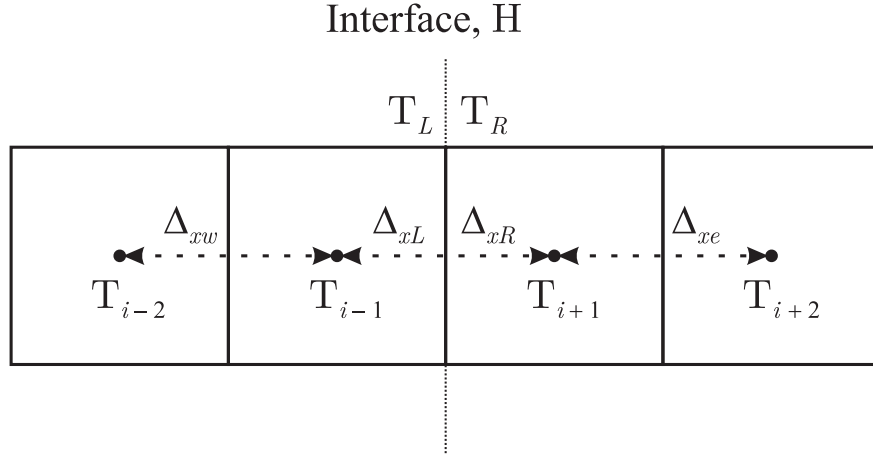


Figure 3. Diagram of a 1-D Material Interface

where T_{i-1} denotes the nearest grid point to the left of the interface, T_{i+1} the nearest grid point to the right of the interface, Δ_{xL} the distance between the point $i - 1$ and the interface, Δ_{xR} the distance between the point $i + 1$ and the interface, and lastly Δ_{xw} the distance between the points $i - 1$ and $i - 2$ to the left, Δ_{xe} the distance between points $i + 1$ and $i + 2$ to the right. In Equation. (25) and (26) we have 4 unknowns: T_{i-1} , T_{i+1} , T_L , and T_R . The temperatures at the grid points everywhere in the simulation, such as T_{i-1} and T_{i+1} are independently solved for using numerical methods such as successive over-relaxation (SOR), and so we need to find expressions to substitute for T_L and T_R . To find these expressions, we use the Taylor series around T_{i-1} and T_{i+1} , the fact that the flux must be continuous on each side of the interface, and the boundary condition itself. The Taylor series around T_{i-1} and T_{i+1} are given by

$$T_{i-1} \approx T_L - \Delta_{xL} \frac{\partial T_L}{\partial x} \quad (27)$$

$$T_{i+1} \approx T_R + \Delta_{xR} \frac{\partial T_R}{\partial x}, \quad (28)$$

while the flux continuity and boundary conditions are

$$\kappa_L \frac{\partial T_{i-1}}{\partial x} = \kappa_R \frac{\partial T_{i+1}}{\partial x} \quad (29)$$

$$\kappa_L \frac{\partial T_{i-1}}{\partial x} = H (T_R - T_L). \quad (30)$$

Using Equation. (27 - 30), T_L and T_R can now be obtained as

$$T_L = \frac{(H\Delta_{xR} + \kappa_R) \kappa_L}{(H\Delta_{xR} + \kappa_R) \kappa_L + H\Delta_{xL}\kappa_R} T_{i-1} + \frac{H\Delta_{xL}\kappa_R}{(H\Delta_{xR} + \kappa_R) \kappa_L + H\Delta_{xL}\kappa_R} T_{i+1} \quad (31)$$

$$T_R = \frac{H\Delta_{xR}\kappa_L}{(H\Delta_{xR} + \kappa_R) \kappa_L + H\Delta_{xL}\kappa_R} T_{i-1} + \frac{(H\Delta_{xL} + \kappa_L) \kappa_R}{(H\Delta_{xR} + \kappa_R) \kappa_L + H\Delta_{xL}\kappa_R} T_{i+1} \quad (32)$$

which can be substituted back into Equation. (25) and (26) to obtain the Laplacian in the neighborhood of the interface. On a uniform grid where $\Delta_{xR} = \Delta_{xL} = \Delta_x$, and letting $H \rightarrow \infty$ it can be shown that the Laplacian reduces to the straightforward case with no interface resistance.

4.0 RESULTS AND DISCUSSION

4.1 Particle-Particle Electron-Phonon Validation

The first validation test for the particle-particle framework in the CMC performed was to initialize a simulation with an out-of-equilibrium phonon distribution. In an adiabatic system with total energy density E_c , the phonon ensemble should ultimately progress towards a Bose-Einstein (B-E) distribution with temperature T_c ($\langle n_{\mathbf{k},p}, T_c \rangle$), which must satisfy the energy vs temperature relationship:

$$E_c(T_c) = \frac{1}{V_c} \sum_p \sum_{\mathbf{k}} \left(\langle n_{\mathbf{k},p}, T_c \rangle + \frac{1}{2} \right) \hbar \omega_{\mathbf{k}} \quad (33)$$

Figure 4 shows the energy distribution at the initial and the final state of the simulation. The initial out-of-equilibrium distribution given to the phonon ensemble is represented by the dashed line, whereas the solid dots represent the correct equilibrium B-E distribution at 216K. The system is allowed to evolve until it reaches steady state (solid line), where we that see the final energy distribution very closely follows the theoretical B-E distribution

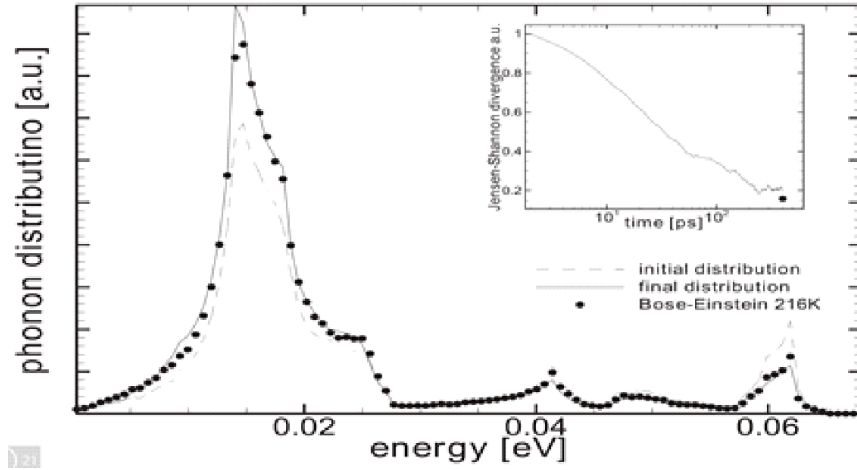
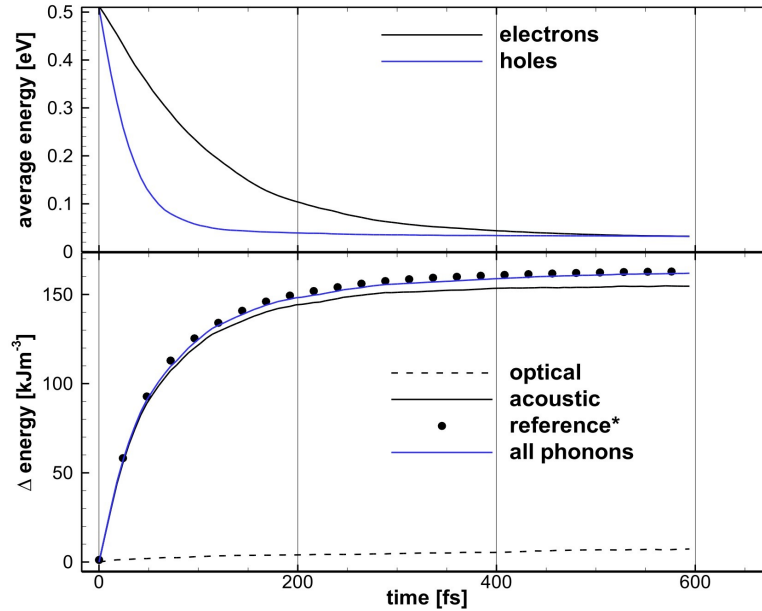


Figure 4. The System Is Initialized With an Out-of-Equilibrium Energy Distribution (Dashed Line), Its Final Distribution (Solid Line), and the Theoretical Distribution (Solid Dots)

Next, a test was performed to check that energy is conserved in a simultaneous simulation of both electrons and phonons. Here, the simulation is begun using an ensemble of high energy electron-hole pairs generated with an optical pulse. Over time, these so-called hot carriers are expected to dissipate excess energy through energy relaxation mechanisms until an equilibrium is reached with the crystal lattice. In other words, the excess energy flows from the hot carriers to the crystal lattice through scattering processes until the two populations reach equilibrium with respect to each other.

Figure 5 (top) shows a plot of the average energy of the electrons and holes, starting at 0.5 eV when they are first generated. The electrons are seen to relax to near their equilibrium energy by $t = 100$ fs, whereas it takes much longer for the holes to do so, at roughly $t = 400$ fs. On the bottom of figure 5 the total energy gained by the phonon ensemble (blue line), as well as the total energy lost by the charge carriers (solid dots) is shown. We see that these two values are in very good agreement, and hence conclude that energy is conserved when transferred from hot carriers to the lattice through scattering processes.



*Energy lost by the charge carriers

Figure 5. Time Evolution of the Carrier Energy in a Synchronous Electron-Phonon Particle Simulation

4.2 Particle-Flux Electro-thermal Validation

To verify the computational framework developed in Secs. 3.6 and 3.7, the tests performed in Hickson *et al.*, Bagnall *et al.*, and Garven *et al.* [12, 17, 18] have been reproduced here using both the Kirchhoff Transformation of Sec. 3.4 and the iterative approach of Sec. 3.5. The results of each approach are compared with the full nonlinear FEA solver in the commercial MATLAB[®] 2018b release [19]. In principle, the full nonlinear FEA solver is capable of solving the full nonlinear EBE in Equation (9) directly.

4.2.1 Convective Interface Conditions

First, the numerical grid and convective boundary conditions of Sec. 3.7 were verified by simulating a 10-layer structure with an associated thermal resistance at each of the interfaces, similar to that in Hickson *et al.* [17]. Note that the heat generation in this test is set to zero. The boundary conditions

imposed are a Dirichlet condition of 400K at $x = 0$ and a Dirichlet condition of 300K at $x = 10$ nm. The layers are in an A-B-A-B structure, with the thermal conductivity in layer A, $\kappa_A = 1$ W/m·K, the thermal conductivity in layer B, $\kappa_B = 0.1$ W/m·K, and the interface resistance, $H = 5 \cdot 10^8$ W/m²·K, which is a reasonable value for a semiconductor-semiconductor interface..

The result is shown in Figure 6 for the cases of a constant conductivity and a temperature-dependent conductivity using both the Kirchhoff transformation and the iterative method. The temperature-dependent solution here closely follows that of the constant conductivity. This is reasonable as each layer is only 1 nm thick. However, the result of the Kirchhoff transformation becomes more inaccurate further from the Dirichlet conditions at $x = 0$ nm and $x = 10$ nm because of the non-linearity. This is seen because the slopes inside the layers are the nearly identical, and the difference in the solution comes from the temperature jumps at the interfaces themselves.

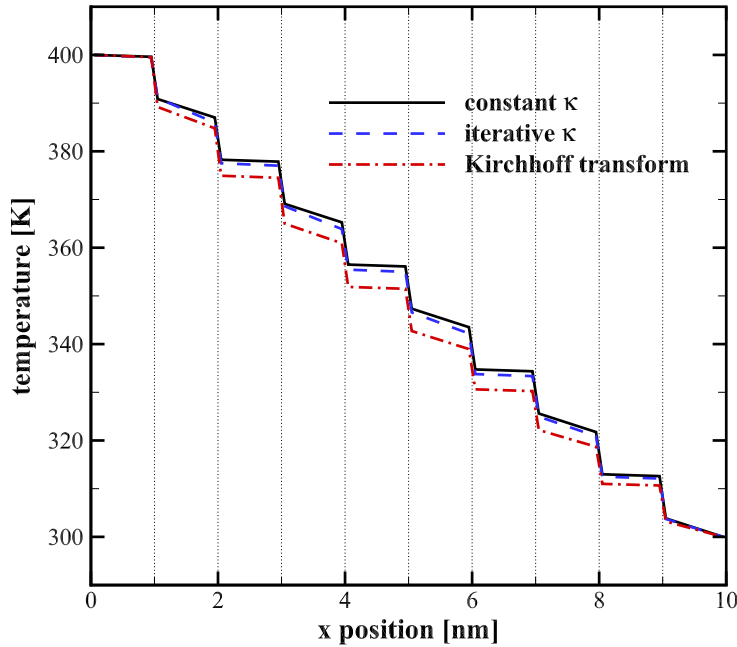


Figure 6. A 10-Layer Structure Simulated Using 1) a Constant Thermal Conductivity, 2) the Iterative Algorithm, and 3) the Kirchhoff Transformation With the Thermal Conductivity Taken at 300K

4.2.2 One-Dimensional Validation

Subsequently, as an initial test of both the Kirchhoff transformation and the iterative approach, the simple layout of Figure 7 is simulated [12]. In this simplest case of a 1-D simulation, we use the material parameters of a 500 μm long by 100 μm thick piece of silicon. The thermal conductivity of silicon at 300K is taken as 150 W/m·K, and the exponent in the temperature power law of Equation (13) is taken as $\alpha = -1.3$ [11, 12]. In other words, the temperature dependent thermal

conductivity is taken as

$$\kappa(T) = 150 \left(\frac{T}{300} \right)^{-1.3}. \quad (34)$$

The boundary conditions used, also indicated in Figure 7, are a constant inward heat flux all along

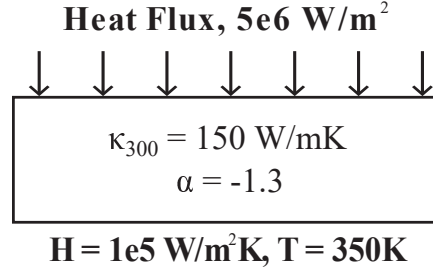


Figure 7. Schematic of the 1-D Heat Transfer Layout

the top boundary of $5 \cdot 10^6 \text{ W/m}^2$, while a convective boundary is set along the bottom of the material characterized by a heat transfer coefficient of $H = 10^5 \text{ W/m}^2\text{K}$ and an ambient temperature of $T_\infty = 350\text{K}$. In other words, the boundary condition is

$$-\kappa \nabla T = 10^5 (T_b - 350\text{K}). \quad (35)$$

The Kirchhoff transformation was used to solve Equation (9) with the convective boundary condition of Equation (4.2.2) in two cases: 1) effectively linearizing the boundary condition under the Kirchhoff transformation by choosing the reference temperature to be that of the average temperature expected at the boundary, and 2) without linearizing the transformation but instead using $T_{ref} = 300\text{K}$ and $\kappa_{ref} = \kappa_{300} = 150 \text{ W/mK}$. In the simple 1-D case, the temperature expected at the convective boundary can be determined analytically as [12]

$$T_b = \frac{\Phi}{H} + T_\infty, \quad (36)$$

where Φ denotes the inwards flux at the top boundary.

As seen in Figure 8, the solution for the Kirchhoff transformation agrees exactly with the full nonlinear FEA solution when the reference temperature in the Kirchhoff transformation is chosen in this manner, such that the transformation of the boundary condition is effectively linearized around the convective boundary. However, this approach requires some knowledge of the solution *a priori*. To illustrate this, an unlinearized Kirchhoff transformation solution, where the reference temperature is taken as 300K, is also shown in Figure 8. The unlinearized version is seen to be inaccurate by 26K when compared to the full nonlinear FEA and the linearized Kirchhoff transformation.

One advantage of the proposed iterative method is that no *a priori* knowledge of the solution is required. To demonstrate this, the same 1-D simulation is performed with the iterative approach using $T_{ref} = 300\text{K}$ and the associated thermal conductivity value. In Figure 9 the iterative solution

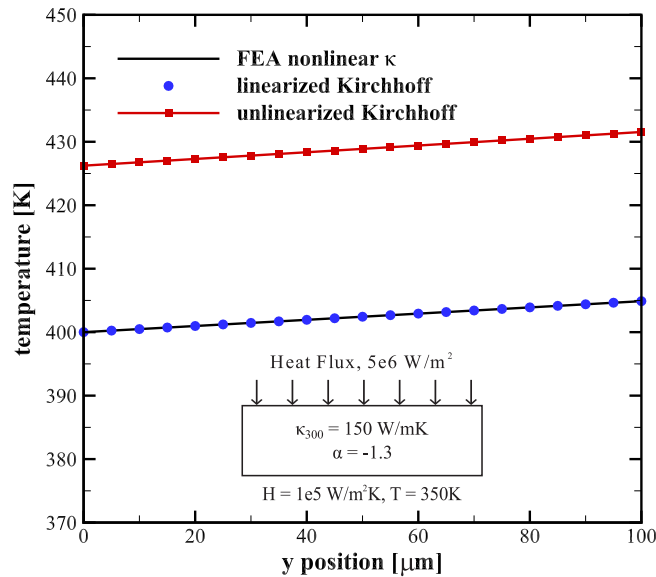


Figure 8. 1-D Heat Transfer Solution for a 100 μm Thick Piece of Silicon Using the Expected Boundary Temperature of $T_{Ref} = 400\text{K}$ (Linearized), and $T_{Ref} = 300\text{K}$ (Unlinearized) in the Kirchhoff Transformation [20] ©2020 ASME

is shown as compared to that of the full nonlinear FEA. The iterative approach is seen to agree exactly with the full nonlinear FEA using both a constant and a temperature dependent thermal conductivity, while requiring no information about the solution ahead of time.

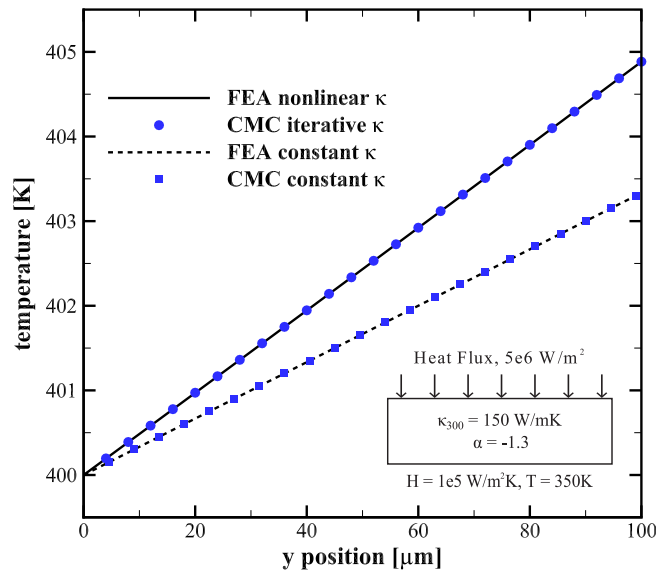


Figure 9. 1-D Heat Transfer Solution for a 100 μm Thick Piece of Silicon Using Both a Constant and Temperature Dependent Thermal Conductivity in the Iterative Algorithm [20] ©2020 ASME

4.2.3 Two-Dimensional Validation

Subsequently, a 2-D rectangular structure was considered where the heat flux applied to the top boundary is only applied at a single central point, rather than uniformly across the entire surface. Three different size dimensions have been considered: 1) a $500\ \mu\text{m} \times 100\ \mu\text{m}$ layout, 2) a $500\ \mu\text{m} \times 5\ \mu\text{m}$ layout, and 3) a $500\ \mu\text{m} \times 2\ \mu\text{m}$ layout. This is because Bagnall et al. [12] found that as the size in the y-dimension of the simulation was decreased, the linearized Kirchhoff transformation became less accurate. The results of these simulations are shown in Figure 10. For the first case shown in Figure 5a, the iterative method shows excellent agreement with the FEA solution for a thickness of $100\ \mu\text{m}$. For thicknesses of $5\ \mu\text{m}$ and $2\ \mu\text{m}$ shown in Figure 5b and 5c, respectively, the iterative method still shows excellent agreement with the FEA solution. However, also shown in these figures is the result using the linearized Kirchhoff transformation that is seen in comparison to become increasingly inaccurate as the size is reduced.

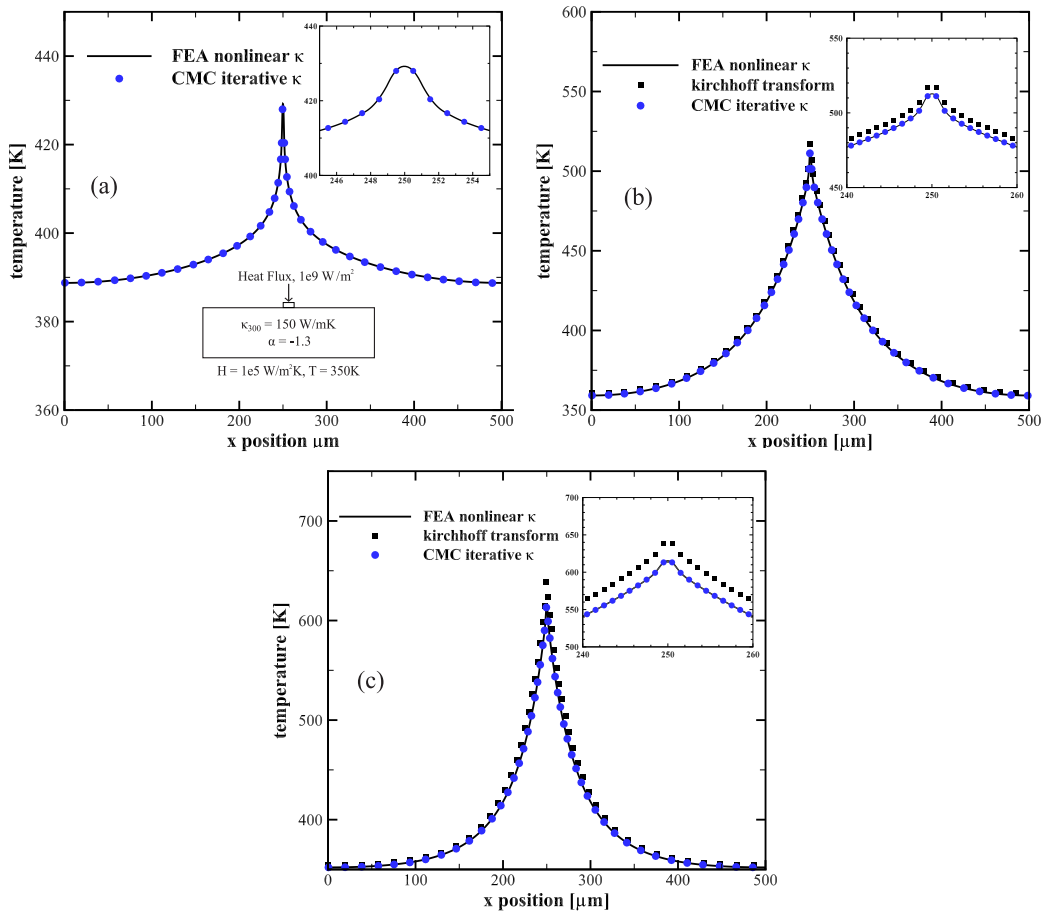


Figure 10. 2-D Heat Transfer Solution for: (a) $100\ \mu\text{m}$ Thick , (b) $5\ \mu\text{m}$ Thick, and (c) $2\ \mu\text{m}$ Thick Piece of Silicon [20] ©2020 ASME

Finally, A robust thermal simulation test found in the literature [12, 18] is that of a package-scale 11-finger gallium nitride (GaN)-on-silicon carbide (SiC) radio frequency (RF) power amplifier, with each device finger modeled as a constant heat source of 10^{10}W/m^2 . The devices are placed along

the top surface of the layout and spaced 50 μm apart, with the first located at $x=25 \mu\text{m}$ along the top of the layout and the final one at $x=525 \mu\text{m}$. The entire simulated layout has dimensions of 1000 μm x 102 μm . In the y-direction, the lower 100 μm is composed of a high thermal conductivity SiC substrate, while the top 2 μm layer is GaN. The thermal conductivities in the iterative method are taken as

$$\kappa_{\text{GaN}} = \kappa_{\text{ref,GaN}}(T/T_{\text{ref}})^{(-1.3)}, \kappa_{\text{SiC}} = \kappa_{\text{ref,SiC}}(T/T_{\text{ref}})^{(-1.4)}, \quad (37)$$

where the reference thermal conductivities are $\kappa_{\text{ref,GaN}} = 150$ and $\kappa_{\text{ref,SiC}} = 420 \text{ W/m}\cdot\text{K}$ as in Bagnall et al. [12]. An initial constant-conductivity solution was obtained to find the average temperature along the convective boundary to use as the reference temperature in the Kirchhoff transformation [12], which was found to be $T = 460\text{K}$. The thermal conductivities used by the Kirchhoff transformation are then

$$\kappa_{\text{GaN}} = 85.8(T/460)^{(-1.4)}, \kappa_{\text{SiC}} = 240.4(T/460)^{(-1.4)}, \quad (38)$$

where the thermal conductivities at $T = 460\text{K}$ are used as the reference values. Additionally, the value of α for GaN is adjusted to $\alpha = -1.4$ in order to have the same functional form as that of SiC, a requirement for the Kirchhoff transformation.

Figure 11 shows the results obtained from the linearized Kirchhoff transformation and the results in an unlinearized Kirchhoff transformation where the reference temperature was taken as $T = 300\text{K}$ and the associated values for the thermal conductivities used in Equation 38. The linearized solution shows reasonably good agreement with a peak temperature discrepancy of 7K compared to the FEA solution, for a peak temperature of 746K vs. 739K. However, the unlinearized version is seen to be extremely inaccurate, and hence *a priori* information is required to obtain reasonable results using the Kirchhoff transformation.

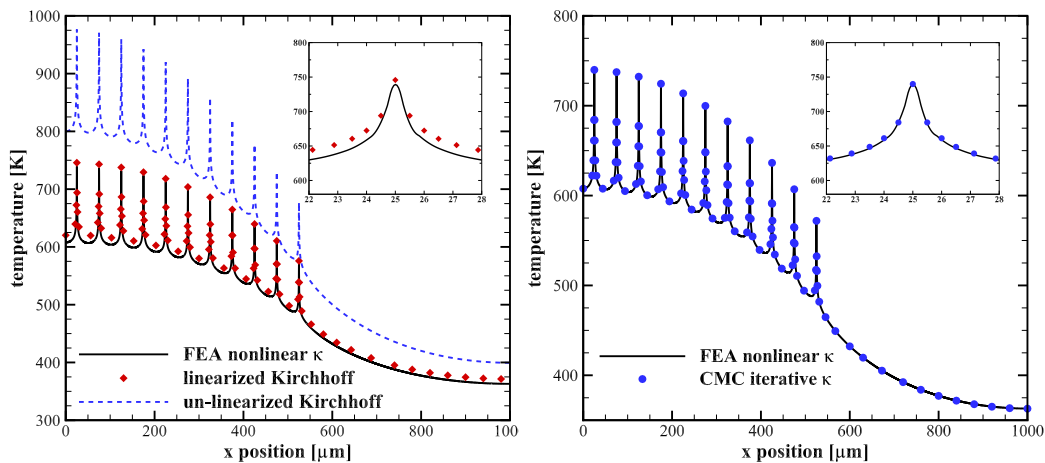


Figure 11. 2-D Heat Transfer Solution for an 11-Finger GaN RF Power Amplifier Modeled Using Constant Heat Sources. A) the Solution Using the Kirchhoff Transformation. B) the Solution Using the Proposed Iterative Method [20] © 2020 ASME

Meanwhile, the iterative approach agrees nearly exactly with the nonlinear FEA, having a peak temperature discrepancy of only 0.7K. Moreover, this is likely due to the iterative method using a fairly coarse grid. In this simulation, the finite element mesh generated by the MATLAB PDE toolbox consists of 236,000 elements, while the grid for the iterative approach contains 383 cells x 205 cells for a total of 78,515 cells.

Subsequently, the same multi-finger layout was then simulated using the thermal conductivity of diamond as

$$\kappa(T) = 2450 \left(\frac{T}{300\text{K}} \right)^{-1.3}, \quad (39)$$

where $\kappa_{300} = 2450 \text{ W/mK}$ and $\alpha = -1.3$. These parameters show reasonable agreement with reported temperature dependent thermal conductivities [21, 22], while using the same value of α as for GaN. The results of this preliminary test simulation are shown in Figure 12 where it is shown that diamonds superior thermal properties, as modeled here, results in a peak temperature reduction of $\approx 233\text{K}$ in the 2-D simulation.

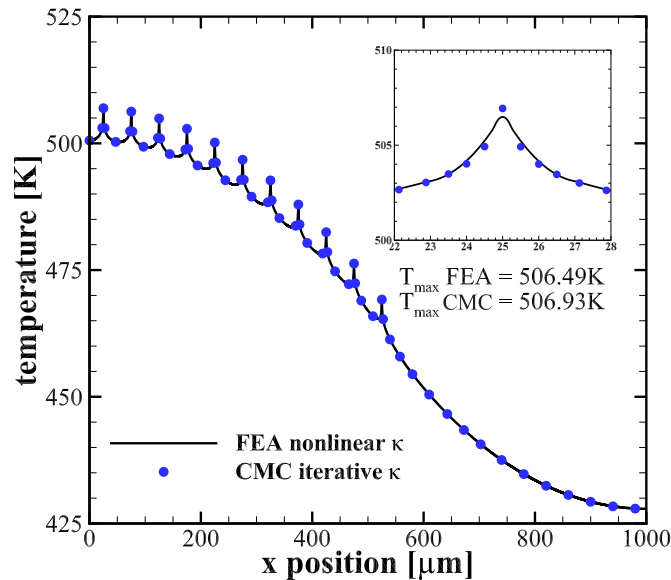


Figure 12. 2-D Heat Transfer Solution for an 11-Finger RF Power Amplifier Modeled Using Constant Heat Sources Composed of Diamond

4.2.4 Electro-thermal Simulation of HEMTs

One advantage for GaN is its high thermal conductivity as compared to traditional semiconductors such as silicon (Si) or gallium arsenide (GaAs). This, in principle, allows GaN to better dissipate the heat generated inside the device. However, convective conditions at material interfaces can be a bottleneck for heat dissipation. Self-heating effects are well known to cause a decrease in operating current, as seen in phenomena such as the well known current collapse in HEMTs. The ability to

design devices accounting also for their thermal characteristics, rather than only the electrical ones, would help in addressing reliability concerns prior to fabrication.

In the following electro-thermal simulations on a GaN/AlGaN HEMT scattering due to both optical and acoustic phonons (both polar and deformation potential), ionized impurities, and impact ionization are considered. The material properties used for GaN are the same as those in Yamakawa *et al.* [23]. To perform the coupled electrothermal simulation, first the electrical CMC is allowed to reach steady-state, just as in an isothermal simulation. Then, we average the power density transferred from the charge carriers to the respective phonon modes over a sufficiently large window to reduce statistical noise. That is, we obtain the value of $\partial W_\mu / \delta t|_{e-p}$ in Equation (9) directly from the CMC simulation. Nevertheless, the energy exchange between the acoustic and optical phonon modes is still treated via the relaxation time approximation, and for GaN assumes values between 2 and 5 ps [24].

The chosen device is that characterized experimentally by Altuntas *et al.* [25]. The experimental layout of this device and the simulated layout consisting of a T-gate structure with a relatively large 1 μm buffer layer is shown in Figure 13 [26].

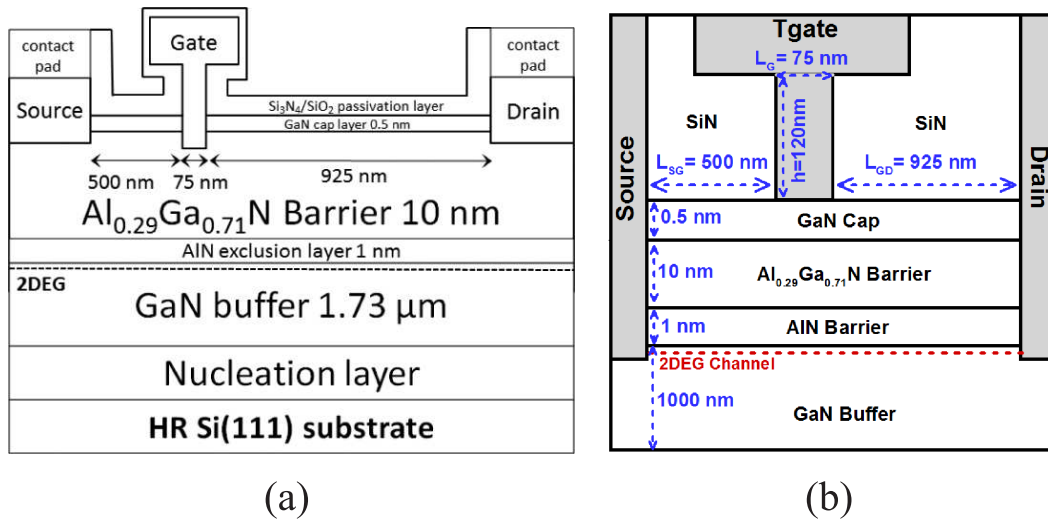


Figure 13. (a) Layout of the GaN/AlGaN HEMT Characterized Experimentally by Altuntas [25] and (b) the Layout Used in the Coupled Electrothermal Simulation [26] ©2019 IEEE

The resulting acoustic mode and optical mode temperatures at the bias point $V_{DS} = 2\text{V}$, $V_{GS} = 10\text{V}$, where both high currents and high electric fields are present, are shown in Figure 14. Here the temperatures are shown as a color map on top of the 3-D surface representing the conduction band to illustrate where the gate, source, drain, and channel regions are located in the device.

The optical mode temperature peaks at near 950K and is highly localized to the drain edge of the gate as should be expected. This is because the optical phonons have very low group velocity, and hence a low thermal conductivity. Hence, the dominant decay path available to them is to decay into acoustic phonons which generally happens at a rate slower than new optical phonons are generated. On the other hand, the acoustic temperature map is much more spread out because of the

acoustic phonon modes' high thermal conductivity, and the peak acoustic temperature is seen to be roughly 375K, also to the drain side of the gate.

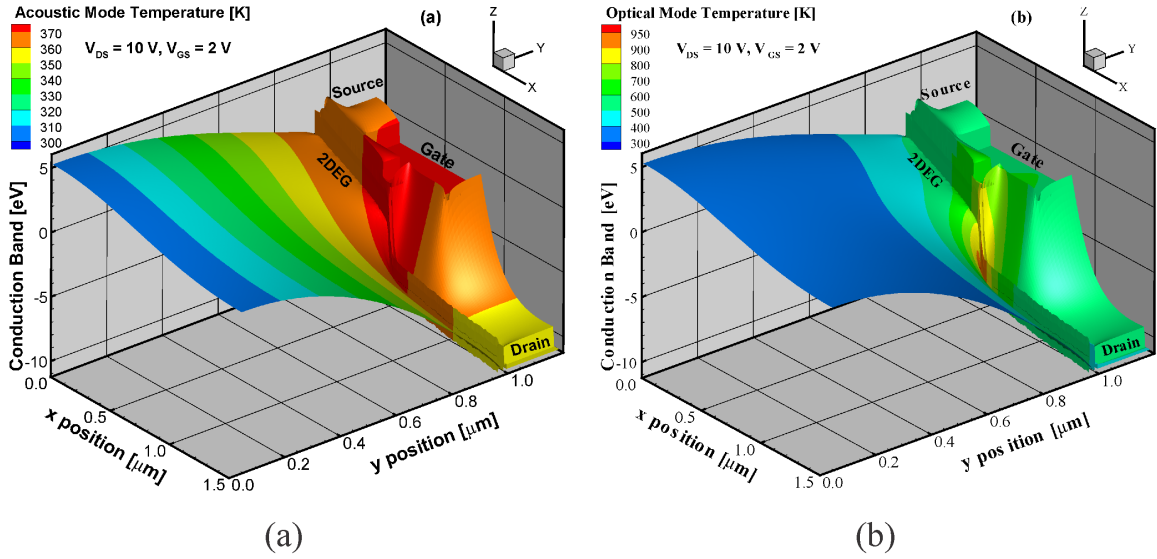


Figure 14. Acoustic (a) and Optical (b) Mode Temperature Maps Obtained for the T-Gate Device at $V_{DS} = 10V$ and $V_{GS} = 2V$ [26] ©2019 IEEE

Finally, the I_{DS} - V_{DS} curves under DC operation from Altuntas [25] along with the those of the electrothermal model presented in this section are shown in Figure 15 [26]. In this case, capturing thermal effects through the Kirchhoff transformation is seen to accurately reproduce the operating currents throughout the entire curve as no convective conditions are present in the model used. In comparison, the isothermal simulations at 300K overestimate the current at higher drain voltages.

Next, the device of Figure 13 is simulated again, this time using the iterative method and subsequently including the effects of convective boundary conditions (a principle advantage of the iterative method).

In the Dirichlet case, the boundary condition at the bottom edge of the device is again taken as a constant 300K, while for the convective condition the boundary condition is that of Equation (17), *i.e.*, $-\kappa \nabla T_{b,C} = H(T_{b,C} - T_{\infty})$ with the ambient temperature, T_{∞} assumed to be a constant 300K, denoted in the results of Figures 18 and 19. All other boundary conditions are assumed to be perfectly insulating Neumann conditions, *i.e.*, a zero flux exiting in the direction normal to the boundary. In other words, we iteratively solve:

$$\nabla^2 T_{\mu,C}^i = -\frac{P_{\mu}(\mathbf{r})}{\kappa_{\mu,C}(T^{i-1})}, \quad (40)$$

subject to either the Dirichlet or convective boundary condition

$$T_b = 300K \quad (41)$$

$$-\kappa \nabla T_b = H(T_{b,C} - 300K), \quad (42)$$

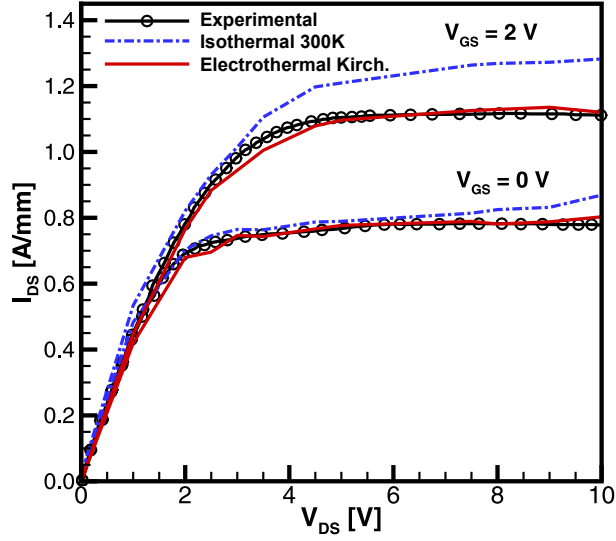


Figure 15. Full Electrothermal I-V Curve for $V_{GS} = 2V$ and $V_{GS} = 0V$ for the GaN/AlGaN HEMT Using the Kirchhoff Transformation With a Dirichlet Boundary Condition. the Isothermal 300K Simulation Result is Shown as a Reference

where $T_{b,C}$ denotes the temperature in each respective boundary cell C along the bottom of the device.

Once the iteration of Equation (40) has converged, in this case using the SOR, the scattering rates are then updated in every cell of the simulation domain according to the new local temperature, and the process is repeated until both the optical and acoustic temperatures have converged to a steady-state value everywhere. The described simulation procedure is depicted in the flowchart of Figure 16. Note that the process depicted in the thermal solver is solved self-consistently in an inner loop, and then convergence is tested based on the change between two successive temperature solutions.

The final temperature maps obtained at the bias point $V_{DS} = 2V$, $V_{GS} = 10V$ are shown in Figure 17. These results can be directly compared to the previous result obtained using the Kirchhoff transformation, and we see good agreement between the two.

Namely, the optical mode temperature peaks at near 950K and is again highly localized to the drain edge of the gate. While on the other hand, the acoustic temperature map is much more dispersive because of their high thermal conductivity, and the peak acoustic temperature is seen to be roughly 380K, also to the drain side of the gate.

Next, the effects of using both convective boundary conditions and convective interface conditions are illustrated, as this is one of the main features of the iterative method.

In Fig 18, the I-V curves for three separate cases of modeling the heat sink are shown as follows: 1) using a simple 300K Dirichlet boundary condition, 2) using a convective boundary condition with $H = 10^8 \text{ W/m}^2\text{K}$, and 3) using a convective boundary condition with $H = 10^7 \text{ W/m}^2\text{K}$. Note that

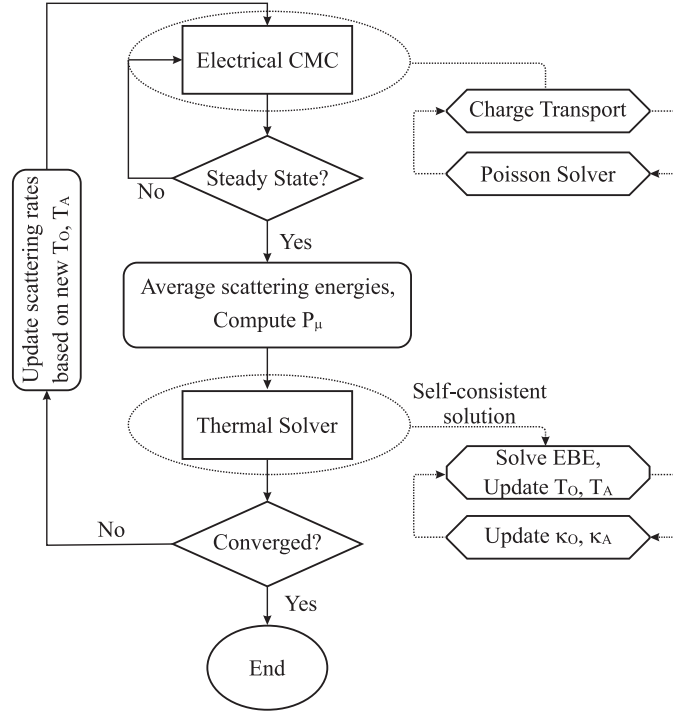


Figure 16. Flowchart of the Electrothermal Simulation Process Using the Iterative Thermal Solver [20] ©2020 ASME

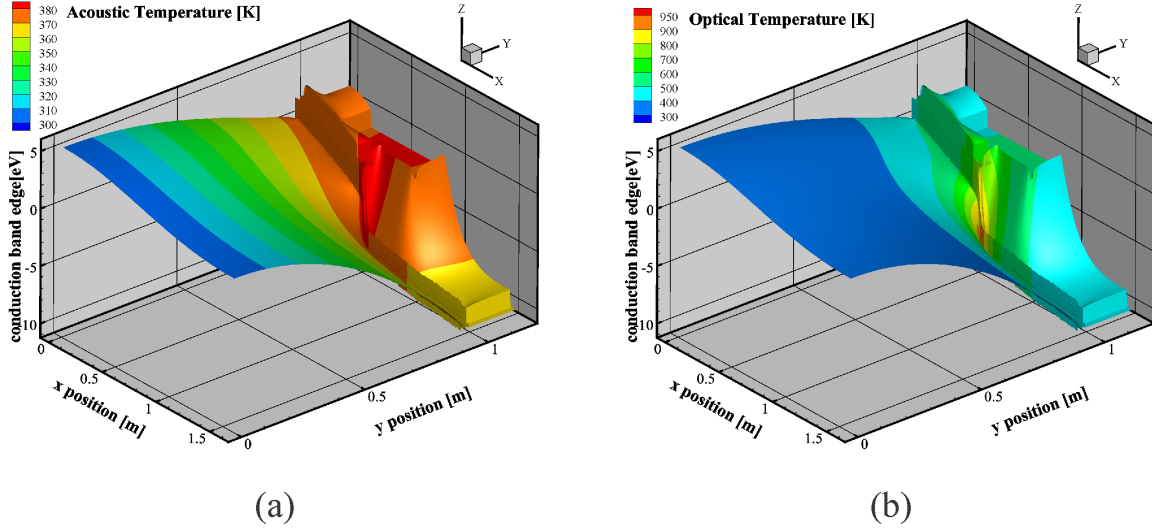


Figure 17. Acoustic (a) and Optical (b) Mode Temperature Maps Obtained for the T-Gate Device at $V_{DS} = 10\text{V}$ and $V_{GS} = 2\text{V}$ Using the Iterative Method [20] ©2020 ASME

the perfect heat sink represented by the Dirichlet boundary condition would be represented by $H \rightarrow \infty$, and also that the most extreme condition of $H = 10^7 \text{ W/m}^2\text{K}$ is an unrealistically poor heat sink, as evidenced by the extremely large temperatures seen in Fig 19. However, the heat transport across semiconductor/substrate material interfaces is often poor, resulting in lower values of H than considered here.

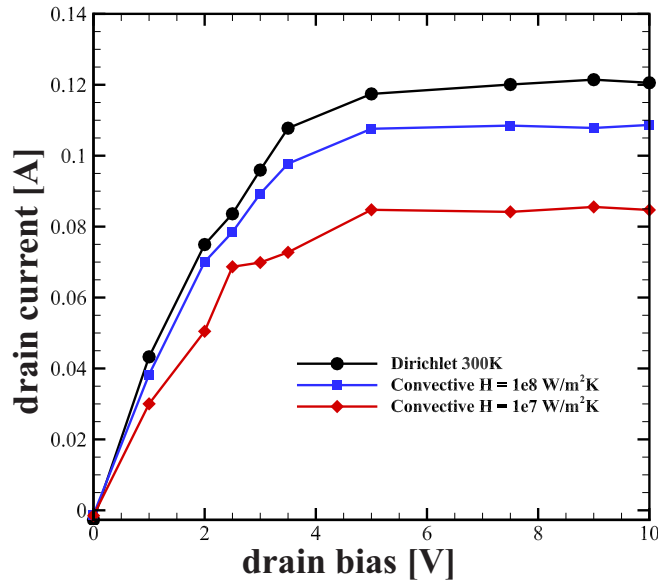


Figure 18. Full Electrothermal I-V Curve for $V_{GS} = 2V$ for the GaN/AlGaIn HEMT Using Both Dirichlet and Convective Boundary Conditions [20] ©2020 ASME

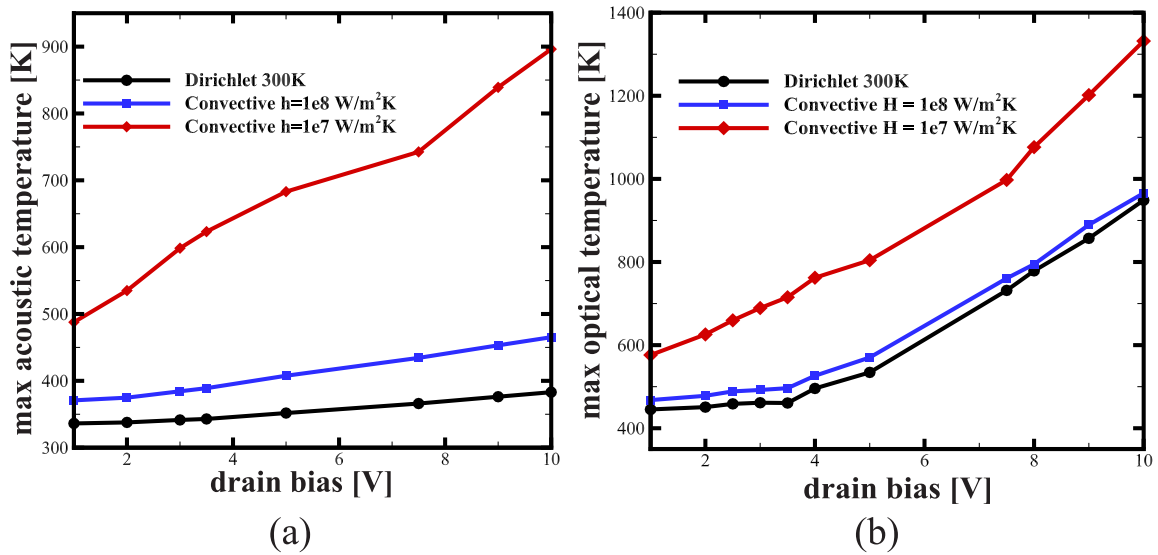


Figure 19. Maximum Optical and Acoustic Temperatures Seen in the Device at Each Simulated Bias Point

Intuitively, as the value of the heat transport coefficient, H , of the heat sink decreases, its ability to dissipate the heat generated in the device is deteriorated, and an associated large decrease in current is seen due to the increase in electron-phonon scattering rates with temperature. Moreover, the current degradation is much more pronounced going from $H = 10^8 \text{ W/m}^2\text{K}$ to $H = 10^7 \text{ W/m}^2\text{K}$ than is seen between the Dirichlet and $H = 10^8 \text{ W/m}^2\text{K}$ boundary conditions. This is due to the large temperature increase when using the $H = 10^7 \text{ W/m}^2\text{K}$ heat sink, which in turn greatly increases the scattering rates seen in the device leading to the reduced current. Therefore, the ability

to simulate non-ideal thermal contacts is highly valuable, as their effect on electrical characteristics are significant even for relatively large values of H , as seen in Figure 18.

4.2.5 Π -Gate Devices and RF Simulation

It has been suggested [27] that rather than using the T-gate structure of Figure 13, hot electron generation can be reduced by splitting the gate into two stems, creating a Π -gate. This layout has the effect of increasing reliability while retaining performance. In essence, this effect is achieved by increasing the electron-phonon scattering rates, which is due to the Π -gate layout producing a higher carrier concentration under the gate as well as a longer transit time due to a spacer region between the two stems [27]. The schematics of these layouts are shown in Figure 20. In particular, in [27] they found that the Π -gate layout with $L_{G,1} > L_{G,2}$ reduced hot electron generation up to 40% under DC operation at bias points corresponding to peak DC power in the dynamic load lines.

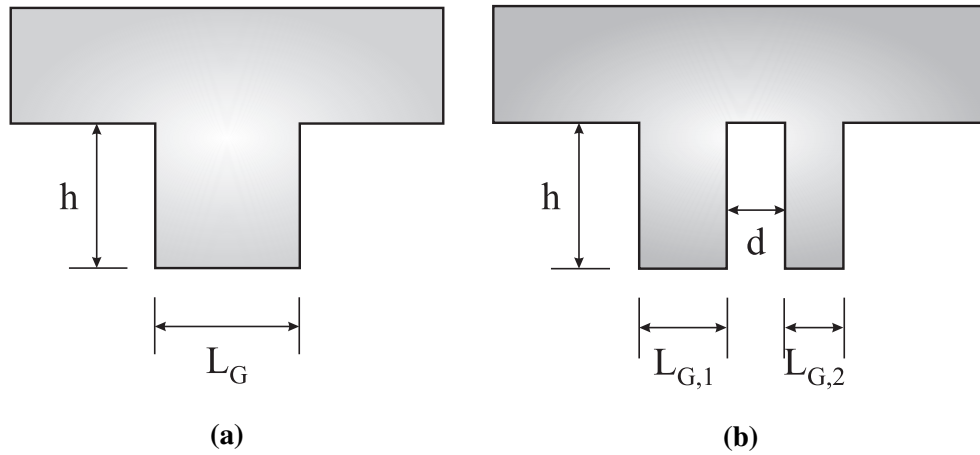


Figure 20. The T-Gate and Π -Gate Structures. Design Rules Require That $L_G = L_{G,1} + L_{G,2}$ [27]

This idea has been applied to the T-gate layout of Figure 13 to produce the Π -gate layout shown in 20b, where $L_{G,1} = 50\text{nm}$, $L_{G,2} = 25\text{nm}$, $d = 25\text{nm}$, and $h = 120\text{nm}$. The source-to-gate and gate-to-drain lengths have been kept constant at $L_{SG} = 500\text{nm}$ and $L_{DG} = 925\text{nm}$, respectively. All other device and simulation parameters are kept constant. As this is expected to decrease hot electron generation, it should correspond to a decrease in peak temperatures obtained from the iterative electrothermal model.

The temperature maps obtained for the bias point $V_{DS} = 10\text{V}$ and $V_{GS} = 2\text{V}$ are shown in Figure 21, with the T-gate results shown in 21a and 21b and those for the Π -gate in 21c and 21d.

In these 3-D plots, the temperature is again plotted as a contour map on top of the 3-D conduction band edge. From this, the acoustic temperature is seen to be uniformly lower throughout the active region of the device near the AlN/GaN barrier at approximately $y = 1\mu\text{m}$, while the difference in the optical temperature distributions are more difficult to discern. To further investigate the temperature maps, the maximum acoustic and optical temperature at each bias point were extracted from the simulation results, and plotted in Figure 22. A decrease of 4K is seen in the peak acoustic

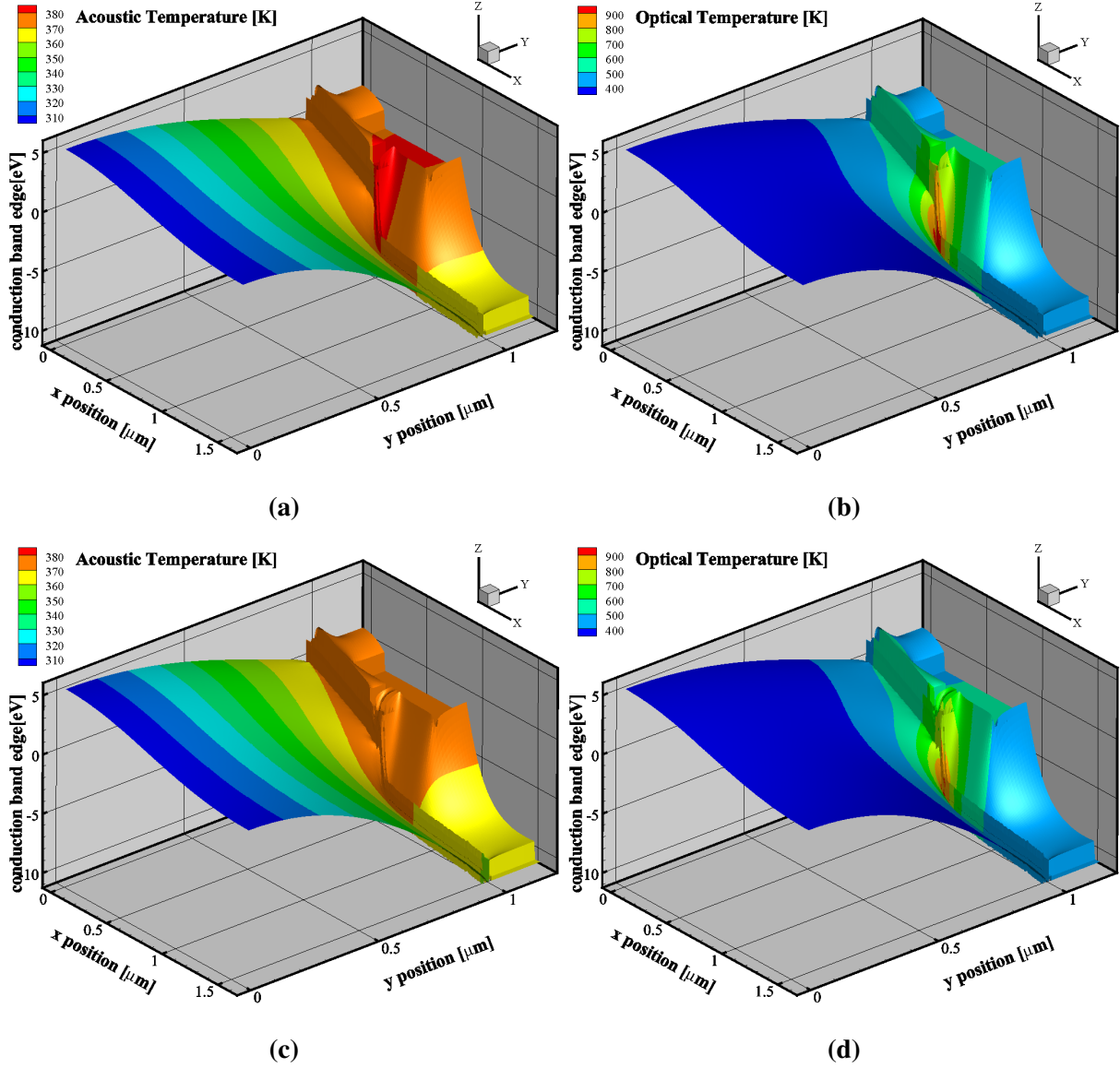


Figure 21. Acoustic and Optical Temperature Obtained for the T-Gate (a,b) and the Π -Gate (c,d) Device Structures

temperature at higher voltages while for the optical temperatures the peak decreases 49K in the asymmetric Π -gate as compared to the conventional T-gate structure. The decrease in the acoustic temperature corresponds to a reduction of 4.8% in the temperature rise above the heat sink temperature of 300K, and for the optical case a 7.5% decrease.

Moreover, the drain current for the two layouts was studied for a $V_{GS} = 2V$ and $V_{DS} = 0 - 10V$. It was found that the drain current for the two layouts in these simulations are nearly identical, and therefore the simulated decrease in temperatures came with no cost in terms of DC performance. Hence, novel gate architectures such as the Π -gate may be a viable path to mitigating undesirable hot electron effects, without drastically reducing device performance.

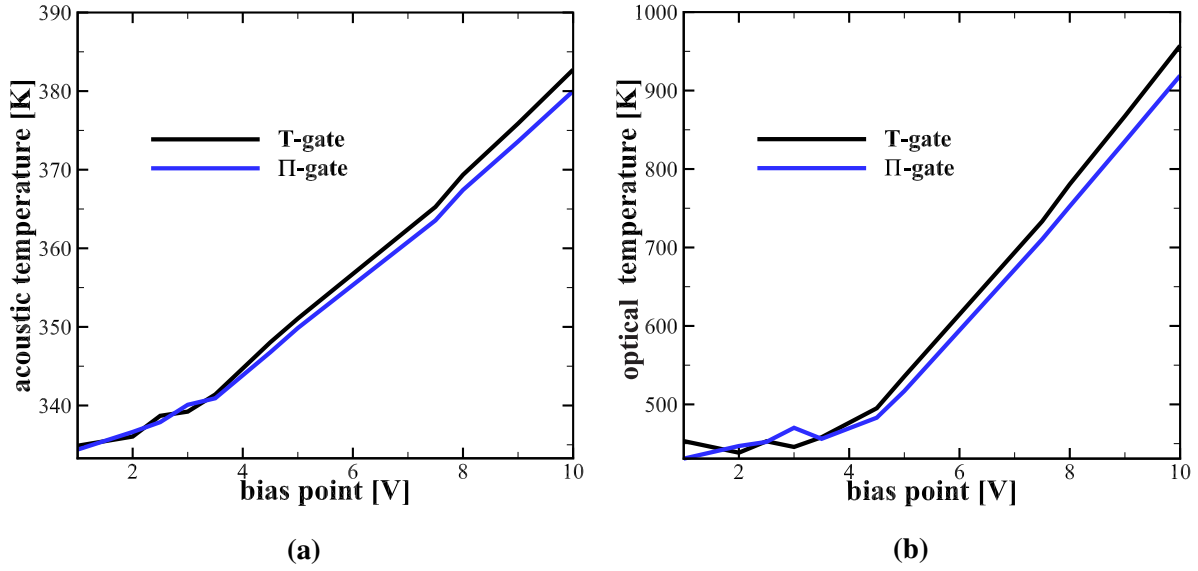


Figure 22. Maximum Optical and Acoustic Temperature Seen in the T-Gate and the Π -Gate Structures

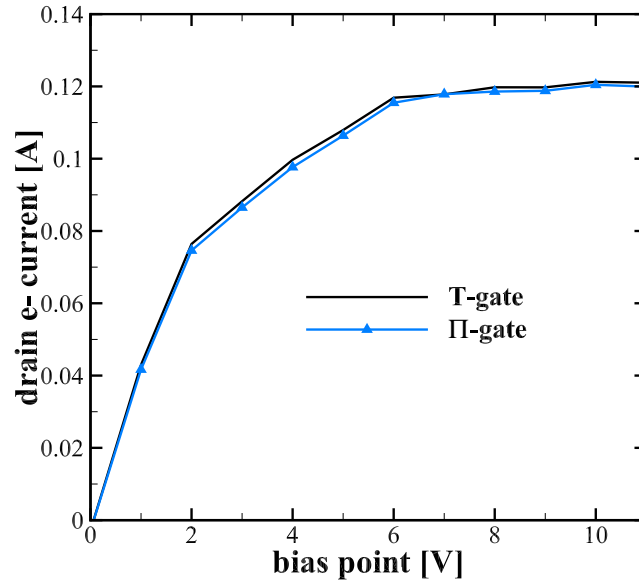


Figure 23. Drain Current vs Drain Bias for the T-Gate and the Π Gate Layouts for a gate voltage of 2V

4.2.6 Electrothermal Small-Signal RF Simulation

The iterative method developed for electrothermal device simulation has also been extended to the domain of small signal AC simulations. In the case of small-signal simulation, it can be assumed that the applied AC signal doesn't have a significant effect on the temperature maps of the device. Hence, the electrothermal simulations from the previous section can be used to generate small

signal RF device characteristics as in [28, 29].

These simulations have been performed as follows: 1) perform a full DC electrothermal characterization of the device, 2) superimpose a small-signal AC sine wave on top of the DC operating point of interest, and 3) extract the relevant RF parameters to determine the cutoff frequency.

In Figure 24a, the results of an isothermal sinusoidal small-signal AC simulation are shown. Using the typical fit line extrapolated to 0dB, for the T-gate layout from [25] a cutoff frequency of 135GHz is found compared to $f_t = 122$ GHz in the Π -gate. However, in [25] the cutoff frequency was experimentally determined to be 116 GHz. It is hypothesized that this discrepancy is due to thermal effects not being taken into consideration.

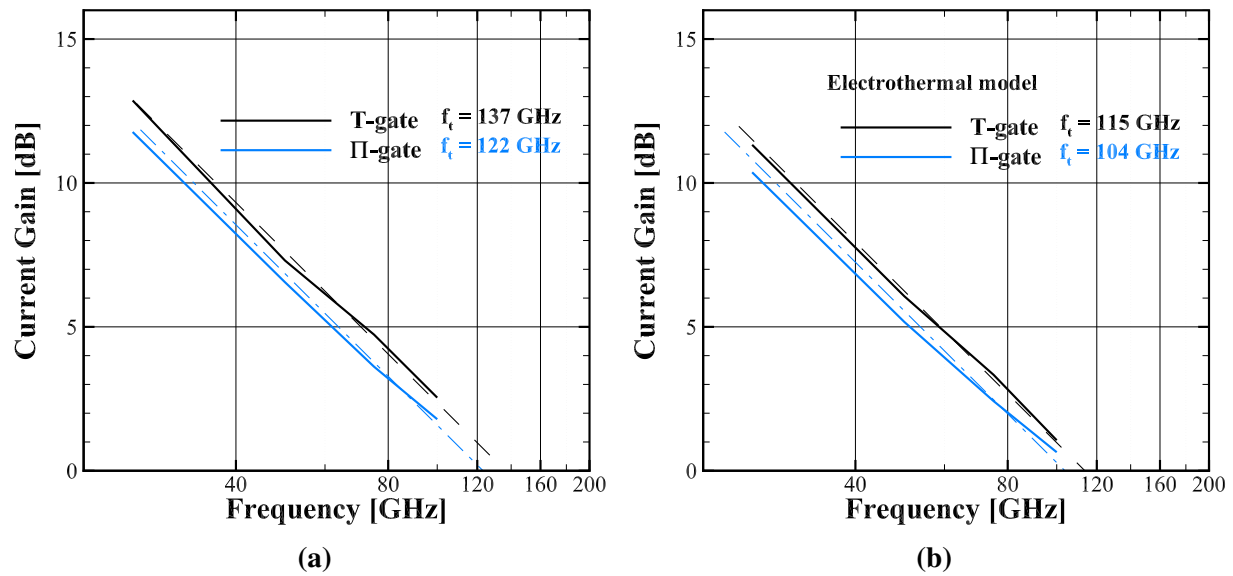


Figure 24. Small Signal Simulation Using Sinusoidal Inputs to Determine the Cutoff Frequency in Both (a) Isothermal and (b) Electrothermal Simulations

To test this hypothesis, the iterative electrothermal model has been applied to both layouts, and the results shown in Figure 24b. Here, a cutoff frequency of $f_t = 115$ GHz is found for the Altuntas device, agreeing very closely with the value of $f_t = 116$ GHz, while for the Π -gate structure a cutoff frequency of 104 GHz is obtained. Hence, the cutoff frequency in the Π -gate structure is slightly less degraded by the inclusion of thermal effects in the model.

However, it is of note that the electrothermal simulation methods studied here are able to obtain much improved results for small-signal AC simulations in addition to those seen for DC operating currents. Therefore, this new model represents an obvious improvement on isothermal simulation

5.0 CONCLUSIONS

Thermal management is nowadays perhaps the largest problem facing semiconductor devices, and is still an area of active research. Methods based on low order moments of the BTE can provide reasonable results in many cases, and lend insight to device characteristics in a relatively short simulation time. However, they necessarily neglect whatever information about the carrier ensemble is contained in the higher order moments that are not taken into account. In addition, assumptions made in order to derive these models in closed form are often only valid near-equilibrium.

Monte Carlo methods, on the other hand, are more computationally expensive but yield a full stochastic solution to the BTE. Furthermore, Monte Carlo methods are invaluable at high electric fields where far-from-equilibrium conditions apply. The CMC approach shifts some of the computational cost to hardware cost by pre-tabulating the scattering rates and loading them into memory at the start of a simulation. This provides a significant decrease of the simulation time as compared to the traditional Ensemble Monte Carlo (EMC), where final states are obtained at run-time for each scattering event. Moreover, the CMC is able to be adapted to local runtime conditions, akin the the EMC algorithm, by employing a rejection method to decide if a “proposed” scattering event should occur or not based on the local conditions.

Still, the use of MC methods in the study of thermal transport along with electrical characteristics has been less widespread until recently. While thermal models have been developed and implemented in MC simulation, they often neglect the temperature dependence of material properties, namely the thermal conductivity. Here we have presented a particle-particle based and particle-flux based electrothermal simulation framework.

The iterative approach for solving an energy balance equation, based on the $n = 2$ moment of the phonon BTE, and including temperature-dependent properties within a Monte Carlo simulation has been detailed here. This approach has been developed to overcome the drawbacks of using the Kirchhoff transformation while still allowing us to solve a linear Poisson-like equation. In particular, it tackles problems including convective boundary conditions, such as material interfaces or non-ideal heat sinks, in a straightforward way which is relatively easy to implement. The importance of solving a Poisson-like equation is that often an efficient finite-difference solver for the Poisson equation is present in any MC electrical device simulator.

However, one potential drawback of the iterative approach is that, since the thermal conductivity is likely to have a different value at each computational gridpoint, multigrid methods are likely to become very inefficient. Fortunately, in an electrothermal simulation, the solution to Poisson’s equation is required much more often (orders of magnitude more times), than that of the phonon EBE.

Furthermore, a novel method for computing the heat generation rate is used in the CMC based directly on the electron-phonon scattering events using energy conservation principles. This provides a physically sound model of heat generation, and is not subject to macroscopic parameters such as the effective mass or carrier mobility.

The iterative method has been shown to work extremely well for thermal large-scale thermal spreading problems, as well as coupled to the CMC framework for full non-linear electrothermal device simulation, *e.g.*, as applied to the GaN HEMT devices. Moreover, it can be used to study the

electrothermal characteristics of novel device layouts with the aim of mitigating thermal effects and improving device performance and reliability. Small-signal AC simulations using the iterative electrothermal model are able to reproduce experimentally determined cutoff frequencies in devices.

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List of Acronyms, Abbreviations, and Symbols

2DEG	2-dimensional electron gas.
B-E	Bose-Einstein.
BTE	Boltzmann transport equation.
CMC	cellular Monte Carlo.
EBE	energy balance equation.
FEA	finite element analysis.
GaAs	gallium arsenide.
GaN	gallium nitride.
HEMT	high electron mobility transistor.
MC	Monte Carlo.
PDE	partial differential equation.
RF	radio frequency.
Si	silicon.
SiC	silicon carbide.
SOR	successive over-relaxation.
α	exponent in power law for temperature dependent thermal conductivity.
H	heat transfer coefficient.
k_{300}	thermal conductivity at 300K.
R_{TH}	thermal resistance.
Θ	Kirchhoff transformed apparent temperature.