SIMULATION OF OPTICAL ENERGY DEPOSITION FOR PULSED LASER-INDUCED SINGLE EVENT EFFECTS TESTING IN MICROELECTRONIC DEVICES

By

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Thesis

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While particle accelerators represent the traditional methodology for inducing single event effects (SEE) in microelectronic devices and circuits, increasing demand coupled with a limited number of particle accelerator facilities has led to scarce availability of testing hours. As a result, alternative testing techniques have been developed that can be carried out with more widely available equipment [1]-[2]. Pulsed laser-induced single event effect (PL-SEE) testing has become a staple testing technique that leverages table top laser systems for charge injection through photon absorption processes as opposed to charge generated from ionizing particles [3]. As charge generation is defined by the spatial and temporal behavior of the optical pulse, PL-SEE testing offers greater spatial and temporal resolution than traditional ion facilities. This confinement has been extensively used within the radiation effects community for spatial mapping of device sensitivities and examination of the role of buried junctions in device geometries [3]-[4].

To generate an electron-hole pair in a material, energy greater than the bandgap of the material must be imparted into an electron to move to an excited energy state. For photon energies greater than the bandgap, a single photon can be used to create a single electron-hole pair that is commonly modelled with Beers’ law and referred to as single photon absorption (SPA). As the absorption coefficient is a wavelength-dependent parameter, the testing wavelength of light can be varied to change the distribution of the charge that is injected into a material. Although measurements employing above-bandgap laser wavelengths are used extensively [5],[6],[7], intensity decay into the material typically restricts the technique to devices that share proximity with an unobstructed surface.

In order to combat these constraints imposed by single photon testing, sub-bandgap wavelengths can be used in conjunction with highly focused laser pulses to deposit charge with multiphoton absorption processes [3]. Multiphoton absorption is a nonlinear optical process that occurs when multiple photons simultaneously interacting with a single electron combine to provide enough energy to generate an electron-hole pair. As multiphoton absorption processes require multiple photons, there is dependence on the intensity of the light and charge generation can be
localized to regions of high intensity [8]. Using focusing optics, sub-bandgap wavelength laser pulses can be used to deposit charge locally at the focal point of the pulse without depositing charge from SPA. This technique, using two photons to produce a single electron-hole pair (TPA), is commonly used for through-substrate illumination of devices with topside metallization as there is minimal energy dissipation in the substrate [3].

Though PL-SEE testing has proven to be an invaluable qualitative technique, a renewed interest in predicting heavy ion response with PL-SEE testing has led to the development of correlation methods between the techniques [9],[10]. A simple technique is empirical comparison of the PL-SEE and heavy ion experimental results with an analytical model to calculate “experimental parameters” that map PL-SEE responses onto heavy ion SEE results [10],[11]. However, techniques that require collection of both heavy ion and pulsed laser measurements prior to correlation lack the predictive capabilities necessary to predict heavy ion SEE results strictly from PL-SEE measurements. A more general approach to predicting heavy ion results from PL-SEE requires comparison of the three-dimensional distribution of generated charge induced by both a laser pulse and a heavy ion [12]. Though simulation capabilities for ionizing particles are extensively developed and validated by the community, equivalent capabilities for pulsed lasers have only recently begun to be developed [13]. Currently, the main approach for simulating PL-SEE measurements requires several approximations that reduce the complexity of the simulation while still showing agreement with experimental results for some types of devices [10],[14]. However, recent work has demonstrated cases in which such approximations are unable to fully capture the PL-SEE measurements, suggesting that more sophisticated simulation approaches are required [12],[15].

In this work, a first-principle simulation approach for PL-SEE experiments is developed and compared with experimental results collected on a large area silicon diode. Development and parametrization of nonlinear optical models (Chpt. II) as well as the characterization of a propagating laser pulse is necessary for simulation of a PL-SEE experimental setup (Chpt. III). A commercial first principles optical solver was adapted to incorporate nonlinear optical processes (Chpt. IV) essential in PL-SEE testing to simulate the three dimensional optically generated charge distributions (Chpt. V). These charge distributions are used as an initial condition for charge transport solvers to simulate the electrical response of the diode to the laser pulse (Chpt. VI). Experimental and simulated collected charge is compared for a variety of bias conditions and pulse
energies and demonstrates excellent agreement, affirming the simulation approach implemented for PL-SEE measurements (Chpt. VII). The first principles approach used in this work has proven integral in understanding PL-SEE measurements as well as capturing additional optical processes that impact optical charge generation.
CHAPTER II

LIGHT-MATTER INTERACTION

As optical processes are used for charge deposition, understanding light-matter interaction is critical for modeling charge injection from a pulsed laser. Light, modelled by Maxwell’s equations, is expressed with amplitude and phase; light-matter interaction is modelled as a modulation of amplitude and/or phase. Understanding material interaction requires consideration the index of refraction and absorption coefficient (Beers’ Law); refractive indices and absorption coefficients are traditionally modelled as linear optical processes. As optical processes are expressed amplitude/phase modulation, nonlinear optical processes can be developed as perturbations to the traditional approach for deriving linear processes. In this chapter, the origin of nonlinear optical processes and their incorporation into Maxwell’s equations are explored in order to facilitate the addition of nonlinear models into optical solvers; the derivation of the origins of nonlinear models roughly follows from Boyd [8].

II.1 Maxwell’s Equation

Classical electrodynamics and optics are built upon the foundation of Maxwell’s equations, which are coupled partial differential equations that define the behavior of electromagnetic fields [16]. The microscopic Maxwell’s equations consider electric fields ($E$) and magnetic flux density ($B$) and the interactions with discrete charges (volumetric charge density, $\rho$) and currents (current densities, $J$).

\[
\nabla \cdot E = \frac{\rho}{\varepsilon_0} \quad \text{(II.1A)} \\
\n\nabla \cdot B = 0 \quad \text{(II.1B)} \\
\n\nabla \times E = -\partial_t B \quad \text{(II.1C)} \\
\n\nabla \times B = \mu_0 (\varepsilon_0 \partial_t E + J) \quad \text{(II.1D)}
\]
In the simplest case, a region without any charge or currents \( (\rho = J = 0) \) reduces the complexity of the equations. It can be shown under these conditions that the wave equation shown in Eqn. II.2 can describe the propagation of the electric field in space and time [16].

\[
\mu_0 \varepsilon_0 \partial_{tt} E - \nabla^2 E = 0 \quad (\text{II. 2})
\]

Since the wave equation is a homogenous Helmholtz equation, the solution takes the form of a complex exponential function, as shown in Eqn. II.3.

\[
E(r, t) = A_\omega e^{i k_0 r - i \omega t} \quad (\text{II. 3})
\]

where \( A_\omega \) is an amplitude, \( \omega \) is the angular frequency of the wave, and \( k_0 \) is the wavevector. In order to define the functional form of the wavevector, the solution (Eqn. II.3) can be plugged back into the wave equation (Eqn. II.2) to form a relationship between the wavevector and the angular frequency, as shown in Eqn. II.4.

\[
\left( \frac{\omega^2}{c^2} - k_0^2 \right) E(r, t) = 0 \quad (\text{II. 4})
\]

where \( \frac{1}{c^2} = \mu_0 \varepsilon_0 \). The wavevector in vacuum is \( k_0 = \frac{\omega}{c} = \frac{2\pi}{\lambda_0} \), where \( \lambda_0 \) is the vacuum wavelength.

**Bulk Materials**

Though it is possible to consider bulk material systems through the microscopic form of Maxwell’s equations, considering individual atoms as charge quickly becomes an intractable problem. Under the influence of an external electric field, electrons bound to individual atoms, unable to move freely in the material, are locally displaced according to the charge of the particles and the direction of external field. This local separation of charge induces an electric dipole moment \( \vec{p} \) associated with individual atoms. Rather than considering each dipole individually, the total population of dipoles per unit volume is used to define a polarization density \( (P) \). In a similar manner, individual atoms can contribute to magnetic dipoles based on the angular momentum of the electrons, and the total contribution per unit volume can be expressed as the magnetization.
density \( (M) \). To accommodate bulk material interactions in the Maxwell’s equations, two additional constitutive fields are defined: the electric flux density or displacement field \( (D) \) and the magnetic field \( (H) \) [16].

\[
D = \varepsilon_0 E + P \quad \text{(II. 5)}
\]
\[
H = \frac{1}{\mu_0} B - M \quad \text{(II. 6)}
\]

Nominally, induced dipoles from an external field are not formed instantaneously, but rather exhibit a response time to the applied field. Given this dependence of the polarization density on not only the current field distribution, but also the past field distributions, the polarization density should be characterized as a response function

\[
P(r, t) = \varepsilon_0 \int_{-\infty}^{t} \int_{-\infty}^{\infty} \chi(r', t' - t)E(r', t')dr'dt' \quad \text{(II. 7)}
\]

where \( \chi \) is referred to as the electric susceptibility of a material [8],[16]. In the most general sense, the polarization density is nonlocal in both time and space, exhibiting a dependence on the fields at all positions in the material for all previous times, but a common approximation is to disregard the spatial nonlocality and therefore the spatial convolution. Due to the temporal convolutions, it is preferable to transform the polarization density from the time domain to the frequency domain, which replaces the convolution with a product of the transformed susceptibility and the electric field.

Typically, first order polarization densities are defined as proportional to the electric field

\[
P^{(1)} = \varepsilon_0 \chi^{(1)} E \quad \text{(II. 8)}
\]

where the proportionality constant \( \chi^{(1)} \) is the linear susceptibility of the material. As the polarization density acts as an additional source of electric fields, the polarization density results in an inhomogeneous Helmholtz function.
\[ \nabla^2 \mathbf{E} - \mu_0 \varepsilon_0 \partial_{tt} \mathbf{E} = \mu_0 \partial_{tt} \mathbf{P} \]  \hspace{1cm} \text{\textbf{(II.9)}}

From the field of differential equations, the solution of an inhomogeneous equation is the sum of the homogeneous solution and a particular solution defined by the additional term. The impact of the polarization density from a material acts as a modification of the behavior derived in vacuum. For the first order polarization density defined above, the wavevector relationship for the material is defined as

\[ \left( -k^2 + \frac{\omega^2}{c^2} + \frac{\omega^2}{c^2} \chi^{(1)} \right) \mathbf{E}(r, t) = 0 \]  \hspace{1cm} \text{\textbf{(II.10)}}

and therefore \( k = k_0 \sqrt{1 + \chi^{(1)}} \). The most common way to characterize linear optical behavior of a material is the complex dielectric function, defined as

\[ n + i \kappa = \sqrt{1 + \chi^{(1)}} \]  \hspace{1cm} \text{\textbf{(II.11)}}

with the real part of the dielectric function referred to as the index of refraction \( (n) \) and the imaginary part referred to as the extinction coefficient \( (\kappa) \). Substituting the wavevector in the material (Eqn. II.11) into the complex exponential solution of the Helmholtz equation (Eqn. II.3), the physical significance of the dielectric function becomes clear, as shown in Eqn. II.12, where it is assumed that the wave is propagating in the \( z \)-direction.

\[ \mathbf{E} = A(\omega)e^{-k_0 \kappa z} e^{ik_0 nz - i\omega t} \]  \hspace{1cm} \text{\textbf{(II.12)}}

Using this functional form, the index of refraction remains in the complex exponential, contributing to the phase of the wave. On the other hand, the extinction coefficient contributes to the amplitude, decaying as the wave propagates into the material. Commonly, amplitude decay is considered as a function of \(|\mathbf{E}|^2\)

\[ |\mathbf{E}(z)|^2 = |\mathbf{E}(0)|^2 e^{-2k_0 \kappa z} \]  \hspace{1cm} \text{\textbf{(II.13)}}
where $E(0)$ signifies the initial amplitude of the light. This intensity decay is parameterized by the propagation distance required to reach an intensity that is $1/e$ of the original intensity

$$\frac{1}{\alpha} = \frac{1}{2k_0\kappa} = \frac{\lambda_0}{4\pi\kappa} \quad \text{(II.14)}$$

where $\alpha$ is referred to as the absorption coefficient. Development of the relationship between material parameters and the induced polarization density is integral for the incorporation of additional physical process to the linear optical response of a material.

### II.2 Lorentz Model

Though not strictly applicable to most material systems, the Lorentz model of the atom provides a framework for qualitatively describing physical processes. The Lorentz model considers an individual atom as a harmonic oscillator, with a bound electron oscillating relative to an effectively stationary nucleus. Approximating this system as a ball and spring model, the displacement $x(t)$ of a bound electron of mass $m_0$ from a driving electric field $E(t)$ can be expressed as

$$d_{tt}x(t) + \zeta d_t x(t) + \frac{1}{m_0} F_{\text{restoring}}(x(t)) = -\frac{q}{m_0} E(t) \quad \text{(II.15)}$$

where $\zeta$ defines a velocity damping term and $q$ is the charge of an electron [8],[16],[17]. Generally, the potential experienced by an electron in a material is complex, lacking a reasonable analytic functional form for integration into the model. Therefore, the restoring force is expressed as a power series expansion in the displacement

$$\frac{1}{m_0} F_{\text{restoring}}(x(t)) = \sum_n \gamma_n x^n(t) = \gamma_1 x(t) + \gamma_2 x^2(t) + \gamma_3 x^3(t) + \cdots \quad \text{(II.16)}$$

with $\gamma_n$ characterizing the contribution of the $n$th displacement term to the total restoring force.
Linear Contribution

Neglecting the nonlinear terms of the restoring force, the displacement differential equation can be rewritten in the frequency domain using Fourier transforms.

\[-\omega^2 x(\omega) - i\omega \zeta x(\omega) + \omega_0^2 x(\omega) = -\frac{q}{m_0} E(\omega)\]  \hspace{1cm} (II.17)

It is common for the coefficient of the linear term of the restoring force to be expressed as \(\omega_0^2\), denoting a resonance frequency of the system. Displacement of the electron induces an individual electrical dipole moment, that in a system of \(N\) electrons per unit volume, induces a polarization density \(P(\omega)\) defined as

\[P^{(1)}(\omega) = -Nq x(\omega) = \varepsilon_0 \left(\frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega \zeta}\right) E(\omega)\]  \hspace{1cm} (II.18)

where \(x(\omega)\) follows from Eqn. II.17 and the plasma frequency is included and defined as \(\omega_p^2 = \frac{Nq^2}{m_0 \varepsilon_0}\) to simplify the expression. A complex-valued susceptibility can be extracted from polarization density by combining Eqns. II.11 and II.18, as shown in Eqn. II.19.

\[\chi^{(1)}(\omega) = \omega_p^2 \left(\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + \omega^2 \zeta^2} + i \frac{\omega \zeta}{(\omega_0^2 - \omega^2)^2 + \omega^2 \zeta^2}\right)\]  \hspace{1cm} (II.19)

The physical significance of the damping term, which is a key contribution to the imaginary component of the susceptibility, relates to the phase delay of the polarization density.

Nonlinear Contributions

Incorporation of the nonlinear terms of the restoring force results in differential equations without known analytic solutions, requiring approximation techniques to develop the analytic models. In the case that the nonlinear terms of the restoring force are small compared to the linear term \(\gamma_1 x \gg \gamma_n x^n\), perturbation analysis is an attractive technique commonly applied to similar problems in quantum mechanics [18],[19]. Perturbation analysis approximates a solution to
complex equation by first considering a simpler, related equation that can be solved by conventional techniques, and then applying small, corrective terms to the solution of the simple equation to approximate the complex solution. Analytically, this is implemented as representing the complex solution as the power series expansion in a small perturbation \( \delta \), commonly referred to as coupling strength [8].

\[
x(t) = \sum_{n} \delta^{n} x^{(n)}(t) = \delta x^{(1)}(t) + \delta^{2} x^{(2)}(t) + \delta^{3} x^{(3)}(t) + \ldots \tag{II. 20}
\]

For the Lorentz model, the initial solution that will be perturbed by correction terms is the model that only considers a linear restoring force. The perturbation expansion of the displacement is incorporated into the differential equation for the spring model (Eqn. II.15)

\[
d_{tt} \left( \sum_{n} \delta^{n} x^{(n)}(t) \right) + \zeta d_{t} \left( \sum_{n} \delta^{n} x^{(n)}(t) \right) + \sum_{n} \gamma_{n} \left[ \sum_{n} \delta^{n} x^{(n)}(t) \right]^{n} + \delta \frac{q}{m} E(t) = 0 \tag{II. 21}
\]

with a first order perturbation term \( \delta \) applied to the driving field component as the driving field is considered in the linear solution. Similar to the linear case, the displacement solution for an individual electron can be used to define a polarization density induced from a system of \( N \) electrons per unit volume. Given that the displacement is related to the polarization density by \( p^{(n)}(\omega) = -Nq x^{(n)}(\omega) \), the definition of \( \gamma_{n} = \gamma_{n} \left( \frac{1}{Nq} \right)^{n-1} \) allows for the equations to represent polarization densities rather than displacement. Following the expansion of the sums in Eqn. II.21, terms with the same power of \( \delta \) can be grouped together. As each power of \( \delta \) is linearly independent, a set of coupled differential equations can be written from the coefficients of each power of \( \delta \) that satisfies Eqn. II.21. The linear component, evaluated in Eqn. II.18, and the first two correction terms are written in Eqns. II.22A-C as an example [8].

\[
d_{tt} P^{(1)}(t) + \zeta d_{t} P^{(1)}(t) + \gamma_{1} P^{(1)}(t) = -\varepsilon_{0} \omega_{p}^{2} E(t) \tag{II. 22A}
\]

\[
d_{tt} P^{(2)}(t) + \zeta d_{t} P^{(2)}(t) + \gamma_{1} P^{(2)}(t) + \gamma_{2} \left[ P^{(1)}(t) \right]^{2} = 0 \tag{II. 22B}
\]

\[
d_{tt} P^{(3)}(t) + \zeta d_{t} P^{(3)}(t) + \gamma_{1} P^{(3)}(t) + 2\gamma_{2} P^{(1)}(t) P^{(2)}(t) + \gamma_{3} \left[ P^{(1)}(t) \right]^{3} = 0 \tag{II. 22C}
\]
From inspection of the equations above, the set allows for a “consecutive” solution approach, with the nth order correction requiring only the solutions to lower order correction terms. The first order solution \( P^{(1)}(t) \) is the polarization density from the linear restoring force, with an analytic solution (Eqn. II.18). With the linear solution, the second order correction term can be expressed as

\[
P^{(2)}(\omega) = -\frac{\gamma_2}{\omega_p^2} \chi^{(1)}(\omega) \int_{-\infty}^{\infty} \left[ p^{(1)}(t) \right]^2 e^{-i\omega t} dt \tag{II.23}
\]

Rather than evaluating the Fourier transform \( \mathcal{F}\left\{ \left[ p^{(1)}(t) \right]^2 \right\} \) directly, \( \left[ p^{(1)}(t) \right]^2 \) can expressed as the product of two inverse Fourier transforms \( \mathcal{F}^{-1}\{ p^{(1)}(t) \} \cdot \mathcal{F}^{-1}\{ p^{(1)}(t) \} \) to rewrite Eqn. II.23 as

\[
P^{(2)}(\omega) = -\frac{\gamma_2}{\omega_p^2} \chi^{(1)}(\omega) \int_{-\infty}^{\infty} \left( \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p^{(1)}(\omega_1)p^{(1)}(\omega_2)e^{i(\omega-\omega_1-\omega_2)t} d\omega_2 d\omega_1 \right) dt \tag{II.24}
\]

Substituting the solution for \( p^{(1)}(\omega) \) and completing the Fourier transform introduces a delta function restricting the frequency content of the induced polarization density [8]

\[
P^{(2)}(\omega) = -\frac{\gamma_2}{\omega_p^2} \chi^{(1)}(\omega) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \chi^{(1)}(\omega_1)\chi^{(1)}(\omega_2)E(\omega_1)E(\omega_2)\delta(\omega - \omega_1 - \omega_2)d\omega_2 d\omega_1 \tag{II.25}
\]

Analogous to energy conservation, the delta function ensures that the frequency of the induced polarization density \( (\omega) \) is the sum of the two driving frequencies \( (\omega_1, \omega_2) \). Typically, the delta function is incorporated, along with other constants, into a second order susceptibility [8]

\[
\chi^{(2)}(\omega; \omega_1, \omega_2) = \left( -\frac{\gamma_2}{\varepsilon_0 \omega_p^2} \right) \chi^{(1)}(\omega_1)\chi^{(1)}(\omega_2)\chi^{(1)}(\omega_1 + \omega_2)\delta(\omega - \omega_1 - \omega_2) \tag{II.26}
\]
which allows the general representation of the second order polarization density shown in Eqn. II.27.

\[ P^{(2)}(\omega) = \varepsilon_0 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \chi^{(2)}(\omega; \omega_1, \omega_2)E(\omega_1)E(\omega_2) d\omega_2 d\omega_1 \]  

(II.27)

**Discrete Field Components – Pockels Effect**

An electric field \( E(t) \) that is the sum of two distinct frequency cosine waves can be represented in the frequency domain with:

\[ E(\omega) = E_1(\delta(\omega - \omega_1) + \delta(\omega + \omega_1)) + E_2(\delta(\omega - \omega_2) + \delta(\omega + \omega_2)) \]  

(II.28)

From this functional form, there are four discrete frequency components of the electric field that can induce sixteen frequency components (nine distinct) of the second order polarization density. Substituting the electric field into the Eqn. II.27 and evaluating the delta functions, the distinct nonnegative frequency content of the induced second order polarization density can be expressed as the sum of the driving frequencies [8].

\[ P^{(2)}(\omega_1 + \omega_1) = \varepsilon_0 \chi^{(2)}(\omega_1 + \omega_1; \omega_1, \omega_1)E_1E_1 \]  

(II.29A)

\[ P^{(2)}(\omega_2 + \omega_2) = \varepsilon_0 \chi^{(2)}(\omega_2 + \omega_2; \omega_2, \omega_2)E_2E_2 \]  

(II.29B)

\[ P^{(2)}(\omega_1 - \omega_2) = 2\varepsilon_0 \chi^{(2)}(\omega_1 - \omega_2; \omega_1, -\omega_2)E_1E_2^* \]  

(II.29C)

\[ P^{(2)}(\omega_1 + \omega_2) = 2\varepsilon_0 \chi^{(2)}(\omega_1 + \omega_2; \omega_1, \omega_2)E_1E_2 \]  

(II.29D)

\[ P^{(2)}(0) = 2\varepsilon_0 \chi^{(2)}(0; \omega_1, \omega_2, -\omega_1, -\omega_2)(E_1E_1^* + E_2E_2^*) \]  

(II.29E)

Generally, this process of creating frequency content not part of the initial driving field is called frequency mixing, with higher order \( P^{(n)} \) capable of producing even more distinct frequency content. These processes are invaluable to optical techniques, such as optical parametric amplification [20] and four wave mixing [21] that seek to exploit the production of new frequency content [22],[23].

In the case that the electric field as defined in Eqn. II.28 has a static electric field component \( (\omega_2 = 0) \), the frequency sum and difference polarization densities can be expressed as
\[
P^{(2)}(\omega_1 - 0) = P^{(2)}(\omega_1) = 2\varepsilon_0\chi^{(2)}(\omega_1; \omega_1, 0)E_1E_2 \\
P^{(2)}(\omega_1 + 0) = P^{(2)}(\omega_1) = 2\varepsilon_0\chi^{(2)}(\omega_1; \omega_1, 0)E_1E_2
\]  

Due to the static electric field component, there are second order induced polarization densities at the same frequency as the driving field. This second order effect present in non-centrosymmetric material, called the Pockels Effect, is commonly modeled as a modification to the dielectric function of the material [8]. Neglecting high order corrections, the total induced polarization density at this driving frequency can be rewritten

\[
P(\omega_1) = P^{(1)}(\omega_1) + 2P^{(2)}(\omega_1 \pm 0) = \varepsilon_0 \left(\chi^{(1)}(\omega_1) + 4E_0\chi^{(2)}(\omega_1; \omega_1, 0)\right)E(\omega_1)
\]  

II.3 Free Carrier Effects

Until this point, polarization densities have been formulated from electrons bound to a stationary nucleus. However, materials such as metals and doped semiconductors have a population of mobile charge carriers that contribute an additional optical response to bulk materials. Conceptually, the difference between a bound and unbound electron in the ball and spring model is the existence of a restoring force. For an unbound electron being driven by an oscillating electric field, the equation of motion becomes

\[
d_t p(t) + \frac{1}{\tau} p(t) = -qE(t)
\]  

where \( p(t) \) is the momentum of the unbound electron and \( \tau^{-1} \) is the momentum scattering time [17]. For an oscillating electric field of the form \( E(t) = E_0e^{-i\omega t} \), the drift velocity of the electron
is going to exhibit similar behavior \( \mathbf{v}(t) = \mathbf{v}_0 e^{-i\omega t} \). Substituting the driving field and the velocity solution into the differential equation of motion (Eqn. II.32), the drift velocity can be written as

\[
\mathbf{v}(t) = -\frac{\tau q}{m_0} \frac{1}{1 - i\tau \omega} \mathbf{E}(t)
\]

which can then be used to define a macroscopic conductivity from the current density using \( \mathbf{J} = -Nq\mathbf{v}(t) = \sigma \mathbf{E}(t) \). An optical conductivity can be defined as

\[
\sigma_{\text{optical}} = \frac{N\tau q^2}{m_0} \frac{1}{1 - i\tau \omega}
\]

that can be used to characterize the optical response of the electrons. The optical conductivity has both real and imaginary terms, implying that the free electron response would induce both real and imaginary polarization densities that contribute to both refraction and absorption.
Pulsed laser microelectronic testing uses a tightly focused laser to achieve high energy densities that spatially probe selected regions of a microelectronic device under test. Hence, understanding the propagation of a focused laser beam is essential for understanding the fundamentals of pulsed laser testing. In most cases, the cross section of the fundamental mode of a laser can be approximated as a radial Gaussian function. When this beam is incident on a focusing lens, the spatial distribution of the phase is modified by the lens, resulting in a beam that remains radially Gaussian but with a beam width and wave front curvature that change as a function of propagation distance. Although not strictly applicable to tightly focused light, an analytical approach to representing focused Gaussian beams using the paraxial approximation is the most common approach for providing a basis of quantitative parameters that can be used to define laser beams and for defining a propagating wave based on initial conditions. The paraxial approximation is most accurate when applied to electric fields that vary gradually in the propagation direction [24].

III.1 Gaussian Optics

For an electromagnetic wave propagating in a lossless, homogenous linear material, the electric field behavior is expressed by the homogenous wave equation, as shown in Eqn. III.1.

\[
(\nabla^2 - \frac{n^2}{c^2} \partial_{tt})E = 0 \tag{III. 1}
\]

Assuming harmonic time dependence for a single frequency wave (Eqn. II.3), the temporal derivative term can be calculated and replaced by the wavevector \( k^2 = n^2 \omega^2 / c^2 \), as shown in Eqn. III.2.

\[
(\nabla^2 + k^2)E = 0 \tag{III. 2}
\]
Then, the spatial solution for the electric field distribution can be written as shown in Eqn. III.3

\[ E(x, y, z) = E_0 e^{-ikz\hat{z}} \]  

where the complex exponential conveys a uniform amplitude wave front propagating in the z-direction (unit vector \( \hat{z} \)). In a small perturbation approach, rather than a uniform amplitude wavefront, we will now suppose that there is a spatial variation perpendicular to the propagation direction that can be expressed as

\[ E(x, y, z) = A(x, y, z) e^{-ikz\hat{z}} \]  

where \( A(x, y, z) \) is a spatial envelope function modulating a complex exponential propagating in the z-direction. Two restrictions are imposed on the spatial envelope function to significantly reduce the complexity of deriving an analytical solution: the change in amplitude along the direction of propagation for a single wavelength is small and the change in amplitude along the direction of propagation is small compared to the change in amplitude in the perpendicular plane [24]. The electric field distribution described by Eqn. III.4 can be substituted into Eqn. III.2 to establish a differential equation for the spatial envelope function, as shown in Eqn. III.5. From the two prior restrictions placed on the spatial envelope function, referred to as the Slowly Varying Envelope Approximation [24],[25], the higher order derivative along the direction of propagation can be neglected to reduce Eqn. III.5 to Eqn. III.6

\[
\begin{align*}
\left( \partial_{xx} + \partial_{yy} \right) A(x, y, z) + \partial_{zz} A(x, y, z) - i2k\partial_z A(x, y, z) &= 0 \\
\left( \partial_{xx} + \partial_{yy} \right) A(x, y, z) - i2k\partial_z A(x, y, z) &= 0
\end{align*}
\]

At this point, it is highly advantageous to move from a Cartesian to cylindrical coordinate system and to assume that the spatial envelope function is radially symmetric to represent Eqn. III.6 as shown in Eqn. III.7.

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial A(r, z)}{\partial r} \right) - i2k\partial_z A(r, z) = 0
\]  

\[ \text{(III.7)} \]
Parabolic differential equation theory provides an ansatz for Eqn. III. 7 of the form

\[ A(r, z) = e^{-i\left(\frac{P(z) + k r^2}{2 q(z)}\right)} \]  

(III. 8)

where \( P(z) \) and \( q(z) \) are complex value functions used to parameterize the distribution [24]. For a given position \( z \) along the propagation direction, the ansatz results in a Gaussian radial distribution that is characteristic of a fundamental mode of a Gaussian beam. Substitution of Eqn. III. 8 into Eqn. III. 7 establishes the differential equation shown in Eqn. III. 9.

\[
\frac{r^2 k^2}{[q(z)]^2} \left(\frac{dq}{dz} - 1\right) - 2k \left(\frac{dP}{dz} + \frac{i}{q(z)}\right) = 0
\]

(III. 9)

As Eqn. III. 9 must be true for all values of \( r \) and \( z \), two separate equations can be constructed.

\[
\frac{dq}{dz} = 1  \quad \text{(III. 10)}
\]

\[
\frac{dP}{dz} = -\frac{i}{q} \quad \text{(III. 11)}
\]

Beginning with Eqn. III. 10, it is apparent that \( q \) must be a linear function of \( z \) with a unitary slope. Further conclusions about \( q \) can be made by referring to the ansatz equation. The function \( q \) is necessarily complex due to the fact that a strictly real value for \( q \) would result in a lack of radial dependence on the amplitude of the envelope function [24],[25]. Therefore, \( q \) is written as

\[
q(z) = z + iz_r
\]

(III. 12)

with the imaginary integration constant \( z_r \) in order to satisfy the complex value requirement. Based on the ansatz, greater utility is found from the inverse of \( q(z) \) as
\[
\frac{1}{q(z)} = \frac{1}{z + iz_r} = \frac{1}{z \left(1 + \frac{z^2}{z^2}ight)} - \frac{i}{z_r \left(1 + \frac{z^2}{z^2}ight)}
\] (III.13)

Substituting Eqn. III.13 into Eqn. III.8, the resulting equation can be decomposed into phase terms and amplitude terms

\[
A(r, z) = \exp(-iP(z))\exp\left(-i\frac{kr^2}{2R(z)}\right)\exp\left(-\frac{kr^2}{2z_r \left(1 + \frac{z^2}{z^2}\right)}\right)
\] (III.14)

where \(R(z)\) (defined in Eqn. III. 15) is the radius of curvature and characterizes spherical contours of equal phase [24],[25].

\[
R(z) = z \left(1 + \frac{z^2}{z^2}\right)
\] (III.15)

Using Eqn. III.14, the constants and terms can be parameterized to measurable quantities. As the radial dependence of the amplitude is Gaussian, a convenient characterization metric is the [1/e] radius and can be derived from Eqn. III.14

\[
w^2(z) = \frac{2z_r}{k} \left(1 + \frac{z^2}{z^2}\right)
\] (III.16)

where \(w(z)\) is referred to as the [1/e] beam radius. The position \(z = 0\) corresponds to the minimal beam radius, termed the beam width \(w_0\), which can be experimentally measured at the focal point of the laser beam. Eqn. III.16 can be used to relate to \(z_r\) to the beam waist and rewrite Eqn. III.16 to include the beam width parameter, as shown in Eqns. III.17-18.

\[
z_r = \frac{kw_0^2}{2}
\] (III.17)
Now that \( q(z) \) has been derived and parametrized, it can be used with Eqn. III.11 to solve for an analytic form of \( P(z) \):

\[
P(z) = -i \ln(z + iz_r) = -i \ln \left( 1 - i \frac{z}{z_r} \right) - i \ln (iz_r)
\]

As the second term of Eqn. III.19 is a constant, it can be neglected when deriving the spatial dependence of \( P(z) \) [24].

\[
P(z) = -i \ln \left( 1 + \frac{z^2}{z_r^2} \exp \left( -i \left( \tan^{-1} \left( \frac{z}{z_r} \right) \right) \right) \right)
\]

In regards to the ansatz function, it can be seen that the first term of Eqn. III.20B modulates the peak amplitude while the second term imposes a uniform phase accumulation. Following the development of analytic functions for \( q(z) \) and \( P(z) \), Eqn. III.13 and Eqn. III.20B can be substituted into Eqn. III.8 to establish the functional form of the electric field distribution (Eqn. III.3) that provides both amplitude and phase information (Eqn. III.21) [24],[25]. In some cases the phase information is not necessary, in which case the intensity (Eqn. III.22) of the electric field is typically used to provide amplitude information. Using Eqn. III.22, a spatial distribution of field intensity can be plotted to demonstrate the spatial confinement of a focused laser beam around a focal point (Fig. III.1). The parameters defined in this section can be related to the intensity distribution of a laser beam to provide physical significance to the parameters (Fig. III.2 and Fig. III.3).
\[
E(r, z) = E_0 \frac{w_0}{w(z)} \exp \left( -\frac{r^2}{w^2(z)} \right) \exp \left( i \left( \tan^{-1} \left( \frac{z}{z_r} \right) - \frac{kr^2}{2R} - kz \right) \right) \hat{z} \tag{III. 21}
\]

\[
I(r, z) = |E(r, z)|^2 = I_0 \left( \frac{w_0}{w(z)} \right)^2 \exp \left( - \frac{2r^2}{w^2(z)} \right) \tag{III. 22}
\]

Figure III.1. Spatial distribution of normalized intensity values to illustrate the spatial confinement of intensity (energy) of a Gaussian beam near the focus and its spread as it propagates away from the focus. Contour lines allow for easier visualization of the spatial confinement from a focused laser beam.
Figure III.2. Intensity contour for a focused Gaussian beam subject to the paraxial approximation where the red curves marks the $[1/e^2]$ decay from the on-axis intensity. Contours provide spatial intuition about the local intensity distribution of the beam and relates it to far-field observables. The labeled variables are defined in Fig. III.3.

<table>
<thead>
<tr>
<th>Parameter Name</th>
<th>Symbol</th>
<th>Formula</th>
<th>Description based on intensity profile</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam width</td>
<td>$w_0$</td>
<td>$w_0$</td>
<td>Smallest radius of the beam, at the focal point of the beam</td>
</tr>
<tr>
<td>Rayleigh range</td>
<td>$z_r$</td>
<td>$kw_0^2/2$</td>
<td>Distance along the central axis to reach half the peak intensity</td>
</tr>
<tr>
<td>Beam waist</td>
<td>$w(z)$</td>
<td>$w_0^2\left(1 + \frac{z^2}{z_f^2}\right)$</td>
<td>Radius of the beam at distance $z$ from focal point</td>
</tr>
<tr>
<td>Total angular spread</td>
<td>$\phi$</td>
<td>$\frac{2\lambda_0}{n\pi w_0}$</td>
<td>Far-field divergence of focused beam</td>
</tr>
</tbody>
</table>

Figure III.3. Parameters and definitions used in the derivation of focused Gaussian optics.
III.2 Energy Density

In a lossless material, energy conservation requires that the energy measured through an infinite plane perpendicular to the axis of propagation is independent of the location of the plane on the axis. Exploiting the radial symmetry of the beam, the energy passing through a circle of radius \( r \) is defined by integrating through the area defined by the circle.

\[
U(r, z) = \int_0^r 2\pi I_0 \left( \frac{w_0}{w(z)} \right)^2 \exp \left( -\frac{2r^2}{w^2(z)} \right) r' dr' = \frac{\pi w_0^2 I_0}{2} \left( 1 - \exp \left( -\frac{2r^2}{w^2(z)} \right) \right)
\]

From this expression, it is possible to estimate the amount of energy contained within a pulse that passes through a plane or volume at an arbitrary position. For example, consider an optical aperture placed in a laser system in order to spatially filter the laser beam. As light not passing through the aperture is excluded from the beam, there is an energy loss associated for inclusion of an aperture in the system. For a circular aperture the energy transmitted through the aperture can be estimated by using the radius of the aperture in Eqn. III.23.

From an experimental perspective, energy conservation means that as long as losses are accounted for, energy measurement at a single point (such as a photodiode) in a setup can be used to calculate the pulse energy at any point in the setup. For a small volume, such as the active region of a microelectronic device, the energy passing through volume can be estimated from the formula above. Moving the volume to different positions in the focused beam changes the amount of energy that passes through the region. Conceptually, this process of scanning the position of the volume to change the amount of energy interacting with the volume resembles the processes of three-dimensional positional scans of microelectronic devices.

Impact of material systems

Though the index of refraction of the material is incorporated in the derivations above, it is quickly assimilated into other parameters that cloud the impact on the beam propagation. Since propagation can be entirely constructed from the beam parameters, accessing the impact of a material on each parameter will entirely describe the impact on the beam. As the beam waist \( w_0 \) is a defined quantity, it is independent of the material, implying that the minimal spot size of the beam does not change from material to material. The only other parameter necessary to
consider is the Rayleigh range ($z_r$), as all other parameters can be defined from the beam waist and the Rayleigh range. Inclusion of the wavevector into the definition of Rayleigh range indicates that there is a proportionality to the index of refraction, resulting in a longer Rayleigh range in a material with higher index of refraction. Using Eqn. III.22, the intensity distributions ($I_0 = 1$) of a focused Gaussian beam in vacuum ($n=1$) and in silicon ($n=3.5$) are depicted in Fig. III.4. In silicon, the longer Rayleigh range results in the intensity extending much further along the axis of propagation than in vacuum.

![Figure III.4](image)

Figure III.4. Spatial distribution of normalized intensity values for paraxial Gaussian optics in air and silicon for the same beam width. For each distribution, normalization ensures that the maximum intensity value is 1.

The elongation of the Rayleigh range in a material has significant impact on energy deposition from focused laser systems incident on materials. One of the biggest advantages of depositing energy using nonlinear absorption, which is commonly done in pulsed laser testing of microelectronic devices, is the ability to minimize the three-dimensional volume in which the energy deposition occurs: the beam waist provides radial confinement and the Rayleigh range
provides confinement along the direction of propagation. The beam waist is constant across
material systems and therefore the radial confinement, and by extension the radial resolution of
the measurement system, is material-independent. However, the Rayleigh range is proportional to
the index of refraction. The Rayleigh range increases and therefore the confinement of the beam
along the axis of propagation lessens in higher index materials. Therefore, as the index of refraction
of the material increases, the beam waist must be reduced in order to attain the same confinement
along the axis of propagation.

It is important to consider material interfaces when exploring the impact of materials on the
beam propagation. In many cases, it is not reasonable to make the assumption that the entire beam
is contained with a single material. When a beam propagating in one material is incident on an
interface with a different material, the spatial distribution of the beam is affected. The most
significant impact of the interface is the movement of the location of the beam waist relative to the
interface. When a focused Gaussian beam propagates from one material ($n_1$) into a different
material ($n_2$), the Rayleigh range of the beam is modulated according to [26]

$$z_2 = \frac{n_2}{n_1} z_1$$

(III.24)

The modulation of the Rayleigh range results in the movement of the beam waist as the Gaussian
beam passes into the different material; the change in focal position is the same proportionality as
in Eqn. III.24 [26]. For pulsed laser testing in materials, it is important to keep in mind the
distinction between beam waist position in air and in a material in order, for example, to properly
relate stage displacement in air with beam displacement in silicon and properly identify the region
of highest intensity within the silicon.
CHAPTER IV

NONLINEAR MODELS IMPLEMENTED IN FDTD

Though there are simplified examples where field distributions can be expressed in analytic terms, most electromagnetics problems require computational techniques to achieve numerical results. Several varieties of algorithms can be used for solving Maxwell’s equations; the most natural technique involves expressing electromagnetic fields as coupled quantities that propagate forward in time. For electromagnetics calculations associated with pulsed laser testing, nonlinear models defined as additional polarization densities terms (see Chapter II) must be included. In this chapter, the finite-difference time-domain numerical technique utilized by the optical solver is defined and the parameterization method used to incorporate the polarization densities that describe nonlinear optical processes in the optical solver is derived. This approach is integral for the development of an optical simulation tool that can be applied to an arbitrary device geometry.

IV.1 Finite Difference Time Domain Method

The two Maxwell’s equations that address wave propagation are the curl equations

\[ \nabla \times \mathbf{E} = -\mu_0 \frac{\partial}{\partial t} \mathbf{H} \]  \hspace{1cm} (IV. 1A)
\[ \nabla \times \mathbf{H} = \frac{\partial}{\partial t} \mathbf{D} \]  \hspace{1cm} (IV. 1B)

which, combined with constitutive equation for the displacement field \( \mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} \), represent a system of coupled differential equations. Implicit in these equations is the interconnectedness of the spatial and temporal behavior of the wave propagation defined by spatial and temporal derivatives. A common technique for solving coupled differential equations is a class of algorithms referred to as finite-difference methods, which attempt to solve differential equations by approximating derivatives with finite difference equations

\[ \frac{\partial_t f(t)}{\Delta t} \approx \frac{f\left(t + \frac{\Delta t}{2}\right) - f\left(t - \frac{\Delta t}{2}\right)}{\Delta t} \]  \hspace{1cm} (IV. 2)
To best serve the spatial computations, a Cartesian lattice with a unit cell defined by lattice constants is used in the spatial discretization process. The simulation space is discretized and numerically represented by the vertices of the lattice. As spatial operations, such as three-dimensional curl operations, are limited to the vertices of the lattice, field components are unable to be calculated at the same spatial location. Consider the approximation of derivatives involved in a three-dimensional curl operation along a basis

\[(\nabla \times \mathbf{E})_x = (\partial_y E_z - \partial_z E_y)\]  \hspace{1cm} (IV.3)

which introduces, in a sense, a nonlocality to field components calculated from the curl equations. The impact of this realization is that while field components will be stored at a node existing at a single point in space, in reality field components will be computed at different spatial locations within the unit cell of the lattice, and if needed, can be interpolated to a single point. This approach to spatial discretization was proposed by Kane Yee in 1965 and is now appropriately referred to as a Yee Cell [27].

![Figure IV.1.](image)

Figure IV.1. An illustration of the decomposition of spatial field information into field components that are calculated at separate locations in a spatial unit cell known as a Yee Cell.

Temporal discretization is a simple process in comparison with the spatial discretization, with a time interval being represented by a chain of nodes in time separated by a time step \(\Delta t\). Given the coupling of the displacement and magnetic fields from Eqns. IV.1A and IV.1B, it is not possible to compute field components for both displacement and magnetic fields at the same point.
in time. Therefore, the temporal chains are offset such that the magnetic field components are computed at the temporal midpoint of displacement field computations creating a ladder approach where displacement fields and magnetic fields are alternately solved. Approximating both the spatial and temporal derivatives by the difference equations, the field components are symbolically represented as $D_x^n(r)$ where the superscript corresponds to the nth time node, the subscript corresponds to field components, and the position corresponds to a computational space node. An example of the update equations for field components can be seen below in Eqn. IV.4. Assuming that the electric field and magnetic field are known at a previous time, the update equations can be used to calculate the fields at the next time step; calculating the displacement field at the time step couples the update equations [27]. Any additional process that are incorporated into the algorithm, such as polarization densities from nonlinear processes, must be considered in the constitutive equation.

\[
H_x^{n+\frac{1}{2}}(r) = -\frac{\Delta t}{\mu_0} \left( \frac{E_z^n(r + \frac{\Delta y}{2} \hat{y}) - E_z^n(r - \frac{\Delta y}{2} \hat{y})}{\Delta y} \right) - \frac{E_y^n(r + \frac{\Delta z}{2} \hat{z}) - E_y^n(r - \frac{\Delta z}{2} \hat{z})}{\Delta z} + H_x^{n-\frac{1}{2}}(r) \tag{IV.4A}
\]

\[
D_x^{n+1}(r) = \Delta t \left( \frac{H_z^{n+\frac{1}{2}}(r + \frac{\Delta y}{2} \hat{y}) - H_z^{n+\frac{1}{2}}(r - \frac{\Delta y}{2} \hat{y})}{\Delta y} \right) - \frac{H_y^{n+\frac{1}{2}}(r + \frac{\Delta z}{2} \hat{z}) - H_y^{n+\frac{1}{2}}(r - \frac{\Delta z}{2} \hat{z})}{\Delta z} + D_x^n(r) \tag{IV.4B}
\]

**IV.2 Wave modulation and generation rates**

As described in chapter II, optical processes can be incorporated into Maxwell’s equations as polarization density terms through the displacement field ($D = \varepsilon_0 E + P$). As the displacement field is used in the finite-difference time domain (FDTD) algorithm, expressing nonlinear polarization densities in functional forms that can be easily solved by the FDTD algorithm is invaluable. The differential form of Beer’s law expresses the change in intensity of light after traveling a distance of $dz$ in a material [16].
\[ dl = -\alpha dl dz \]  

(IV.5)

The intensity decay constitutes energy dissipation in the material that can be decomposed into individual process that can be considered separately. For energy dissipation associated with generation processes, a generation rate can be defined by dividing the energy lost to the process by the creation energy of the processes. As the intention of PL-SEE is charge injection, modeling the generation rate of free carriers from absorptive processes is the required output of the optical simulations. For example, electron-hole pair generation rate for single photon absorption would be

\[ \dot{N}_{SPA} = \frac{\alpha I}{\hbar \omega} \]  

(IV.6)

where \( \hbar \omega \) expresses the energy of the single photon used to generate the single electron-hole pair [28],[29].

With this Beer’s law approach, absorptive processes and any associated generation can be incorporated into the differential model (Eqn. IV.5) by treating each process individually and summing the contributions. As two photon absorption is characterized by an intensity dependent absorption, two photon absorption is expressed with a differential form of

\[ dl = -\beta I^2 dz \]  

(IV.7)

where \( \beta \) is a material dependent parameter called the two photon absorption coefficient [28],[29]. The energy lost from two photon absorption contributes to the production of an electron-hole pairs; a generation rate can be defined as

\[ \dot{N}_{TPA} = \frac{\beta I^2}{2\hbar \omega} \]  

(IV.8)

with \( 2\hbar \omega \) capturing the energy of the two photons absorbed in the generation of a single electron-hole pair. In the case that the only electron-hole pair generation processes are SPA and TPA, the total generation rate of the model is expressed as
\[ \dot{N}_{\text{total}} = \dot{N}_{\text{SPA}} + \dot{N}_{\text{TPA}} = \frac{\alpha I}{\hbar \omega} + \frac{\beta I^2}{2\hbar \omega} \] (IV. 9)

Free carriers can still absorb incident photons to move to higher energy states within the same energy band, producing no additional free carriers in the process. Free carrier refraction is expressed as a function of the free carrier density in the material

\[ dI_{\text{FCA}} = -\sigma_{\text{FCA}} N_{\text{total}} Idz \] (IV. 10)

where \( \sigma_{\text{FCA}} \) is the absorption cross-section of free carriers, a material parameter [28],[29]. Considering absorption processes from single/two photon absorption and free carrier absorption, the total absorption can be expressed as the sum of the contributions from the processes.

\[ dI = -\alpha Idz - \beta I^2 dz - \sigma_{\text{FCA}} N_{\text{total}} dz \] (IV. 11)

**Phase Accumulation**

Similar to the intensity decay, phase accumulation from propagating through a length \( dz \) of a material is expressed as the differential

\[ d\phi = n k_0 dz \] (IV. 12)

where \( n \) is the index of refraction of the material and \( k_0 \) is the free space wavevector [16],[17]. Additional phase accumulation contributions are summed together to provide the total phase accumulated. Based on the intensity-dependent self phase modulation from the Kerr effect, an additional phase accumulation can be expressed as an intensity dependent term

\[ d\phi_{\text{kerr}} = k_0 n_2 Idz \] (IV. 13)

with \( n_2 \) being a material dependent parameter that is often referred to as the nonlinear refractive index with units of cm\(^2\)/W [28],[29]. Free carriers provide additional photon-interactions, resulting in a free carrier density dependent phase accumulation factor
\[ d\phi_{FCR} = k_0\sigma_{FCR}N_{total}dz \]  

(IV.14)

where \( \sigma_{FCR} \) is a material parameter called the free carrier refraction cross-section \([28],[29]\). Considering refractive processes from single/two photon absorption and free carrier absorption, the total phase accumulation can be expressed as the sum of the contributions from the processes.

\[ d\phi = nk_0dz + k_0n_2ldz + k_0\sigma_{FCR}N_{total}dz \]  

(IV.15)

**IV.3 FDTD Implementation**

To incorporate additional physical processes into a FDTD algorithm to calculate free carrier generation, additional polarization terms must be defined that contribute to the displacement field defined by the constitutive equation \( \mathbf{D} = \varepsilon_0\mathbf{E} + \mathbf{P} = \varepsilon_0\varepsilon\mathbf{E} \). The optical processes associated with a typical dielectric function are expressed as a complex value linear polarization density by defining a relative permittivity \( \varepsilon \)

\[ \varepsilon = \varepsilon_r + i\varepsilon_i = (n + i\kappa)^2 = (n^2 - \kappa^2) + i2n\kappa \approx n^2 + i2n\kappa \]  

(IV.16)

where a polarization density is defined by \( \mathbf{P} = \varepsilon_0(\varepsilon - 1)\mathbf{E} \) \([16],[17]\). In semiconductors, the real component of the dielectric function is typically much larger than the imaginary component \( n \gg \kappa \) allowing for the neglection of smaller terms to simplify the relative permittivity expression, and therefore the polarization density. Considering higher order optical processes as modification of the linear response, then a perturbation to the dielectric function \( (n_0,\kappa_0) \) is expressed as perturbations \( (\Delta n, \Delta \kappa) \) to the relative permittivity used to define polarization densities.

\[ \varepsilon_r + \Delta\varepsilon_r + i(\varepsilon_i + \Delta\varepsilon_i) = (n_0 + \Delta n)^2 + i2(n_0 + \Delta n)(\kappa + \Delta \kappa) \]  

(IV.17)

As the nonlinear processes are contained in the perturbation terms of the relative permittivity, once the products are simplified, the base permittivity terms \( (\varepsilon_r, \varepsilon_i) \) are subtracted out. Further simplifications can be made by neglecting smaller order terms in a similar fashion to the linear relative permittivity.
\[
\Delta \varepsilon_r + i \Delta \varepsilon_i = 2n_0 \Delta n + (\Delta n)^2 + i2(n_0 \kappa_0 \Delta n + \kappa_0 \Delta n + \Delta \kappa \Delta n) \approx 2n_0 \Delta n + i2n_0 \Delta \kappa \quad (IV.18)
\]

From this formulation, higher order processes can be defined as polarization densities with phase modulation processes being described by perturbing the real part of the dielectric function and absorptive processes described by perturbing the imaginary part of the dielectric function. While the phase modulation nonlinear processes have already been described as a refractive index perturbation and hence dielectric function perturbation (Eqn. IV.12), absorptive processes to this point have been defined by absorption coefficients and absorption cross-section rather than a dielectric function (Eqn. IV.5). Rearrangement of the absorption coefficient definition discussed in Chapter II (Eqn. II.14) allows for the expression of the imaginary component of the dielectric function as [16],[17]

\[
\kappa = \frac{ac}{2\omega} \quad (IV.19)
\]

From Eqn. IV.19, the imaginary component of the relative permittivity \( (\varepsilon_i) \) can be written as a function of the absorption coefficient using Eqn. IV.18.

\[
\varepsilon_i = \frac{n_0 c \alpha}{\omega} \quad (IV.20)
\]

**Nonlinear Polarization Densities**

Beginning with the third order nonlinear optical processes, two polarization density contributions from the Kerr effect and TPA were defined using the dielectric perturbation. From the differential representation of two photon absorption (Eqn. IV.7), the polarization density can be written as

\[
P_{TPA} = -\frac{\varepsilon_0 n_0 c \beta}{i\omega} |E| = -\frac{n_0^2 c^2 \varepsilon_0^2 \beta}{2i\omega} |E|^2 E \quad (IV.21)
\]
where the intensity of plane wave \( I = \frac{1}{2}cne_0|E|^2 \) is used to express the polarization density as a function of the electric field [29]. Assuming an instantaneous field response, the polarization density associated with the Kerr effect (Eqn. IV.13) is written as

\[
P_{Kerr} = \varepsilon_0 2n_0 n_2 |I|E = \varepsilon_0^2 c n_0^2 n_2 |E|^2 E
\]  

As free carriers at sufficiently high concentrations impact optical propagation, it is necessary to not only consider the initial concentrations from the doping of the materials, but also the generated carriers as the pulse propagates through the material. The temporal envelope of the laser pulse requires instantaneous modeling of free carriers because carriers generated by the leading edge of the pulse impact the propagation of the lagging edge. From Eqn. IV.9, the generation rate from SPA and TPA is expressed as [29]

\[
\partial_t N_t = \partial_t N_{SPA} + \partial_t N_{TPA} = \frac{aI}{\hbar \omega} + \frac{\beta I^2}{2\hbar \omega} = \frac{acn_0 \varepsilon_0}{2\hbar \omega} |E|^2 + \frac{\beta c^2 n_0^2 \varepsilon_0^2}{8\hbar \omega} |E|^4
\]  

With an expression of the free carrier concentrations, a polarization density for both free carrier refraction and free carrier absorption can be expressed as a function of the free carrier density from Eqns. IV.14 and IV.10 respectively [29].

\[
P_{FCR} = 2\varepsilon_0 n_0 \Delta n_{FCR}(N_t) E
\]  

\[
P_{FCA} = -\frac{\varepsilon_0 n_0 c \sigma_{FCA}}{i \omega} N_t E
\]

It is possible to create more complex functional analytic forms for the carrier dependence of FCA and FCR. In this fashion, these more complex models can be still be incorporated, as is demonstrated by the free carrier density function \( \Delta n_{FCR}(N_t) \) in Eqn. IV.24A.

The displacement field can be expressed as the sum of polarization contributions from linear processes, captured by the dielectric function, and nonlinear process as defined above.

\[
D = \varepsilon_0 E + \varepsilon_0 \chi_L E + P_{FCR} + P_{Kerr} + P_{FCA} + P_{TPA}
\]  

(IV.25)
Substituting the defined polarization densities into displacement field

\[ D = \varepsilon_0 \left( E + \frac{P_L}{\varepsilon_0} + 2n_0 \Delta n_{FCR} E + \varepsilon_0 n_0^2 n_2 c |E|^2 E - \frac{1}{i\omega} \left( n_0 c \sigma_{FCA} N_t E + \frac{n_0^2 c^2 \varepsilon_0 \beta}{2} |E|^2 E \right) \right) \tag{IV.26} \]

which has been written to accentuate that absorption polarization terms have a \((-i\omega)^{-1}\) factor.

Transitioning into the time domain by replacing \(-i\omega\) with temporal derivatives \((\partial_t)\), the displacement field can be written in a form that can be discretized using difference equations [29].

\[ \partial_t D = \varepsilon_0 \left( \partial_t \left( E + \frac{P_L}{\varepsilon_0} + 2n_0 \Delta n_{FCR} E + \varepsilon_0 n_0^2 n_2 c |E|^2 E \right) + n_0 c \sigma_{FCA} N_t E + \frac{n_0^2 c^2 \varepsilon_0 \beta}{2} |E|^2 E \right) \tag{IV.27} \]

The FDTD algorithm dictates that at time \((n + 1)\Delta t\) the displacement field \(D^{(n+1)}\) is calculated from the curl of the magnetic field \(\left( \nabla \times E^{(n+1/2)} \right)\), as discussed in section IV.1. Using \(D^{(n+1)}\), the constitutive equations can be used to calculate \(E^{(n+1)}\), which in turn can be used to calculate the magnetic field at the next time step. Therefore, once discretized, the displacement equation should be rearranged to solve for \(E^{(n+1)}\). In the interest of clarity, the expansion of the displacement field with difference equations is performed by considering each polarization term separately (see components of Eqn. IV.27) and then recombining them [29].

\[
\begin{align*}
\partial_t D^{(n+1/2)} &= \frac{D^{(n+1)} - D^{(n)}}{\Delta t} \quad \text{(IV.28A)} \\
\partial_t \left( E^{(n+1/2)} \right) &= \frac{E^{(n+1)} - E^{(n)}}{\Delta t} \quad \text{(IV.28B)} \\
\partial_t \left( \chi L E^{(n+1/2)} \right) &= \frac{E^{(n+1)} - E^{(n)}}{\Delta t} \quad \text{(IV.28C)} \\
\partial_t \left( 2n_0 \Delta n_{FCR} \left( E^{(n+1/2)} \right) E^{(n+1/2)} \right) &= 2n_0 \frac{\Delta n_{FCR} \left( E^{(n+1)} \right) E^{(n+1)} - \Delta n_{FCR} \left( E^{(n)} \right) E^{(n)}}{\Delta t} \quad \text{(IV.28D)} \\
\partial_t \left( \varepsilon_0 n_0^2 n_2 c \left| E^{(n+1/2)} \right|^2 E^{(n+1/2)} \right) &= \varepsilon_0 n_0^2 n_2 c \frac{\left| E^{(n+1)} \right|^2 E^{(n+1)} - \left| E^{(n)} \right|^2 E^{(n)}}{\Delta t} \quad \text{(IV.28E)}
\end{align*}
\]

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As the absorptive processes (i.e., FCA, TPA) do not have a temporal derivative component (see Eqn. IV.27), conversion between half time steps uses the average formula

\[ 2E^{(n+\frac{1}{2})} = E^{(n+1)} + E^{(n)} \]

\[ \varepsilon_0 n_0 c \sigma_{FCA} \frac{N_t^{(n+\frac{1}{2})} E^{(n+\frac{1}{2})}}{2} = \varepsilon_0 n_0 c \sigma_{FCA} N_t^{(n+\frac{1}{2})} \left( E^{(n+1)} + E^{(n)} \right) \]  

(IV.29A)

\[ \frac{n_0^2 c^2 \varepsilon_0^2 \beta}{2} \left| E^{(n+\frac{1}{2})} \right|^2 E^{(n+\frac{1}{2})} = \frac{n_0^2 c^2 \varepsilon_0^2 \beta}{8} \left( \left| E^{(n+1)} \right|^2 + \left| E^{(n)} \right|^2 \right) \left( E^{(n+1)} + E^{(n)} \right) \]  

(IV.29B)

As free carrier absorption and refraction considers the free carrier concentration at the current time step, the free carrier generation must be considered in the same manner as polarization densities. Discretization of the temporal derivative associated with the free carrier generation allows for the creation of an update equation for the free carrier concentration

\[ N_t^{(n+\frac{1}{2})} = \frac{\Delta t c n_0 \varepsilon_0}{2h\omega} |E^n|^2 + \frac{\Delta t \beta c^2 n_0^2 \varepsilon_0^2}{8h\omega} |E^n|^4 + N^{(n-\frac{1}{2})} \]  

(IV.30)

where the initial free carrier concentration is the doping of the material [29]. Following the expansion of the individual polarization densities, the discretized displacement field can be assembled to solve for the electric field

\[ E^{(n+1)} = \frac{D^{(n+1)} - D^{(n)}}{V_+ E^{(n+1)}} + \frac{V_- \left( E^{(n+1)} \right)}{V_+ \left( E^{(n+1)} \right)} E^{(n)} \]  

(IV.31)

where
\[ V_+(E^{(n+1)}) = \varepsilon_0 + \varepsilon_0 \chi_L + 2\varepsilon_0 n_0 \Delta n_{FCR} (E^{(n+1)}) + \varepsilon_0^2 n_0^2 n_2 c |E^{(n+1)}|^2 + \frac{\Delta t \varepsilon_0 n_0 c \sigma_{FCA} N_t^{(n+\frac{1}{2})}}{2} \]
\[ + \frac{\Delta t n_0^2 c^2 \varepsilon_0^2 \beta}{8} \left( |E^{(n+1)}|^2 + |E^{(n)}|^2 \right) \] (IV.32A)

\[ V_-(E^{(n+1)}) = \varepsilon_0 + \varepsilon_0 \chi_L + 2\varepsilon_0 n_0 \Delta n_{FCR} (E^{(n)}) + \varepsilon_0^2 n_0^2 n_2 c |E^{(n)}|^2 - \frac{\Delta t \varepsilon_0 n_0 c \sigma_{FCA} N_t^{(n+\frac{1}{2})}}{2} \]
\[ - \frac{\Delta t n_0^2 c^2 \varepsilon_0^2 \beta}{8} \left( |E^{(n+1)}|^2 + |E^{(n)}|^2 \right) \] (IV.32B)

It should be noted that Eqns. IV.31 and IV.32 are simply compact forms used to denote the equations; there is not physical significance ascribed to the functional form [29].

The expression for \( E^{(n+1)} \) shown in Eqn. IV.31 does not have an analytic solution, and requires the use of numerical techniques to arrive at a solution. Given the single \( E^{(n+1)} \) term, one potential solution technique is an iterative approach, though there is concern with number of iterations required for convergence. An implementation of this solution technique has allowed for anecdotal observations that convergence was consistently reached within a couple iterations. Newton’s Method, a root finding technique, has been successfully employed to solve Eqn. IV.33 for \( E^{(n+1)} \).

\[ \frac{D^{(n+1)} - D^{(n)}}{V_+(E^{(n+1)})} + \frac{V_-(E^{(n+1)})}{V_+(E^{(n+1)})} E^{(n)} - E^{(n+1)} = 0 \] (IV.33)
CHAPTER V

OVERVIEW OF OPTICAL SIMULATION CAPABILITIES

Before attempting to create an optical simulation, reviewing the physical system that is being emulated will help inform the development of the simulation deck. Considering the entire pulsed laser measurement setup (Fig. V.I.), a majority of the instrumentation is devoted to routing and characterizing the laser pulse. All of this information can be reduced to the definition of an incident laser pulse characterized by the pulse information and the objective lens used for focusing the light onto the sample. Therefore, the entire simulation can be defined with the geometry of the device, with complete material and doping information, and the parameterization of the laser pulse (Fig V.II.). With this information, a simulation can be defined by creating the geometry from primitive objects of selected materials before defining injected electromagnetic waves and the spatial mesh to be used for the discretization of the simulation region.

Figure V.I. Pictographic representation of the PL-SEE measurement system at Vanderbilt University [30]. Optical simulations capture all components associated with the laser pulse.
Lumerical is a commercial, multi-physics software suite that seeks to provide optical modeling of capabilities from light interaction with nanoscale features [31],[32],[33] to photonic integrated circuits [34],[35]. FDTD Solutions is a material level simulation tool that simulates the electromagnetic response of user defined structures based on the FDTD algorithm [36]. Given the spatial discretization of the FDTD algorithm, the only limit on device complexity is the resolution of the spatial mesh and the computational resources necessary to run the simulation. While there are other FDTD solver packages [37]-[38], FDTD Solutions provides an easy to use GUI as well as additional functionality to improve simulation accuracy, reduce resource consumption, and reduce wall time. This chapter does not attempt to provide a comprehensive overview of FDTD Solutions, as the large application space of the tool would make this a formidable task. Rather, this chapter serves as documentation of functionality that is germane to emulating optical energy deposition from pulsed lasers.

V.1 Simulation Mesh

By default, the spatial mesh is generated during the initialization of the simulation using a routine that considers the device geometry, the refractive index of the materials used, and the wavelength spectrum of the injected fields. User input is taken in the form of a “Mesh Accuracy” parameter, a whole number ranging from one to eight corresponding to mesh points per material wavelength. However, this is only a factor in the final spatial mesh. Due to the rapidly increasing resource consumption associated with decreasing the mesh step size, it is recommended to initially
use a small “Mesh Accuracy” (1 to 3) and gradually increase only when a finer mesh is necessary. It is possible to specify a “minimum mesh step” that acts a global minimal boundary of a mesh step size, but care should be taken as bounding the mesh step size could produce a spatial mesh not suitable for an accurate simulation [39].

**Mesh Override**

Lumerical generates a non-uniform mesh to try to minimize computation time while not compromising accuracy for a given “mesh accuracy” value. However, there are cases where the Lumerical mesh needs to be adjusted in the sub-regions of the simulation. For example, consider a single bowtie photonic crystal cell placed inside a silicon waveguide [33],[40]. The dimensionality of the bowtie requires a very fine mesh to resolve the center of the bowtie, but the waveguide can be represented by a much coarser mesh to save resources. Though the non-uniform meshing attempts to adequately mesh the structure, it is possible that the single “Mesh Accuracy” parameter results in some regions being too coarsely or finely meshed. A “Mesh Override” region defines a spatial extent in which the spatial step size in each individual Cartesian direction can be specified, independent of the meshing routine invoked for the simulation. This allows for adjusting the mesh in only one direction, while maintaining the non-uniform meshing in the other directions. While there are clear advantages to applying mesh overrides, care should be taken as continuity requirements of the Cartesian mesh can result in mesh refinement in some subregions forcing mesh refinement to be enacted on neighboring regions.

**V.2 Boundary Conditions**

After defining the spatial extent of a simulation region, it necessary to define the behavior of electromagnetic fields at the interface. When considering boundary conditions, it is essential to remember that boundaries are a numerical consequence of a finite simulation, and in the ideal case would be indistinguishable in the simulation of the physical system. FDTD Solutions provide an assortment of boundary conditions that can be used to emulate open and closed boundaries, essential for dictating the behavior of the fields at the boundaries of the simulation. Spatial extent of the simulation region is a critical feature of any simulation as it impacts resources and wall time of the simulation; care must be taken to ensure that the extent is large enough to ensure that any numerical error induced by the boundaries is negligible.
**Perfectly Matched Layers (PML)**

In most cases, the dimensionality and fabrication of a device allows for the decomposition of the device in the simulation regime into two regions, relevant and extraneous. For example, topside illumination of devices likely means that once light propagates into the substrate, it is likely no longer impacting the device response. To simulate only the region of interest, the spatial boundaries of the simulations need to absorb incident electromagnetic waves, without creating reflections from the impedance mismatch of an absorbing layer, to physically emulate an open boundary. Numerically, this is accomplished by creating a series of absorbing layers that are tapered from low impedance to high impedance, a concept referred to as perfectly matched layers [41]. Care must be taken when used with source objects that spatially extend through a boundary as non-physical scattering can be induced by the source injecting in the layers. The spatial uniformity of a plane wave source will always experience non-physical scattering due to absorption at the boundaries [42], but as long as the spatial extent of the simulation region is large enough to allow for the radial distribution of a Gaussian beam to sufficient decay before the boundary, the non-physical scattering is negligible.

**Periodic**

For some devices it is possible to decompose the total device into a unit cell geometry that is repeated, such as in photonic crystal and metamaterials devices [31]–[33], [43]. Conceptually, a single unit cell of a device can be used to emulate an entire device by understanding that any light leaving a unit cell must be injected back into the unit cell since light leaving a single unit cell is entering the adjacent unit cell. Numerically, this is implemented for periodic boundaries by connecting the minimum and maximum boundary of an axis, resulting in fields impinging on one boundary being injected at the other boundary without any phase delay. For certain physical situations, such as an angled injection, it is necessary to generalize the periodic boundary condition to assign a phase delay to the fields injected by the boundaries, referred to as Bloch boundaries [44]. While these boundaries can greatly reduce simulation times and resource consumption, care must be taken to understand the extrapolation of a unit cell simulation to a total device; a unit cell simulation excited with a single dipole source is not equivalent to an entire device excited with a single dipole source. In this case, the duplication of the source for every unit cell removes spatial control over the location of the source in the overall structure.
**Metal**

Metal boundary conditions define the boundary of the simulation region as a perfect electrical conductor, resulting in unity reflection at the boundary that prevents energy escaping the simulation through the boundary. While the physical analogue of a such a metal boundary condition is unlikely to be present in many devices, there are numerical advantages afforded by using metal boundary conditions instead of PML boundaries in certain circumstances. For geometries where the optical energy reaching the boundary is negligible, such as light confinement in optical structures away from the boundaries, the behavior of the boundary is irrelevant. Contrary to PMLs, the unity reflection of metal boundaries does not require additional numerical techniques to emulate the boundary behavior, resulting in faster simulations with less likelihood of unintentionally introducing nonphysical behavior from the boundaries. Even in geometries where metal boundaries are not appropriate, an initial troubleshooting step for divergent simulations is setting all boundaries to metal. In the event that the simulation completes, the divergence is likely a consequence of the PML boundaries; if the simulation still diverges, it is likely connected to dispersive materials or the meshing of the geometry.

**Symmetric/Anti-Symmetric**

In the event that an entire simulation, including any injected and induced fields, exhibits planar symmetry along a Cartesian axis, the effective resource consumption and wall time of the simulation can be reduced by a factor of two by exploiting the symmetry and only simulating the unique region. This functionality is implemented by designating the minimum boundary of the axis that is normal to the plane of symmetry as “Symmetric/Anti-Symmetric” to denote the symmetry. Physically, planar symmetry implies that some field components must be equal to zero at the boundary, so the boundary forces the necessary field components to zero to satisfy the corresponding symmetries. A symmetric boundary requires that normal electric and tangential magnetic field components be zero at the boundary, while an asymmetric boundary requires that tangential electric and normal magnetic field components be zero at the boundary. Given the lack of internal validation of the symmetry boundaries, it is critical that the correct symmetries are used in order to ensure accurate simulations; agreement between simulations with and without symmetry boundaries affirm proper configuration of the symmetries.
V.3 Materials

The primary application space of Lumerical is broadband simulations [40],[45]-[46]. Therefore, it is important to accurately express the refractive indices of materials over the frequency band of interest. This frequency band is defined for a given simulation in the global properties and can be manually adjusted but should always be at least large enough to capture all relevant effects, such as the frequency spectrum of the source and, when appropriate, higher harmonic generation. In most cases, the default materials provided by Lumerical are sufficient for simulations, but in the case that a material is not provided or is insufficiently defined for a frequency band, new material models can be created for use in simulations. A discrete spectrum of the refractive index of a material can be experimentally measured (such as with ellipsometry [47]), taken from literature [48], or generated from an analytical model (such as optically conductivity) can be used to create a numerical model that is used for the material in simulations. Though specifics of the numerical model are proprietary, Lumerical provides functionality through a tool called “Material Explorer” for visual inspection of the numerical model compared with the discrete spectrum values. For every material, the dielectric function defined over the frequency spectrum of the simulation region can be plotted to inspect the quality of the analytic model. In the event that the quality of the model is poor, either increasing the number of coefficients used in the model or decreasing the spectrum width will likely result in increased fidelity. Due to the mathematical implications of increasing the available coefficients, such as increased ringing between discrete points (Runge’s phenomena) and increased runtime, it is typically better to adjust the frequency spectrum first. This preference is further enforced by the narrow frequency band required for simulation of energy deposition for ultrafast pulses.

Dielectric Function (Multi Coefficient Model)

In most cases, materials are incorporated into Lumerical’s Material database through a tabular format where wavelengths and the corresponding complex index of refraction are stored in order to represent a discretized spectrum of the optical coefficients. Lumerical uses what is referred to as a Multi Coefficient Model, a proprietary methodology, to fit the discrete spectrum with an analytic model with a functional form conducive to the necessary transform for use in the time domain solution algorithm. Ideally, the number of wavelengths used to discretize the spectrum will be sufficient to capture the dispersive nature of the spectrum, but that is not the only concern
in modeling materials accurately. The dielectric functions of real materials are the amalgamation of many distinct processes which complicates the analytic expression over a large frequency spectrum. Since the same analytic model is applied regardless of the domain, the fidelity of the analytic model will begin to suffer with regions of large amounts of dispersion.

**Analytic Models**

While it is highly preferable to use the tabular format in order to accurately capture material dispersion, it is not always possible to produce a dielectric function spectrum for new/exotic materials. In lieu of the tabular format for the dielectric functions, explicit analytic models for the dielectric model, such as a constant index of refraction, can be specified by providing the required parameters. Furthermore, some models can be used to augment base materials by appending additional terms to the dielectric function to create a new material \( \varepsilon_{base} + \varepsilon_{model} \). Though there are many provided analytic models, some models, such as metals and uniform index of refractions, are used more regularly than others. A common analytic model for describing the dielectric function of conductive materials is

\[
\varepsilon_{metal} = \varepsilon_{base} + i \frac{\sigma}{2\pi f \varepsilon_0} \tag{V.1}
\]

where \( \sigma \) is the optical conductivity, \( f \) is the optical frequency, and \( \varepsilon_{base} \) is a real permittivity value [17]. The inverse frequency dependence of the resultant dielectric function in comparison with real metals conveys the importance in restricting the frequency range in which this model is applied to minimize the error introduced by the approximation. In the case of \( \sigma \to \infty \), the model becomes the model of a perfect electrical conductor, resulting in frequency-independent unity reflection from light interacting at the boundary of the material.

**Custom Defined Models**

In addition to the default material models in the Lumerical material library, user defined models can be incorporated into the software through the flexible material plugin feature. Additional material models can be incorporated into the algorithm through the development of polarization densities that contribute to the total displacement field being simulated. The implementation of
this feature requires the development of a function in C++ that can be invoked by the solver during simulations to compute the electric field from previous field components provided by the solver. Once the function has been written, it must be compiled into a library file (.dll in Windows, .so in Linux) that can be added to the material subdirectory of the source code.

```
g++ -c -fpic UserMaterial.cpp
g++ -shared -o UserMaterial_example.so UserMaterial.o
```

For example, if the Kerr effect is incorporated into Lumerical, a model would be created that modifies the refractive index of the material consistent with Eq. IV.13. This is equivalent to using a base material model, such as silicon, and user defined model to add additional effects to the base material. Each instance of the material model can be created with a base material, such as silicon, and a parametrized model, such as the Kerr coefficient.

### V.4 Sources

Optical injection regions are defined by a line or plane, for 2D and 3D respectively, which define the spatial extent in which electromagnetic fields will be generated. For every node in the source region, the injected fields can be expressed as the product of a temporal function and spatial function. Spatially, every node is assigned a normalized amplitude and phase required to influence wave propagation for the intended behavior, with the amplitude providing an initial distribution of the field and the phase providing the evolution of that initial distribution as the wave propagates. The simplest realization is a uniform plane wave, which requires a spatially invariant amplitude and phase. A more complex, but more realistic source configuration is a focused Gaussian pulse, which requires both spatial distributions of amplitude and phase. Fortunately, these distributions are computed based on parameters provided by the user. Focused Gaussian optics can be defined by two methods, a Gaussian optics approximation and a full vectoral consideration where the delineation between methods is the legitimacy of the Gaussian optics approximations to the modeled systems. For either method, the distance of the injection plane relative to the beam waist and the convergent behavior of the beam must be specified. Due to the analytic model (chapter IV), the convergence of the Gaussian optics model can be specified as either the divergence angle or beam waist. For full vectoral consideration, the numerical aperture (NA) of the lens is required.
to characterize the convergence of the source. In the case of focused pulsed laser testing, the full vectoral description is used to most accurately capture an overfilled objective with tight focusing.

Temporal behavior of the pulse can be specified either in the temporal or the frequency domain, with corresponding parameters being calculated for the unspecified domain.

- Frequency: Central frequency of the pulse [THz]
- Pulse Width: FWHM of the temporal intensity profile of the pulse [fs]
- Offset: Time between the start of the simulation and the max amplitude of the pulse [fs]

Or

- Bandwidth: FWHM of the frequency band of the pulse [THz]

For most nanophotonic applications, a short pulse is used to measure a broadband spectrum so pulse-specific parameters are unimportant due to the frequency normalization; in these cases, setting the bandwidth is the preferred method of defining the light source. However, for the purpose of energy deposition from single pulses, defining the temporal profile of the pulse by the experimentally determined temporal parameters is essential to accurately modeling the pulse.

![Figure V.III. GUI used to parametrize the temporal/frequency content of the laser pulse injected into the simulation.](image-url)
**Pulse Energy**

Given the method that is used to define sources, it is not directly possible to initially define the source with a given pulse energy. Power propagating within a wave is expressed by the real part of the Poynting vector, one of the field quantities that can be computed at every node [16]. Integration of the temporal Poynting vector over an infinite plane normal to propagation computes the energy flux of the pulse, and in a lossless, homogenous medium, spatial integration over any infinite plane perpendicular to propagation calculates the energy within the pulse. Given the significant reduction in resource consumption, it is preferable to perform this operation in the frequency space, permitted by Parseval’s theorem [16], where a spectral average of the pulse replaces the temporal integration. For every source, following a successful simulation, it is possible to extract the spectral average of the injected fields integrated over the injection plane of the source, which provides the energy that was injected into the simulation. Once the pulse energy for a unique source configuration is calculated for reference, adjustment of the pulse energy is accomplished by tuning the electric amplitude by a simple proportionality

\[
|E_{\text{new}}| = |E_{\text{ref}}| \sqrt{\frac{U_{\text{new}}}{U_{\text{ref}}}}
\]  

(V.2)

where \(|E|\) is the amplitude of the source and \(U\) is the energy of the pulse.

**V.5 Monitors**

The resource-intensive nature of this algorithm requires that the software be adapted to reduce memory consumption during the simulation as well as the data stored at the conclusion of the simulation. Due to the first order discretization of the time derivatives, the default algorithm structure requires temporary storage of the field component for the previous and current timestep at every spatial node in the mesh. Following the competition of a simulation, Lumerical saves field components from the simulation to an output file that can be accessed by the user. For resource conservation and smaller output file size, Lumerical defaults to not storing field components from any previous time steps and only stores field components from mesh points contained with a specified subregion of the simulation. It is therefore the responsibility of the user to define temporal
ranges and subregions of interest to store field components within the simulation region; this can be done through the incorporation of nonphysical simulation objects known as monitors. For an individual monitor, the spatial extent is specified to define a point, line segment, rectangular plane, or rectangular parallelepiped that will record field components at every spatial node defined within the monitor. More than likely, not every field component is needed and therefore individual field components can be toggled on/off in order to ensure that only the desired field components are recorded. In the event that only the flux through a surface is need, it is possible to specify that only the spatial integration of the flux density through the monitor is recorded to further reduce memory consumption.

**Time Monitor**

Given the time domain of the FDTD algorithm, a source with a user-defined temporal profile, \( s(t) \), is used to excite the simulation region and the electromagnetic components are computed as a function of time. The temporal behavior of the field components can be stored by the inclusion of time monitors to capture the device response to a specific, user defined excitation. In addition to the standard field components, a point monitor can be used in conjunction with a user-defined material to record internal variables that are used in the implementation of the material. Due to the large number of time steps, it becomes impractical to store all field components for larger monitor extents and Lumerical provides the capability to restrict the initial time to start recording as well as the number of time steps to record to reduce the memory consumption.

**Frequency Monitor**

The user-defined temporal profile, \( s(t) \), and the corresponding induced field components can be expressed in the frequency domain

\[
\tilde{s}(\omega) = \int e^{i\omega t} s(t) dt
\]  

(V. 3)

\[
\vec{E}_{sim}(\vec{r}, \omega) = \int e^{i\omega t} \vec{E}(\vec{r}, t) dt
\]  

(V. 4)

Post-processing of field components produces the spectral density of the fields at every spatial node that can be stored by frequency monitors in a manner similar to a time monitor. The desired
frequency range and frequency spacing can be specified to ensure that only necessary data is stored to reduce memory storage. In most cases, frequency monitors consume less memory than time monitors due to the number of discrete frequency points being less than discrete time steps in a simulation. As opposed to time monitors, if the simulation only considers linear processes, then frequency monitors can be further processed to calculate the continuous wave response of the device for every frequency contained within the frequency band of the simulation. This additional processing is referred to as continuous wave normalization (“cwnorm”) and is toggled on by default. In order to use frequency monitors in nonlinear simulations, it is essential to toggle the additional processing off (“nonorm”).

Linear vs. Nonlinear

FDTD algorithms are a popular computation method for electromagnetic wave calculations for nanophotonic applications due to the wide frequency band simulation potential of a single simulation performed in the time domain [40],[45]-[46]. A linear system excited by a delta function in time produces a response consistent with a uniform excitation of all frequencies, referred to as an impulse response. However, delta functions present numerical stability issues, and are practically approximated as a smooth, short duration pulse. By limiting the scope of optical processes to the linear regime, a single simulation can be used to extract the impulse response of a simulated structure by normalizing the spectral density of the fields by the spectral density of the injected fields. This technique allows spectral densities to be calculated for the specific pulse simulated $\vec{E}_{sim}$ (nonorm) as well as an impulse response $\vec{E}_{imp}$ (cwnorm)

\[
\vec{E}_{sim}(\vec{r}, \omega) = \int e^{i\omega t} \vec{E}(\vec{r}, t) dt \tag{V.5A}
\]
\[
\vec{E}_{imp}(\vec{r}, \omega) = \frac{\vec{E}_{sim}(\vec{r}, \omega)}{s(\omega)} \tag{V.5B}
\]

For a linear simulation, consider the injected field profile at a source plane which can be expressed as a product of a spatial and temporal functions

\[
\vec{E}(\vec{r}, t) = \vec{E}_0(\vec{r})s(t) \tag{V.6}
\]
As discussed previously, the spectral density of the pulse and corresponding fields can be expressed as \( \tilde{s}(\omega) \) and \( \tilde{E}_{\text{sim}}(\omega) \) respectively. From the time profile of the field, the \( \tilde{E}_{\text{sim}} \) and \( \tilde{E}_{\text{imp}} \) can be calculated as

\[
\tilde{E}_{\text{sim}}(\vec{r}, \omega) = \int e^{i\omega t} \tilde{E}(\vec{r}, t) dt = \int e^{i\omega t} \tilde{E}_0(\vec{r}) s(t) dt = \tilde{E}_0(\vec{r}) \tilde{s}(\omega) \quad (V.7A)
\]
\[
\tilde{E}_{\text{imp}}(\vec{r}, \omega) = \tilde{E}_0(\vec{r}) \quad (V.7B)
\]

The lack of frequency dependence in \( \tilde{E}_{\text{imp}} \) ensures that the normalization results in a uniform injected field across the spectral range.

**V.6 Post Simulation Processing**

Following the successful completion of a simulation, data recorded by monitors can be accessed through the GUI, but practicality dictates using the Lumerical scripting language to navigate and process the data. For the purpose of this work, the output of the optical simulations is a spatial distribution of optically generated charge that can be incorporated into a charge transport solver. In order to extract the three-dimensional distributions of optically generated charge from the simulations, scripts have been written that extract the data from the monitors, format the distribution, and write the data to a Matlab file. For large simulations with too much stored data to reasonably work with on a personal computer, the script files can be executed on the cluster computer and the Matlab files can be recovered from the cluster to a personal computer.

**V.7 Additional Considerations**

*2D & 3D*

The dimensionality of the simulations can be selected to either be two or three dimensions, with two dimensional simulations consuming less resources and wall-time compared to three dimensional simulations. Unfortunately, there is no option for 2-D cylindrical simulations, which simulate radially symmetric 3-D structures as a 2-D structure cut along the radius and rotates the results around a central axis to produce a 3-D simulation. From a simulation perspective, the
transition from a 3D to 2D simply removes a dimension that light can propagate from or into, effectively reducing the simulation to an isolated spatial plane. Qualitatively, this reduction is relatively benign when applied appropriately and still captures the relevant physical process of a device, like a cavity, while losing some auxiliary processes, like losses from out of plane scattering. It is critical to understand the implications of reducing 3-D simulations to 2-D simulations to verify the validity of the reduction as well as appropriately interpret the simulation results.

The treatment of a 2-D simulations as isolated planes requires that any extension into three dimensions be performed by uniform extrusion along the third dimension, effectively being reduced to applying a normalization length in a manner similar to charge transport solvers. Physically, this can become problematic when capturing three dimensional phenomena, such as a focused laser pulse. In a simplified 3-D view, focusing squeezes the light into a point for 3-D simulations, but is squeezed into a line when simulated in 2-D and extruded. Confinement in only a single dimension eliminates the possibility of manually creating 2-D cylindrical simulations using the 2-D simulation as the radial cut, as the lack of confinement in a second direction results in breaking conservation of energy in the pulse. Therefore, while it is beneficial from a resource and wall-time perspective to run simulations in two dimensions when possible, the physical implications on injecting light in 2-D simulations largely prohibits use in quantitative energy deposition simulations.

**Autoshut off**

The maximum duration of simulated time is provided by the user as the “simulation time”, which in conjunction with the temporal step, is used to compute the maximum number of time steps to be used in the simulation. From the Courant stability condition, the maximum temporal step is computed internally as a function of the materials and spatial step size of the meshes and cannot be edited by the user. By default, the maximum temporal step is used in order to minimize wall time of the simulation, but in some situations it is necessary to reduce the temporal step to increase stability of the simulation. The “dt stability factor” can be set in the open interval of zero to one, acting as scaling factor applied to the maximum temporal step.

To reduce wall time and resource consumption, the simulation time should be set as small as possible without truncating any field propagation to ensure that there is minimal time in the simulation devoted to negligible field behaviors. “Auto shutoff” is a feature that monitors the ratio
of the energy in the simulation space at the current time step to the total injected energy, which triggers the conclusion of the simulation, before the simulation time is reached, once the ratio falls below the “Auto Shutoff Min” threshold specified by the user. This energy ratio can also be used to determine if the simulation is likely diverging due the ratio growing larger than the “Auto Shutoff Max” threshold. Due to the utility, the default simulation states enables these functions, though in some cases it is necessary to disable one or both of the functions.
CHAPTER VI

INTEGRATION WITH TCAD

From the perspective of simulating PL-SEE testing, optical simulations capture the optical pulse, passing through a device and depositing a spatial distribution of charge in a device. However, the measurement that is taken is an electrical signal collected that represents the movement of the deposited charge through the device and circuit. Similar to electromagnetics, charge transport is governed by partial differential equations that can be solved using numerical techniques; these solvers are integral tools for electrical characterization of devices. Therefore, to completely model a PL-SEE from laser pulse to measurement, the simulated spatial distribution of charge from the pulse needs to be used as an initial condition in a charge transport code. In this chapter, the functionality of a charge transport solver is examined and the integration processes between the optical solver and charge transport solver are described.

VI.1 Tool Suite Overview

Sentaurus is a suite of technology computer-aided design (TCAD) software tools developed for the simulation of semiconductor device behavior and reliability. Rather than a single tool being responsible for the entire simulation process, Sentaurus decomposes the simulation process into subtasks that are performed by individual tools in the suite. For example, defining a simulation geometry and producing a simulation mesh is performed using the Sentaurus Device Editor while physical simulations on a device defined by a mesh is performed by Sentaurus Device. The interconnectedness of the tools is predicated on the writing and reading of data files that are used to store information, such as meshing or simulation results. This distributed approach to simulations becomes advantageous when a single output data file is able to be used as the input to multiple simulations.
VI.2 Device Physics

The spatial distribution of charge in a device, both mobile and immobile, induce an electrostatic potential distribution that can be described by the Poisson equation [49]

$$\nabla \cdot (\varepsilon \nabla \varphi) = -q(p - n + N_D^+ - N_A^+) - \rho_{\text{trap}}$$  \hspace{2cm} (VI.1)

with the charge contributions from electron density (n), hole density (p), ionized donor density ($N_D^+$), ionized acceptor density ($N_A^+$), and fixed/trapped charge density ($\rho_{\text{trap}}$). Electric permittivity ($\varepsilon$) captures the impact of screening of the potential from the material system. Conservation of charge ensures that the carrier current density flowing out from a spatial point is the net contribution of generation (additive) and recombination (subtractive) processes

$$\nabla \cdot J_n = q(R_{\text{net}} + G_{\text{net}})$$ \hspace{2cm} (VI.2)

$$-\nabla \cdot J_p = q(R_{\text{net}} + G_{\text{net}})$$ \hspace{2cm} (VI.3)

where $R_{\text{net}}$ is rate of removing carriers and $G_{\text{net}}$ is the rate of generating carriers [49]. Carrier current densities $J_n, J_p$ can be modelled with a variety of physical models for carrier movement, such as movement induced by thermal or potential gradients. Physically, the integration of optically generated charge with device physics is accomplished with generation processes. Therefore, to incorporate optically generated charge, the spatial distribution of optically generated carriers must be used as a spatial generation rate.

VI.3 Generation Models

Any physical process that creates electron-hole pairs is incorporated into device physics through the generation rate term in the continuity equation. As the continuity equations are defined over the spatial extent of semiconductor regions of a device, inclusion of a generation process requires the definition of a spatial distribution $G(x, y, z)$ over the same extent [50],[51]. This general description of generation processes demonstrates that the physical model of a generation process is responsible for defining $G(x, y, z)$, either through an analytical, empirical, or simulation model.
For example, the spatial distribution of electron-hole pairs generated from a heavy ion passing through a material is often expressed as a simplified analytical model

$$G(r, \theta, z) = G_{LET}(z)R(r)$$

( VI. 4 )

where the spatial distribution is expressed as the product of a function along the path of the particle $G_{LET}(z)$ and a function describing generation along a direction normal to the path $R(r)$.

Sentaurus provides several generation models that use parametrized equations to define spatial distributions, such as heavy ion and avalanche generation [52]. Computational techniques for computing optically generated carrier distributions, including FDTD and beam propagation solvers that can be invoked either before or during a device simulation, are available with the “OpticalGeneration” physics model. For this work, optical simulations are completed using Lumerical (Chapter V) prior to device simulations and the generated carrier distributions are stored in a TDR file as datasets labelled “OpticalGeneration” to be imported into device simulations. The name of the dataset in the TDR file is critical for the model as the importation of a distribution from a TDR file is performed by searching the file for datasets labelled as “OpticalGeneration”. The name of the TDR file containing the optical generation distribution is provided in the “File” section of the command file, and the model is directed to read the distribution from the file. Distributions read from “OpticalGeneration” datasets are not processed, other than an optional scale factor, and therefore relies on any necessary computations be performed prior to storage in the TDR file [52].

```plaintext
File {
   OpticalGenerationInput = <TDR File Name>
}

OpticalGeneration {
   ReadFromFile(
      Datasetname=OpticalGeneration
   )
}
```

Figure VI.1. Commands to enable optical generation from a file.
Temporal

Generation models can be defined as the product of a spatial profile $G(x, y, z)$ and a temporal envelope $F(t)$

$$G_r(x, y, z, t) = G(x, y, z)F(t) \quad (\text{VI. 5})$$

This functional form allows for the establishment of a steady-state generation by setting $F(t)$ equal to unity, while also allowing for a temporal envelope that is typically used to toggle a model for a given time interval [52]. Temporal envelopes that are only nonzero on a subinterval of the simulation time can be used to inject a finite amount of charge distributed over the subinterval, such as a suitably defined Gaussian or square pulse. Ideally, the temporal envelope is only associated with the act of injection of charge and not the total amount of charge, and therefore requires the inclusion of a scaling factor such that $\int F(t)dt = 1$. It is critical to understand the time scale of the physical process that is being emulated in the simulation. For instance, charge injected by an ultrafast laser pulse or ionizing particle occurs over a much shorter time scale than from a burst of particles distributed in time.

Temporal dependence for generation models is incorporated into a simulation by definition of a “TimeDependence” command within the physics model statement. Three different temporal envelopes are provided: trapezoid, pseudo-Gaussian, and user defined requiring the path to a text file defining the temporal behavior [52]. For this work, a pseudo-Gaussian envelope defined as shown in Eqn. VI.6

$$F(t) = \begin{cases} 
\exp \left( -\left( \frac{t - t_1}{\sigma} \right)^2 \right) , & t < t_1 \\
1 , & t_1 \leq t \leq t_2 \\
\exp \left( -\left( \frac{t - t_2}{\sigma} \right)^2 \right) , & t_2 < t 
\end{cases} \quad (\text{VI. 6})$$

where $t_1, t_2, \sigma$ are user defined constants in the command. A typical Gaussian envelope can be defined from Eqn. VI.6 by setting $t_1 = t_2$. From this functional form, the scaling factor can be calculated by integration of $F(t)$ to be $\frac{1}{\sqrt{\pi \sigma}}$ for $t_1 = t_2$ to ensure that there is not a net contribution
of charge from the temporal envelope. For both pulsed laser and heavy ion simulations, charge
deposition occurs at a time scale much shorter than any charge transport phenomena, and therefore
the charge injection should occur over a time interval that is essentially instantaneous compared
to the device response. While it may be tempting to select a time interval that is arbitrarily small,
umerical stability concerns dictate that the optimal time interval is the largest interval that does
not impact the device simulation [50].

```plaintext
TimeDependence {
   WaveTime = (<t1>, <t2>)
   WaveTSigma = <sigma>
   Scaling = <scale>
}
```

Figure VI.2. Commands for defining a temporal envelope.

**VI.4 TDR Files**

During the creation of the simulation mesh, information provided to the meshing tool is used
to create metadata necessary for the data structure, such as name labels and region materials, used
in the TDR files [53]. The spatial mesh constitutes the necessary information to reconstruct a
device, storing data defining the boundaries and material types of the individual regions, as well
as the location of electrical contacts. Categorized by their metadata, the spatial mesh is stored as
coordinates of individual nodes as well as the connectivity with neighboring nodes [54]. Datasets
store data associated with physical quantities of the device at each individual spatial node. For
instance, a dataset could store the doping profile or the spatial distribution of avalanche generation
for an individual region.

**TDR Interfacing**

As depicted in the simplified TDR structure in Fig. IV.3, the data storage is structured similarly
to a directory structure, where a single structure can hold many distinct sets of data. A single TDR
file can contain multiple geometries, with each geometry defining a mesh that can be used to store
datasets. An individual geometry contains information relating to the regions that are used to
construct the simulation mesh, and the data related to the physical properties of the device. An
individual state stores all defined physical quantities across all regions for a given device.
configuration. Since a dataset stores data for a single physical quantity defined over a single region, a single state likely has multiple datasets for a single physical quantity.

![Diagram of data structure hierarchy](image)

Figure VI.3. Visual representation of the data structure hierarchy used in .tdr files [53].

TDR files are a binary file, requiring additional software tools to interact with the data stored in the files. Sentaurus provides a tool, called DataExplorer, which makes use of an adapted TCL programming language to create commands and scripts for navigating the internal data structure in TDR files by specifying “paths” to data values [53]. In keeping with the file system analogy, the “path” to a single value stored in a dataset would be “File/Geometry/State/Region/Dataset/”. Though each directory has a unique name label, subdirectories of a directory are arrayed and addressed by an index. For each directory, commands are available to return the number of available subdirectories. The number of subdirectories can be used to index through all subdirectories (TDX indexes from zero) and check metadata associated with each subdirectory, such as name labels.
For many applications, the spatial distribution of physical quantities is of interest. To assemble the spatial distribution of a physical quantity, both the physical quantity and the physical coordinates of every node must be extracted. Commands are provided to extract this spatial and physical information from a single value in a dataset. These commands can be used with loops to iterate over every value in every dataset for a physical quantity to extract the necessary information to construct a spatial distribution of the physical quantity.

 VI.5 Command File

The device physics simulator Sentaurus Device is primarily controlled by a command file that constitutes the information necessary to instruct the tool to conduct a numerical experiment. Command files are subdivided into sections that are responsible for individual components of a
device simulation. Within each section, keywords can be defined to enable functionality, such as physical models and data storage, that are critical in accurately capturing a numerical experiment. The following section definitions are necessary for the implementation of optical generation in the device simulations [52].

**File Section**

The “File” section is related to the file management associated with a device simulation, with specific keywords for defining input/output files for specific applications. Though there are several input keywords associated with extra functionality, the only required input is a TDR file containing a device mesh; this mesh file is specified with a “Grid” keyword. The dimensionality of the simulation is determined by the dimension of the geometry stored in the “Grid” TDR file. Output keywords designate the filenames from data produced from the device simulations. Electrical contact data (“Current”) and log files (“Output”) are stored as text files. Spatial distributions (“Plot”) are stored in a TDR file.

```plaintext
File {
    Grid = "<GridName>"
    Plot = "<PlotName>"
    Current = "<CurrentName>"
    Output = "<OutputName>"
}
```

Figure VI.6. “File” keyword in a command file.

**Plot Section**

Every time data related to the physical state of the device is recorded, it is possible to record every quantity that is stored on the spatial mesh, such as doping concentrations or the spatial profile of trap-assisted recombination, in the output file. To assist with resource conservation, only quantities defined within the “Plot” section will be stored in the output files. In some cases, the volumetric integral defined over one or more regions is of more significance than the spatial distribution. This functionality can be included by the keyword “Integrate()”, with the domain of integration provided as an argument. The resulting quantity is stored in the “current” output file defined in “File”.

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Physics Section

Physical processes are incorporated into device simulations by modification of terms in the constitutive equations of device physics. A large number of these physical processes have been modeled and provided to the user as keywords, some with additional arguments, that can be toggled on by definition in the “Physics” section. Many physical models are defined with default material-dependent parameters that can be overwritten by the inclusion of parameter files, that contain user-defined model parameters, in the “File” section using keyword “Parameter”.

VI.6 Integration with Lumerical

Conceptually, the optically generated carriers are characterized as a continuous spatial distribution $G(x, y, z)$ defined over a domain, such that any point contained within the domain can be mapped to a value in the distribution. As the simulated optically generated charge is to be used as an initial condition for the charge transport, the continuous spatial distribution discretized by the optical simulations is the same distribution that is being discretized by the charge transport code. Therefore, in order to transition from the optical mesh generated by Lumerical to the TCAD mesh, an interpolation technique, such as cubic interpolation, is used to map the distribution onto the TCAD mesh. The spatial mesh of the optical simulation is easily extractable, but the spatial mesh of the TCAD simulations are more challenging to extract. Using the tool to interact with the data files, bash scripts have been written to access the mesh information. Interpolation between the two simulation meshes are performed using MATLAB scripts. Following the interpolation, the
distribution of optically generated carriers interpolated on the TCAD mesh is written back into the data files.

Figure VI.9. For the same spatial distribution, two distinct meshes (black and red) can used to discretize the spatial extent into sets of nodes. As the two meshes represent the same distribution, data stored on one mesh (black) can be used to calculate the data to be stored on a different mesh (red). Common interpolation techniques take in a spatial position and uses neighboring nodes to calculate the data at that spatial point.

Figure VI.10. Block schematic of the integration of the output of Lumerical FDTD Solutions into TCAD using Bash scripts.
CHAPTER VII

COMPARISON WITH EXPERIMENTS

The previous chapters of this thesis describe the development of a simulation infrastructure to simulate PL-SEE testing from laser pulse to electrical measurement of a device. Following completion of the simulation tools, comparison with analytic models and experimental results is essential in establishing the validity of the tools. Simple analytical models can be used to verify the accuracy of the free carrier optical models and the impact of doping profiles on the optical simulations. An epitaxial silicon diode was used as the experimental device under test. Current transients were captured for a variety of pulse energies, voltages, and focal positions, and measured values compared well with simulated results. The benefit of the first principles approach to the optical simulations on the experimental results is also discussed in this chapter.

VII.1 Incorporated Free Carriers

Due to the importance of free carrier effects from doping in the materials, it is critical to validate the free carrier models. As the native output of FDTD Solutions is electromagnetic fields, it is preferable to compare simulated results with analytical models. Due to the modular structure of the material models, it is possible to toggle models independently of other models, allowing for the decoupling of free carrier and free carrier refraction.

Free Carrier Refraction

A plane wave incident on a smooth interface between two materials will experience both reflection and transmission at the interface, with the proportionality of the light transmitted and reflected dictated by the index of refraction of the two materials. For light traveling from a material with index of refraction \( n_1 \) into a material with index of refraction \( n_2 \) at normal incidence, the Fresnel equation for reflected light intensity from the interface [16],[17] is expressed as

\[
R = \frac{|n_1 - n_2|^2}{n_1 + n_2} \tag{VII. 1}
\]
From the free carrier refraction models (Eqn. IV.14), the density of free carriers contributes to the total refraction of the material, represented by the modification of the real part of the dielectric function of the bulk material. In the absence of any optical free carrier generation, the concentration of free carriers in the material is controlled by the doping of the material. The introduced free carriers from a given doping concentration in the material, \( N_{doping} \), will result in free carrier refraction, which is expressed as an additional term of the index of refraction of the material \( \Delta n_{FCR} \left( N_{doping} \right) \) [17]. Under these conditions, the Fresnel equation can be rewritten to highlight the dependence of the reflection coefficient on the doping of the material, as shown in Eqn. VII.2 where it is assumed that material 2 is doped.

\[
R(N_{doping}) = \left| \frac{n_1 - (n_2 + \Delta n_{FCR}(N_{doping}))}{n_1 + (n_2 + \Delta n_{FCR}(N_{doping}))} \right|^2
\]  

(VII.2)

For the purposes of benchmarking simulations against the analytical model, consider a smooth interface between vacuum \( (n_1 = 1) \) and a material \( (n_2 = 3.5) \) that is illuminated from the vacuum. Using the free carrier refraction parameters defined for silicon, the reflection coefficient of the doped material can be simulated as a function of doping concentration. Comparisons of the results of numerical simulations carried out in Lumerical, with the nonlinear FCR model enabled, with the analytical model shown in Eqn. VII.2 are compiled in Fig. VII.1. The excellent agreement between the numerically calculated data points and analytical model affirms the proper implementation of the free carrier refraction models within FDTD Solutions.
Figure VII.1. Reflection coefficient from free carrier refraction as a function of doping level. Red points correspond to results of optical simulations. The black line is defined by the analytic theory.

**Free Carrier Absorption**

A plane wave propagating through a material will experience intensity attenuation as function of the distance in the material. For linear absorption, the intensity of light as a function of propagation depth can be expressed with Beer’s Law

\[ I(z) = I_0 e^{-\alpha_0 z} \]  

(VII. 3)

with \( \alpha_0 \) parameterizing the absorption of material [16],[17]. From the free carrier absorption models (Eqn. IV.10), the density of free carriers contributes to the total absorption of the material, represented by the modification of the absorption coefficient of the bulk material. Neglecting free carrier generation processes implies the free carrier density of the material is dictated by the doping concentration \( N_{doping} \) of the material. Free carriers introduced by the dopant atoms contribute to total absorption in the material, which is modelled by a modification of the absorption coefficient \( \Delta\alpha_{FCA}(N_{doping}) \) [17]. With these considerations, the intensity of light as a function of propagation depth can be rewritten to highlight doping dependence.

\[ I(z, N_{doping}) = I_0 e^{-\left(\alpha_0 + \Delta\alpha_{FCA}(N_{doping})\right)z} \]  

(VII. 4)
Consider a material with all losses being attributed to FCA \((\alpha_0 = 0)\). From Eqn. IV.10, the FCA absorption coefficient is the product of the free carrier density and a FCA cross-section. A free carrier absorption cross-section of \(10^{-22} \text{ m}^2\) was used to simulate normalized intensities depth profiles as a function of doping density, compiled in Fig. VII.2. Strong agreement of the simulations with the analytical models affirms the proper implementation of the free carrier absorption models within FDTD Solutions.

![Intensity decay curves](image)

Figure VII.2. Intensity decay curves for different doping concentrations (listed next to curve). Data points correspond to values from the analytical model. Lines come from optical simulations using the incorporated free carrier models.

**VII.2 Pulsed Laser Testing on a Silicon Diode**

Though free carrier optical models implemented in Lumerical FDTD can be verified against analytic models, comparison of simulations against experimental measurements is critical to evaluating the simulation infrastructure. Pulsed laser testing was conducted on a large area silicon diode manufactured by Beijing Microelectronics Technology Institute to serve as a test structure. A cross section of the device is shown in Fig. VII.3. Circular holes with a diameter of 14 microns were included in the top contact to allow for topside illumination of the device without perturbing the electrostatics of the device. Pulsed laser measurements were conducted with a variety of reverse bias conditions that modulate the collected charge and current transient shape as well as the dominant physical processes governing charge collection. Prior to conducting optical
simulations on the Si diode, it is necessary to show that there is no need to consider the reverse bias in the optical simulations.

Figure VII.3. Epitaxial silicon diode geometry and doping information [12],[55].

VII.3 Doping Profile

As free carrier refraction and absorption are dependent on the density of free carriers, defining an initial distribution of free carriers in the device is necessary for accurate optical simulations of the device. While electronic devices are diagrammed as comprising finite regions with distinct doping in those regions, in practice, introduction of doping atoms through ion implantation typically results in non-abrupt transitions between material regions. The process of reaching electrostatic equilibrium within a device further redistributes the free carrier densities modulated by the potentials applied to the device. For example, a symmetrically doped $p$-$n$ junction produces a depletion region around the interface between the two doped regions, with significantly less free carriers than the surrounding material [49]. Spreading resistance measurements can be carried out to reveal the actual doping profile of a device, which can then be incorporated into a device model in Sentaurus TCAD for simulation of the equilibrium state of the diode at a given bias configuration. Free carrier density distributions can be extracted from equilibrium simulations that represent the spatial distribution of free carriers (from doping) in a device for a given bias. Using
the same process as Eqn. VII.4, Fig. VII.4 contains the total free carrier density as a function of depth in the silicon diode (Fig. VII.3) for three device states: doping profile (no bias), 5V reverse bias, and 90V reverse bias.

![Graph of carrier density vs depth](image)

**Figure VII.4.** Free carrier distribution in the silicon diode (Fig. VII.3) at equilibrium for reverse bias conditions: doping profile (no bias), 5 V, and 90 V.

From the free carrier density distribution, a corresponding distribution of absorption coefficients and refractive index modulation can be calculated using a FCA model in silicon (Eqn. IV.10). Neglecting carrier generation processes, the normalized intensity of light propagating through the electrostatically equilibrizied device can then be modeled using a modified Beers’ law (Eqn. VII.4) with a depth dependent absorption coefficient (Fig. VII.5(a)). Fig. VII.5(b) shows intensity curves as a function of depth for three device geometries: a doping profile (no bias) and electrostatically equilibrized devices with 5 Volt and 90 Volt reverse biases. Since free carrier densities associated with the doping levels in an active region of a typical device result in minimal free carrier absorption, the local reduction of carrier densities in the proximity of material junctions only further reduces the free carrier absorption. In a similar fashion, the refractive index modulation from FCR results in minimal impact on the material of the device. Approximate equivalence between the three geometries suggests that from an optical perspective, a simplified,
bias-independent doping model, rather than an electrostatic equilibrium model of free carriers, can be used to define the initial state of the device without a loss of accuracy.

Figure VII.5. (a) Absorption coefficient from free carriers ($\alpha_{FCA}$) as a function of depth for the different biases on the diode. (b) Normalized intensity as a function of depth for the different bias conditions: all curves lie on top of each other.

VII.4 Optical Simulations

For the optical simulations, the simulation geometry comprised the simplified doping diagram in Fig. VII.3, complete with the hole in the 2 micron thick aluminum contact. Two photon absorption pulsed laser testing (1260 nm) was conducted at the Naval Research Laboratory, which reports 130 fs temporal pulse width while using a microscope objective with a 0.5 numerical aperture [56]. The nonlinear parameters used for silicon in the optical simulations [13],[14] were $\beta = 1 \text{ cm/GW}$, $\sigma_{FCA} = 5 \times 10^{-21} \text{ m}^2$, and $n_2 = 4 \times 10^{-18} \text{ m/W}$; the model defined for free carrier refraction in silicon by *Soref* was utilized [29],[57]. In order to emulate experimental campaigns, simulations were conducted for three different pulse energies (400 pJ, 750 pJ, 990 pJ), with depths scans (changing focal position) at each pulse energy. The experimental parameters of the measurement setup were incorporated into the optical simulations to characterize the pulse and the amplitude of the simulated pulse was adjusted to inject the pulse energy used in a measurement. For every optical simulation conducted, a three-dimensional distribution of optically generated charge was produced, which is subsequently imported into TCAD simulations. For comparisons,
two dimensional cuts of the optically generated carrier distributions for each pulse energy at two different focal positions are displayed in Fig. VII.6.

**VII.5 TCAD Simulations**

Optically generated charge carrier densities were extracted from the optical simulation and incorporated into TCAD simulations to simulate the collection of injected charge as described in chapter VI. Device simulations were conducted using a 2D cylindrical simulation in order to reduce resource consumption and wall time. In order to capture the capacitive nature of the large area junction, the width of the diode was adjusted in order to ensure that the total area of the simulated diode is equivalent to the area of the real device. Though a smaller diode width could be used to reduce resource consumption, the reduced junction capacitance alters the temporal shape of the transient. Following the injection of the optically generated charge, the collection of charge by the junction results in a current transient that can be “measured” from the contacts of the diode in the simulation. One metric commonly considered is the total charge collected by the junction, which is characterized by the integration of the current transient. For each pulse energy and position, experimental data was collected at two reverse bias conditions (-5 V and -90 V) to compare to the simulations. Simulations and experimental results for these conditions can be collated together and are summarized in Fig. VII.7. Overall, there was good agreement between simulated and experimental results, validating the accuracy of the optical simulations.
Figure VII.6. Cross sectional cut of optically generated carrier distributions for three different pulse energies: 400 pJ, 750 pJ, and 990 pJ. For each pulse energy, two focal positions are shown: at surface and ~11 microns deep in the diode. The color bar is consistent for simulations of the same pulse energy.
Figure VII.7. Depth profiles of the silicon diode for three pulse energies for two reverse bias conditions: 5V (left) and 90V (right). Experimental error bars represent one standard deviation based on 200 collected transients.
**Current Transients**

Using mixed-mode TCAD simulations to capture the circuit components associated with the measurement system, such as the bias tees, in the simulation environment, it is possible to emulate the entire pulsed laser measurement technique, from laser pulse to electric response of the device. This approach allows for comparison of the simulated current transient with the experimental current transients, with an example shown in Fig. VII.8. Comparing transient shape as well as collected charge allows information about the physical mechanisms impacting charge collection to be extracted from both the simulations and experimental results.

![Figure VII.8. Comparisons between experimentally measured current transient and simulated current transient generated by incorporating results of optical simulations into TCAD device simulations. Conditions: 90 V reverse bias, 750 pJ, focused at surface.](image)

**VII.6 Advantages of FDTD**

One of the main reasons that an optics solver that uses an FDTD algorithm was selected to model optical energy deposition was the ability to accommodate arbitrarily complex device structures. In some cases, it is feasible to approximate a device as a slab of a single material, but that is not always applicable, even for a simple structure like the large area silicon diode used in this work. For example, consider the dimensionality of the hole in the top contact relative to the beam radius for focal positions near the surface of the diode and for focal positions deep into the
diode, as depicted in Fig. VII.9. For focal positions near the surface, the presence of the metal contact is negligible for optical simulations. However, for focal positions deeper into the material, the metal contact acts as a pseudo-pinhole, excluding a non-trivial amount of energy from entering the material.

Figure VII.9. Normalized intensity of a simulated laser pulse with experimental parameters at the front of the metal hole for two focusing conditions: at surface and deep into the substrate. The boundary of the hole is described by the dashed lines.

Another consequence of considering the whole diode structure rather than a single slab of silicon is the added attenuation associated with the heavily doped substrate region. Consider the optically generated carrier distribution for two focal positions, one near the surface and one focused deeper into the material, depicted in Fig. VII.10. For the focal position near the surface, most of the optically generated charge is being generated in lightly doped areas and the distribution is largely unperturbed by the material system. However, when the laser pulse is focused in the heavily doped region, the heavily doped region begins to attenuate the amount of charge that can be deposited, and therefore collected, due to free carrier absorption. Both the hole in the contact and the impact of the doped regions illustrate the power and necessity of using a first principles
approach to model optical energy deposition; in general, the idiosyncrasies of specific devices are captured by the FDTD algorithm making this approach more robust for modeling pulsed laser testing.

Figure VII.10. Cross-section of optically generated carriers focused at the substrate interface for two different pulse energies. The white dashed lines highlights the perturbation of the generated charge due to the presence of the substrate region (starting at 25 microns). The highly doped substrate results in more FCA and FCR perturbing the pulse.
CHAPTER VIII

LUMERICAL AND VANDERBILT RER

Though this document represents the first time the complete integration of Lumerical FDTD Solutions and Sentaurus TCAD has been described in detail, I have used Lumerical FDTD Solutions for understanding and predicting PL-SEE testing at Vanderbilt University while this thesis was in preparation. In many cases, even qualitative optical simulations prove invaluable to radiation effects research.

**Correlation of PL-SEE and Heavy Ion**

A key numerical technique in SEE testing is the definition of a region that collects charge deposited within the region. These regions can be used in conjunction with charge deposition profiles to compute collected charge without charge transport simulations. Heavy Ion and PL-SEE measurements, compiled with heavy ion simulations and the simulation infrastructure discussed in this work, were used to show that sensitive volumes from pulsed lasers and heavy ions are different. This observation is significant to the correlation of PL-SEE testing and heavy ion testing.


**Nanophotonics Impacting Charge Generation**

A significance advantage of conducting optical simulations with a first principles approach to solving Maxwell’s equations, like FDTD, is that it inherently captures complex optical phenomena. As device feature sizes become subwavelength, nanophotonic processes begin to complicate the approximation of a device as a bulk material. Lumerical FDTD Solutions has been
used to examine the impact of surface plasmon polaritons on charge deposition and collection in FinFETs, and demonstrate that the polarization direction of the light impacts PL-SEE measurements. This represents the first time that nanophotonic processes have been shown to impact charge deposition in a device.


Interpreting Experimental Results

Two photon absorption PL-SEE testing was applied to examine charge collection mechanisms in silicon carbide power MOSFETS and power Schottky diodes. Spatial scans of the laser across the MOSFET demonstrated enhanced charge collection isolated to the gate region of the device. Lumerical FDTD Solutions was used to demonstrate that the enhanced charge collection cannot be attributed to reflections from metal/passivation layers.

CHAPTER IX

CONCLUSION

As PL-SEE testing is increasingly being used to augment heavy ion testing facilities, there has been a renewed interest in establishing a quantitative basis to the experimental technique. The intent of this work is to present a simulation infrastructure that simulates PL-SEE measurement from the laser pulse to the electrical measurement of the device. This simulation infrastructure provides a predictive capability for PL-SEE testing as well as facilitates the comparison of the physical processes impacting charge collection from charge deposited by heavy ion and laser pulses. This simulation approach decomposes PL-SEE testing into optical simulations to calculate charge deposition from a laser pulse and charge transport simulations of the deposited charge. The simulation approach outlined in this work represents the first instance of modeling PL-SEE testing from pulse to electrical response using first-principle simulation tools, satisfying a critical need for understanding the distribution of optically generated carriers in comparison to carriers generated from ionizing particles.

Optically, a laser pulse depositing charge requires understanding light-matter interaction and the propagation of a focused laser pulse. Due to high energy densities associated with pulsed lasers, it is critical to consider nonlinear optical processes that modulate the laser pulse, and therefore the spatial distribution of optically deposited charge. As electromagnetic waves are governed by Maxwell’s equation, all light-matter interaction must be incorporated as additional field sources. To facilitate the development of the nonlinear models, the origin of linear optical processes is examined and then perturbed to induce nonlinear order optical effects (Chpt. II). Though not strictly applicable to highly focused lasers, Gaussian optics are useful in providing intuitive understanding of focused laser pulses propagating in a material. Furthermore, it allows for the connection of common experimental parameters of a laser system with the spatial distribution of light around the focus (Chpt. III).

Knowledge of light-matter interaction and light propagation are integral for the creation of optical simulations. A common technique applied to solving Maxwell’s equations, with minimal approximations, was described to motivate the functional form of the nonlinear models that were
incorporated into the FDTD solver (Chpt. IV). Lumerical FDTD Solutions, a commercial three-dimensional FDTD optical solver, was adapted to calculate the spatial distribution of optically generated charge from a laser. Typically applied to solve complex nanophotonic material systems, Lumerical was selected as it allows for the creation of complex structures and creation of custom material models. Functionality of the solver relevant to the simulation of charge deposition from a laser pulse is highlighted (Chpt. V).

The output of the optical simulations is a three-dimensional distribution of optically generated charge. In order to simulate the electrical response of a device, the optically generated charge is incorporated into Sentaurus TCAD as injected charge. To integrate the optical solver with TCAD, the operation of TCAD is examined and the technique to incorporate optical results is discussed (Chpt. VI). The integration of the optical simulations with a charge transport solver creates a simulation infrastructure that models PL-SEE testing from pulse to electrical signal.

Following completion of the simulation infrastructure, comparison against experimental results verifies the functionality of the simulation results. A large area silicon diode was used as a test vehicle; data was taken for multiple pulse energies, bias conditions, and focal positions. The experimental conditions were input to the simulation infrastructure and the simulation results were compiled alongside the experimental results. Excellent agreement between simulation and experiments across a variety of experimental conditions is demonstrated; use of a charge transport solver permits the simulation of current transients for comparison with experiments. A significant advantage afforded by this first principle approach to simulations is that it captures the impact of complexities from device fabrication, such as metallization layers of a device (Chpt. VII).
REFERENCES


