Simulation of a DBR Edge Emitting Laser with External Air Gap Tuning Mirror

Abstract
A methodology for simulating an edge emitting laser is demonstrated that incorporates a distributed Bragg Reflector (DBR) as one of the mirrors, with the other being a variable air gap external planar mirror that is used as a method for fine tuning the lasing wavelength. This type of calculation requires non uniformity of the dielectric's static and dynamic (pumping) properties in both the transverse and longitudinal directions, together with self consistent coupling to the external tuning cavity. A key challenge addressed is the proper treatment of the open nature of the cavity, such that the amplitudes of the outgoing waves leaving the facets are consistent with the cavity interior and facet reflectivity. Mode competition and hopping are natural consequences of the methodology developed. In the model developed here, the spatial hole burning effects, cross and self-saturation effects can be included while accounting for the degree of spatial overlap of modes. We also account for diffraction losses at the output facet which can become important in the case of strong index guiding.

Key Words: Laser, DBR, External Mirror Air Gap Tuning Cavity, Effective Medium Method, Electro-Optic modulation

Introduction
Distributed Bragg reflectors (DBR) play an important role in optical filtering and as mirrors. They are used for frequency selective mirrors to shape the spectral response of laser cavities in both vertical cavity surface emitting and edge emitting lasers. DBRs employ Bragg reflection to attenuate propagation of light through their grating structure, thus creating a highly reflective band in their transmission function. Bragg reflection is used to an opposite effect in distributed feedback lasers (DFB), in which the resonator modes are the Bragg waves allowed to propagate through the grating structure that extends over the entire cavity. However, the main structural aspect common to both types of lasers is the essential non-uniformity of their refractive index along the direction of mode propagation. Of critical importance to their operation and performance are also the pumping induced non-uniformity in their interior refractive index and optical intensity. An important aspect of all laser cavities is also the fact that they are open systems from which light escapes to the outside.

In our previous articles on edge emitting (EEL) and vertical (VCSELs) lasers, we exploited the cylindrical symmetry to treat non-uniform cavities, while simultaneously keeping the problem essentially 2D or 1D. We treated the cavity as an open system only in the case of VCSELs, and ignored the longitudinal non-uniformity (along the propagation direction) in the case of rectangular EELs. Here we describe a hybrid - a rectangular edge emitting open laser cavity with a DBR at one end, and in which we take longitudinal non-uniformity fully into account. We go a step further and allow for an external air gap tuning cavity by including the effects of coherent longitudinal propagation within the air gap, but with beam diffraction treated approximately as an additional loss mechanism. The longitudinal mode spectrum is calculated self consistently with electrical and thermal induced variations in the cavity refractive index.

Continued on page 2 ...
In the hybrid DBR edge emitting laser described here, the requirement to resolve the localized optical intensity patterns is fundamentally a 3D problem, since the DBR reflector must resolve optical standing waves along the propagation direction, and the gain cavity must resolve modal intensities transverse to this direction. However, the problem can be reduced to 2D for cavities that are structurally uniform in one of the transverse directions, with vanishing electric field at all boundaries of the plane, which is a reasonable approximation to real systems featuring index guiding.

The open nature of the cavity is due to the partially reflective surfaces at both ends, so that a fraction of the field propagating inside transmits across the facets, and radiates out to infinity. Solving for modes that are consistent with this condition requires matching both the amplitude and the derivative of the field to the outgoing plane waves in the space outside the resonator. This boundary condition, and the frequency dependence of the dielectric function inside the cavity, result in a nonlinear eigenvalue problem for its optical modes. These modes are called quasi-normal modes to emphasize the fact that their associated eigenfrequencies are complex, whose imaginary part gives the finite lifetime of the field inside the cavity. The above boundary condition and the complex dielectric function mean that the lifetime of the mode accounts for both the absorptive losses in the cavity interior and the photon escape due to the open boundary. For readers familiar with the literature in this field, we remark that the modes found here are characterized by real valued wavevectors outside the resonator, and complex wavevectors (in general) inside. Thus, they are actually constant flux states[1, 2].

In contrast to the longitudinal mode spectrum given by \( \omega_n = \pi c/(nL) \) for a cavity of length \( L \) and refractive index \( n \), the quasi-normal modal frequencies must be determined from solutions of the complex Helmholtz equation. A straightforward application of this strategy can result in a prohibitively slow simulation. However our code makes use of the effective medium method as in the VCSEL simulations, as well as various software level techniques, so that the simulations described below can be completed within 1-2 hours each.

This article is organized as follows. We begin by outlining the methodology for creating the structure and the mesh to setup the simulation. We briefly recount the important theoretical steps of the calculations carried out by the new code, and discuss their scope. We then discuss the results of several illustrative simulations for a GaAs/AlGaAs DBR laser, followed by concluding remarks.

2 Methodology

2.1 Structure Creation and Meshing

In order to facilitate easy creation of the two fundamentally different regions of a DBR edge emitting laser, namely the active laser regions and the distributed brag reflector (DBR), a combination of the normal region statements coupled with automated DBR creation statements are used. The few layers constituting the active laser regions are defined first, followed by the automated creation of the DBR mirror, which over-writes the previously created active laser regions and is at right angles to them. The entire complicated material structure can therefore be created in just a few lines.

Meshing is further simplified by separation of the structure meshing from the mesh used in the optical active laser simulations. In the case of DBR laser, the laser mesh is automatically modified to include the DBR regions generated by structure meshing. The laser mesh can then be fine tuned to properly include dielectric modulations within the laser cavity, independent of the DBR regions.

2.2 Theoretical Approach

Model of the Laser Cavity

In frequency space, the electric field satisfies the Helmholtz equation[3],

\[
\nabla^2 \mathbf{E}(\mathbf{r}, \omega) + \frac{\omega^2}{c^2} n^2(\mathbf{r}, \omega) \mathbf{E}(\mathbf{r}, \omega) = 0, \quad (1)
\]

where \( c \) is the speed of light, and \( n(\mathbf{r}, \omega) \) is the spatially and frequency dependent refractive index. We assume \( n(\mathbf{r}, \omega) \) to have a step discontinuity at the cavity facets, so that \( n = 1 \) outside and takes arbitrary values inside the cavity, while constrained by the condition of causality. With the coordinate frame shown in Figure 1, we take \( \mathbf{E}(\mathbf{r}, \omega) = 0 \) at the cavity boundaries in the xz plane. At the rear (\( y = 0 \)) and front (\( y = L \)) facets, we impose the open boundary conditions that force the field just outside the cavity to be an outgoing plane wave,

\[
\frac{\partial}{\partial y} \mathbf{E}(\mathbf{r}, \omega) + ik_y(\omega)\mathbf{E}(\mathbf{r}, \omega) = 0, \quad y = 0^-; \quad (2)
\]

\[
\frac{\partial}{\partial y} \mathbf{E}(\mathbf{r}, \omega) - ik_y(\omega)\mathbf{E}(\mathbf{r}, \omega) = 0, \quad y = L^+; \quad (3)
\]

where \( k_y(\omega) = \text{Re}[\omega/c] \). Since the wavevector is real outside the cavity, it yields a physical plane wave in contrast to quasi-bound states that diverge or vanish at infinity. In recent literature on open cavities, these modes have been termed constant flux states[1].

The frequency \( \omega \) is real-valued so far, but it is continued analytically to complex values. The Helmholtz equation (1) is an eigenvalue equation, with eigenvalues \( \omega \) corresponding to frequencies of the modes supported by the cavity. Due to the frequency dependence of the refrac-
tive index, \( n(\mathbf{r}, \omega) \), and the \( \omega \)-dependent boundary conditions, it is a non-linear eigenvalue problem. To solve this eigenvalue problem, we follow our previous modeling of VCSELs (see also Wenzel et al. [4]).

For a fixed \( \omega_0 \) and letting \( k_z = \omega_0 / c \), (1) transforms into a linear problem for a dimensionless eigenvalue \( \nu \),

\[
\nabla^2 \mathbf{E}(\mathbf{r}, \omega) + k_0^2 n(\mathbf{r}, \omega_0) \mathbf{E}(\mathbf{r}, \omega) = \frac{\nu k_0^2 n(\mathbf{r}, \omega_0)}{c^2} \mathbf{E}(\mathbf{r}, \omega), \tag{4}
\]

where \( n(\mathbf{r}, \omega) \) is the group refractive index,

\[
n(\mathbf{r}, \omega) = \frac{\partial [\text{Re}(n(\mathbf{r}, \omega))]}{\partial \omega}. \tag{5}
\]

We assume that the laser cavity is uniform and large in the \( z \) direction and identify the modes predominantly TE or TM like, which is a good approximation when the field confinement in \( z \) direction is not significant. We write the field amplitude in a separable form,

\[
\mathbf{E}(\mathbf{r}, \omega) = X(x; y)Y(y) \sin \left( \frac{\pi z}{L} \right),
\]

where \( h \) is the cavity depth in the \( z \) direction, and we have omitted the \( \omega \) dependence of \( X \) and \( Y \) for clarity. The function \( X(x; y) \) depends parametrically on \( y \), and satisfies a scalar 1D Helmholtz equation in variable \( x \). It generates the transverse mode profile, with effective index \( n_{\text{eff}}(y, \omega_0) \), and defines an effective medium described by two re-fractive indices \( n_{\text{eff}}(y, \omega_0) \) and \( \langle n_{\text{eff}}(y, \omega_0) \rangle \),

\[
n_{\text{eff}}(y, \omega_0) = \frac{\int dx [r(\mathbf{r}, \omega_0) - n(\mathbf{r}, \omega_0)] X^2(x; y)}{\int dx X^2(x; y)}, \tag{6}
\]

\[
\langle n_{\text{eff}}(y, \omega_0) \rangle = \frac{\int dx [r(\mathbf{r}, \omega_0) - n(\mathbf{r}, \omega_0)] X(x; y)}{\int dx X^2(x; y)}. \tag{7}
\]

The longitudinal propagation of the mode, with profile \( Y(y) \), is then a 1D propagation inside this effective medium, governed by these effective indices. We incorporate the continuity of the fields at the boundaries, and the arbitrary variation of the refractive index in the cavity, to compute \( X(x; y) \) and \( Y(y) \) to construct a transfer matrix for the cavity. We refer to this matrix as \( Q(\omega) \) and its element, \( Q_{ij}(\omega_0) \), is the inverse transfer function of the cavity for outgoing modes. The transfer function then provides the mode frequencies, and its multiplication with the frequency dependent spontaneous emission rate yields the amplified spontaneous emission spectrum[5] of the resonator.

For concreteness, we mention that for a Fabry-Perot cavity with facet reflectivities equal to \( r_f \) and \( r_p \), the modes of this transfer function correspond to the familiar condition \( 1 - r_f r_p e^{2 \pi n_0 \lambda / c} = 2 \), where \( \alpha \) and \( g \) are internal loss and gain respectively. As in the Fabry-Perot cavity, finite loss due to \( r_f r_p < 1 \) and \( \alpha - g \) implies that the poles lie at complex values of \( \omega \).

Our method lends itself naturally to modify the optical properties at the output facets by accounting for the effects of transverse confinement on mode reflectivities and coupling to external cavities, as described below. In our methodology, the rear interface can be modeled as a film of specified power reflection coefficient, and the front facet as either a film, or an external air gap cavity.

**External Air Gap Cavity**

An air gap cavity can be included in our model by specifying the location of an external mirror facing the resonator output facet. The external mirror location is outside the Atlas mesh, and therefore the cavity can be modeled without extending the laser mesh. The air gap formed between the facet and the mirror extends the cavity in both the longitudinal and transverse directions. The extension in the longitudinal direction shifts the mode spectrum due to increase in the effective optical length of the cavity. The extension in the transverse direction introduces diffraction due to free space propagation within the gap. After a round-trip in the air gap, the diffracted beam re-entering the waveguide couples to all its guided, leaky, and radiation modes. Since we aim to model cavities operating (and lasing) at a single transverse mode, this coupling becomes an effective loss mechanism for the transverse mode.

At frequency \( \omega_0 \), the modes of the air gap are superpositions of plane waves propagating back and forth between its two ends. From this field, and the purely outgoing field at the outer face of external mirror, we construct an effective transfer matrix for the front facet due to the presence of an external mirror and the diffraction within the air gap [6]. The interface transfer matrices are then multiplied into the cavity transfer matrix to construct an effective transfer function for the entire structure.

**Self-consistency**

Simulation of lasing must always account for the drastic changes in the refractive index to account for the bias induced changes from absorption to gain over an expanding frequency range. In addition to this, thermal effects associated with the power flow further modify the frequency dependence of the refractive index. From the above discussion of theory, it is clear that the mode spectrum would also shift as a result of these changes to the refractive index. Thus it is important that the simulated mode spectrum is self-consistent with the electrical and thermal conditions of the cavity. In our methodology, we begin with modes of a cold cavity, and converge to the solutions of coupled Helmholtz, drift-diffusion, and photon rate equations. The computation uses a look-ahead strategy to compute mode spectrum only when it shifts by more than the mode line width. This results in much faster simulation, with little effect on accuracy of the solutions.
Simulations

We performed simulations for the structure shown in Figure 1. The structure consists of 100 micron long AlGaAs waveguide, with a 100 nm GaAs gain region in the center. The waveguide has a GaAs/AlGaAs DBR mirror made of 40 half cycles with widths tuned to the photon energy of 1.4 eV. In the present simulations, we use a real refractive index (set IMAG.INDEX=0 on MATERIALS statement) everywhere except in the active layer. Within the active region, we use the standard gain model implemented in Atlas, with the prefactor, GAIN0 = 6000, and we broadened the gain spectrum by a Gaussian of linewidth 5 meV. We also included free carrier absorption within the gain region by using the model

\[ f = f_n n_c + f_p n_p, \]

where \( f \) is the free carrier absorption, and \( n_c \) and \( n_p \) are the electron and hole densities. The parameters \( f_n = 10^{-18} \text{cm}^2 \) and \( f_p = 2 \times 10^{-18} \text{cm}^2 \) were used to phenomenologically set the carrier related absorption loss to about 20 cm\(^{-1}\). We also activated frequency dependent modal reflectance including diffraction losses at the front facet by specifying MODAL.REFLECTANCE and LOSS.DIFFRACTION on the LASER statement. The band gap of the active medium was set to 1.39 eV.

The laser model described here is activated by the parameter HYBRID on the LASER statement. We set (NMODE=1) and (MAX.LMODES=12), to force Atlas to search upto a maximum of 12 TE like modes with the fundamental transverse mode, within the energy range 1.384 eV to 1.415 eV. Atlas performs this search at all bias points, updating the transfer function magnitude \(|Q_{11}(\omega)|^{-1}\) as the refractive index changes.

In Figure 2, we show the amplified spontaneous emission spectra at a sub-threshold bias of 1.4 V: the blue corresponds to the laser cavity without any external mirror, and the red to the presence of an air gap 0.6 micron wide and formed by a mirror with power reflectivity of 40%. The effectively larger cavity results in redshift of the spectrum. The frequency dependence of reflectivities, the transmission function of the external cavity, and the refractive index further modulate the spectrum. The ASE with air gap also exhibit smaller linewidths, which is due to the slightly smaller escape rate caused by a mirror of higher reflectance than the approximately 30% reflection from the waveguide face alone (see Figure 3).

We now turn to the simulation of electrical pumping of the above structure (with no air gap). Figure 4 shows the photon densities as a function of anode current for the three most populated modes. Single mode lasing is distinctly visible in this graph. Using the SPECTRUM parameter on
the SAVE statements, we also saved the spectra of cavity transmission \(|Q_{11}(\omega)|^{-1}\), and modal photon densities at sub-threshold (1 mA and 1.2 mA denoted as A and B in 4), and above threshold current of 1.6 mA (denoted as C).

Figure 5 shows the evolution of the cavity transmission function \(|Q_{11}|^{-1}\) as the bias current is tuned far into the lasing regime. These curves convey two important physical points. First, the peaks blue shift due to reduction in the real part of the refractive index, which in turn is the result of rising gain. This effect can be understood roughly from the Fabry-Perot picture where the modal frequencies are given by \(\omega_m = \pi mL/ (n_r c)\) for integer \(m\) and real refractive index \(n_r\). Second, the slowly varying modulation of the spectra shows a remarkable change as we move above threshold. This is caused by gain compensation of the net loss due to both absorption and escape from facets. We can see from this spectrum, and confirm from a plot of photon energies of the modes, that lasing occurs near the highest peaks in \(|Q_{11}|^{-1}\).

The actual modal frequencies are slightly shifted from the location of peaks in the transmission function. The location of a pole relative to the peak on the real axis is controlled by the overall phase of the function \(Q_{11}(\omega)\). In addition, by allowing the refractive index to change linearly in the complex domain, we effectively tune the optical path length of the wave, which becomes \(n(\omega_0)(1 - \nu/2)\). This results in shift of the modal frequencies with respect to the reference frequencies identified from Figure 5.

In Figure 6, we plot the photon densities at modal energies at the three operating points shown in Figure 4. We found that the real part of the complex resonator eigenfrequencies were shifted relative to the peaks of the transmission function by about 0.04 meV. This additional shift arises from the phase accumulation within the cavity, the DBR, and the phase shifts associated with the output facet. This additional shift is often small enough to be ignored. If these shifts are significant, then this particular behavior of modes must be closely scrutinized with respect to the material models, parameters, and the geometry of the laser. We do not investigate this further here due to the scope of this introductory article.

Conclusion

In summary, we have demonstrated a methodology for simulating rectangular laser cavities with nonuniform dielectric along the propagating direction of the cavity, while also taking the open nature of the resonator into account when computing its modes. This strategy allows one to study effects such as dynamic shifts in modal spectrum due to pumping, mode competition, and the addition of external air gap to fine tune the lasing mode wavelength. We also found that while overall blue and red shifts in the spectra can be understood robustly as...
arising from changes in the intensity weighted refractive index, additional shifts (less than 1 meV) also exist, which are controlled sensitively by the material and geometrical modeling of the resonator.

References
**Atlas Simulation of a Wide Bandgap Ga$_2$O$_3$ MOSFET**

**Introduction**

Single-crystal gallium oxide (Ga$_2$O$_3$) has attracted increasing attention as a promising material for power device applications. It possesses excellent material properties and has the potential for mass productivity of low-cost and high-quality bulk crystals by using methods such as the edge-defined film-fed growth (EFG) method [1].

Table 1 shows Ga$_2$O$_3$ material properties compared with major wide bandgap semiconductors, 4H-SiC and GaN. It is remarkable that Ga$_2$O$_3$ has a wider bandgap and several times larger value of Baliga’s figure of merit (BFOM) than those of 4H-SiC and GaN. This indicates that Ga$_2$O$_3$ has an advantage in minimizing conduction losses of power FETs, and it can be expected to exceed 4H-SiC and GaN performances when used for high-power and high-voltage applications.

On the other hand, from a numerical simulation point of view, the wider the bandgap becomes the more difficult it is to get stable convergence, because the intrinsic carrier concentration becomes too low to estimate exact leakage current in the carrier continuity equations.

The objective of this article is to show the Atlas applicability for this new wide bandgap oxide semiconductor material Ga$_2$O$_3$ and to reveal what kinds of physical models and settings (traps and charges, etc.) are needed in order to reproduce experimental I-V data.

**Device Structure and Material Parameters**

The experimental data used in this benchmark were selected from a recently reported paper on the first demonstration of Ga$_2$O$_3$ MOSFET [3]. The simulated device structure cross section and doping profile are shown in Figure 1.

The substrate is a semi-insulating single-crystal β-Ga$_2$O$_3$, and a 300 [nm] thick n-type Ga$_2$O$_3$ channel layer was grown on it. The dopant concentration of the layer is $7\times10^{17}$ [1/cm$^3$] and about half of this is considered to be activated. The source and drain contact regions were formed by multiple Si implantations with 150 [nm] deep box profile whose concentration is $5\times10^{19}$ [1/cm$^3$]. Judging from C-V measurement data shown in the paper [3], we assumed that $3\times10^{19}$ [1/cm$^3$] were activated. The distance between the source and the drain box regions is 20 [um] and a 20 [nm] thick Al$_2$O$_3$ gate dielectric film was formed with a 2 [um] long Ti/Pt/Au metal gate on top.

Some of the material parameters of Ga$_2$O$_3$ are not fully established yet. We calculated the local conduction band density of states $N_c=3.72\times10^{18}$ [1/cm$^3$] from the value of an electron effective mass of 0.28$m_0$ [4]. The electron affinity of β-Ga$_2$O$_3$ and the work function of the gate were assumed to be 4.0 [eV] and 5.23 [eV] respectively from ref. [5].

<table>
<thead>
<tr>
<th></th>
<th>4H-SiC</th>
<th>GaN</th>
<th>β-Ga$_2$O$_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bandgap $E_g$ [eV]</td>
<td>3.3 (3.23)</td>
<td>3.4 (3.43)</td>
<td>4.8</td>
</tr>
<tr>
<td>Electron mobility $\mu$ [cm$^2$/Vs]</td>
<td>1000 (460)</td>
<td>1200 (400)</td>
<td>300</td>
</tr>
<tr>
<td>Breakdown field $E_b$ [MV/cm]</td>
<td>2.5</td>
<td>3.3</td>
<td>8</td>
</tr>
<tr>
<td>Relative dielectric constant $\varepsilon$</td>
<td>9.7 (9.7)</td>
<td>9.0 (8.9)</td>
<td>10</td>
</tr>
<tr>
<td>BFOM $\varepsilon \times \mu \times E_b$</td>
<td>340</td>
<td>870</td>
<td>3444</td>
</tr>
<tr>
<td>Intrinsic carrier concentration $N_i$ [1/cm$^3$]</td>
<td>(1.73E-8)</td>
<td>(1.06E-10)</td>
<td>(1.79E-22)</td>
</tr>
</tbody>
</table>

Table 1. *Material properties of wide bandgap semiconductors. These figures are taken from reference [2] except for the figures in parentheses which are from Atlas device simulator.*
Simulation Results and Discussions

Simulated ID-VD curves and a ID-VG curve are shown in Figure 2 and Figure 3 with corresponding experimental data.

We selected simple device models as much as possible. Only the LAT.TEMP parameter was set on the MODEL statement to solve the heat flow in the device and a constant thermal conductivity model was used. A basic constant low-field mobility model was selected with the lattice temperature coefficient for the temperature dependence of electron mobility $\mu_{n0} = \frac{\mu_{n0}}{300} - TMUN$ in equation (I).

$$\mu_{n0} = \frac{\mu_{n0}}{300} - TMUN$$  \hspace{1cm} (I)

Other parameters used for fittings are shown in Table 2.

<table>
<thead>
<tr>
<th></th>
<th>Electron mobility [cm²/Vs]</th>
<th>N-type active dopant concentration [1/cm³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Channel layer</td>
<td>118</td>
<td>$1.1 \times 10^{17}$</td>
</tr>
<tr>
<td>Semi-insulating</td>
<td>20</td>
<td>$1.5 \times 10^{16}$</td>
</tr>
<tr>
<td>substrate</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2. Fitting parameters used in this simulation.

The parameter figures in Table 2 appear to be within reasonable bounds. In this MOSFET case, it is noticeable that a complex model, trap and interface charge were not necessary to reproduce the experimental I-V curves.

In addition to the Atlas device simulation above, we applied the Athena process simulator for reproducing the multiple Si implantation profile [6] using a BCA amorphous material implants model. The implantation energies were 175, 95, 60, 30, and 10 [keV] with corresponding dose ratio of 0.64, 0.15, 0.11, 0.07 and 0.03. The total dose was $1 \times 10^{15}$ [1/cm²].

The comparison between simulation and SIMS experiment is shown in Figure 4.

Although the channeling effect was not considered, it seems that Athena is also useful for a rough estimation of multiple implantation profile.
Conclusion

We demonstrated Atlas device simulation of a Ga$_2$O$_3$ MOSFET’s DC and transfer characteristics. Fairly good agreements with experimental data were obtained using constant mobility model even without any defect trap and interface charge. Also, Athena BCA Monte Carlo implantation simulation was applied to simulate doping profiles successfully. In view of these results, Ga$_2$O$_3$ is a promising material free from serious crystal defects which are suitable for device fabrication, and expected to surpass 4H-SiC and GaN materials in power device applications.

References


Q. How do I Simulate Rapid Thermal Annealing Temperature Transients in Vacuum?

A. When a wafer is clamped only at its edges and is heated with an infra-red source in a vacuum, the majority of the heat loss occurs through black body radiation. The vacuum prevents thermal conduction mechanisms for the majority of the wafer area. It is also important to realize that if both sides of the wafer are exposed to the vacuum without contact to a conductive heat sink, both the front and back sides of the wafer will radiate heat and so black body heat radiation must be simulated from both surfaces for accurate results.

In Atlas, black body radiation is simulated with an additional logical parameter, “BLACKBODY” added to the “THERMCONTACT” statement. This allows the user to set up multiple thermally radiative boundary conditions in their structure.

The power per unit area lost to black body radiation for an ideal radiator, is known absolutely for any given temperature, K. The power absorbed by that same body from its surroundings, is also known absolutely from the temperature of those surroundings. The net power loss or gain, to or from, any body by infra-red radiation, is therefore simply the difference between the power lost to its surroundings and the power absorbed from its surroundings.

The formula in Atlas is given by:

\[
\{ \text{ALPHA} \left( T - \text{EXT.TEMP} \right) \} + \{ \text{STEFAN} \left( T^4 - \text{EXT.TEMP}^4 \right) \} \text{ W/cm}^2
\]

Where:

• “ALPHA” is the coefficient to take account of thermal conductivity to the wafer holder, and should be set to zero if all the heat loss is through radiative processes only
• “T” is the temperature of the surface calculated by Atlas
• “EXT.TEMP” is the external temperature of the surroundings, usually 300K if the equipment is located in normal laboratory conditions
• “STEFAN” is the black body radiation constant

For reflective surfaces, the surface emissivity correction can be taken account of by reducing the value of the “STEFAN” parameter from the ideal black body radiation value of 5.67051x10^{-12} W/cm²/K⁴, which is the default value. The area of the thermal contact is also calculated in Atlas by integrating of the area of all mesh points in contact with the user defined thermal contact.

As a practical application of black body radiation simulation, Figure 1 shows simulated and measured temperatures of an edge clamped wafer in a vacuum, heated by infra-red heat lamps. The main part of the graphic shows the black body radiation cooling of the wafer after being heated. Good correlation with experiment was easily achieved.

So in summary, for an ideal black body radiator, only the background temperature “EXT.TEMP” need be specified on the “THERMCONTACT” statement, the rest will be calculated by Atlas. For reflective surfaces, with less than ideal radiation characteristics, the effective emissivity coefficient can be taken account of by using the appropriate value of the “STEFAN” parameter. Simply multiply the default value of “STEFAN” by the emissivity coefficient. For pure radiative cooling, also set the thermal conductivity coefficient, “ALPHA” to zero.

**Note:** Simulation of black body radiation effects using the methods described in this article requires Atlas version 5.19.24.C or later.

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**How do I get the best performance out of MixedMode 3D on multi-CPU machine?**

The Atlas MixedMode module is a useful method for evaluating the performance of novel devices within a circuit environment. It allows physically-based devices to be embedded within a SPICE circuit simulator and DC, AC and transient simulations to be performed.
To get the best performance out of MixedMode it is necessary to understand how it works. The conductance matrix, which describes how the current at each terminal changes with changing bias, is calculated for every element in the circuit. The circuit simulator uses this information to create a matrix representing the entire circuit and this is solved to determine the nodal voltages.

For a compact model (i.e. SPICE element), the conductance matrix is calculated from an analytical equation. However, the calculations for the physically-based numerical device are more complex and require the solution of a system of partial differential equations. With some mathematical manipulations, this system can be calculated from the standard drift-diffusion Jacobian matrix by using multiple Right Hand Side (RHS) vectors, each of which depends on an electrode. This means that for a device with four electrodes, four linear systems have to be solved for every circuit iteration in addition to the linear system solved in the Newton step.

If a direct solver is used to solve these linear systems, then the inverted drift-diffusion Jacobian matrix from the current bias point can be re-used and a back-substitution step used for each electrode entry. This is extremely fast. Unfortunately, direct solvers are not practical for large 3D problems and an iterative solver must be used to solve these systems. Using an iterative solver means that no inverted Jacobian is available and each electrode entry requires a full linear solution, which can be time-consuming. However, if a machine with multiple CPUs is available then each conductance matrix entry can be solved simultaneously by MixedMode 3D, resulting in a speed-up of the overall simulation time.

Specifying ELEC.PARALLEL on the .NUMERIC statement in the SPICE part of the input deck enables MixedMode 3D to use the maximum number of CPUs available on the machine to solve the conductance matrix. Specifying ELEC.PARALLEL.NUM instead allows the user to specify the maximum number of CPUs to be used.

Example: Three-stage ring oscillator

This example shows the speed performance of a three-stage ring oscillator. Each inverter stage consists of two Atlas devices, so that six Atlas devices are simulated in total.

Figure 1. Three-stage oscillator input deck.

Figure 2. Voltage at nodes 1 and 2 versus time.

Figure 3. The ring oscillator was simulated using varying numbers of CPUs, showing an increase in simulation speed of over 4x when run on 12 CPUs.

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