

Optimization and Design Numerical Modeling and Advances in Fabrication Technologies to Optical Performance

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Abstract—Photonic crystals and Nano photonics have received a great deal of attention over the last decade, largely due to improved numerical modeling and advances in fabrication technologies. To this day, fabrication and optical behavior remain decoupled during the design phase and numerous assumptions are made about “perfect” geometry. As research moves from theory to real devices, predicting device behavior based on realistic geometry becomes critical. In this dissertation, a set of numerical tools was developed to model micro and nano fabrication processes. They were combined with equally capable tools to model optical performance of the simulated structures. Using these tools, it was predicted and demonstrated that 3D nanostructures may be formed on a standard mask aligner. A space-variant photonic crystal filter was designed and optimized based on a simple fabrication method of etching holes through hetero-structured substrates. It was found that hole taper limited their optical performance and a method was developed to compensate. A method was developed to tune the spectral response of guided-mode resonance filters at the time of fabrication using models of etching and deposition. Auto cloning was modeled and shown that it could be used to form extremely high aspect ratio structures to improve performance of form-birefringent devices. Finally, the numerical tools were applied to metallic photonic crystal devices.

INTRODUCTION

As research moves from theory to real devices, predicting device behavior based on realistic geometry becomes critical [1-7]. Even small distortions can lead to dramatic changes in optical behavior [8]. In this dissertation, a set of numerical tools was developed to model micro and nano fabrication processes. They were combined with equally capable tools to model optical performance of the simulated structures. Using these tools, nano-optical elements were designed and optimized by coupling fabrication to optical behavior. Experimental results achieved in the lab verify the concepts developed in this manuscript. Devices used in high speed optical communications networks comprise a wide array of material systems [1]. Among the key material systems are silica (both fiber and silica-on-silicon), silicon oxynitride, sol-gel, dielectric thin film, lithium niobate, gallium arsenide, indium phosphide, magneto-optic materials, birefringent crystals, and polymer. Such a wide array of material systems is necessary because of the unique requirements of the constituent passive or active components [2]. Passive devices in integrated optics include simple waveguides, arrayed waveguide gratings, Bragg gratings, thin film filters, and microring resonator filters. Important active integrated optical devices include modulators (using electro-optic, acousto-optic, or electro-absorption effects), amplifiers (using heterostructures, quantum wells, or rare-earth doping), and switches (using electro-optic, thermo-optic, electro absorption, or micro-electro-mechanical means). These building-block passive and active components are fundamental in higher-function devices such as optical add/drop multiplexers, interleavers, routers, variable optical attenuators, gain flattening filters, sources, receivers, and detectors. While

semiconductor and other inorganic materials have been extensively investigated and developed during the past decades to meet the demands of high-speed optical communications and large-scale integrated optical circuits [3], the stringent requirements of next-generation optical communications networks are pushing the limits of conventional materials. As a new material available for optical integrated optics, polymer materials remain among the lesser studied and developed materials despite having properties amenable to future requirements. Recently, however, more attention has been given to polymeric materials for use in integrated optical devices because of several advantageous features [4]. These features, and manipulation of these features to accomplish feats impossible or not easily achieved with traditional inorganic materials, are the subject of this manuscript.

I. NANO-OPTICAL ELEMENTS

Conventional micro and diffractive optics consists of macroscopic surface-relief structures usually designed using scalar methods [9]. Basic passive optical components such as lenses [10-12], prisms [13], and mirrors [14] can be miniaturized and arbitrary shapes realized. These devices have found a host of applications in imaging [15, 16], adaptive optics [17], sensors [18, 19], microscopy [20, 21], communications [22-24], micro-fabrication [2, 5, 6, 25], beam shaping [24], and more. Material properties, however, remain a fundamental limitation. Photonic crystals (PC) are structures with sub-wavelength periodic material properties that can produce sharp electromagnetic resonances. These structures provide a means of controlling and engineering the bulk

electromagnetic properties of materials. Many novel and useful phenomena have been observed that promise significant impact on future photonic systems. Useful properties include forbidden transmission [21] and unique dispersive properties like negative refractive index [22].

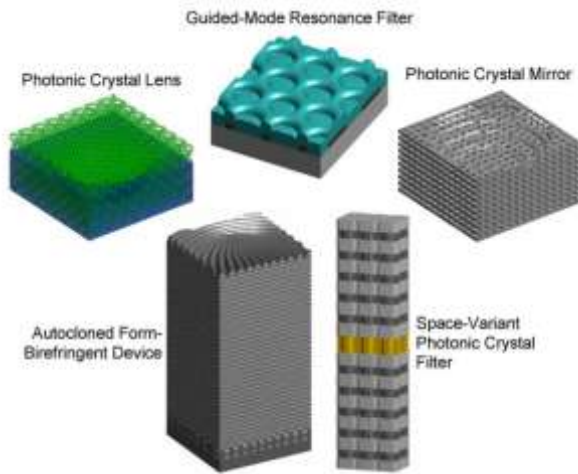


Figure 1: Nano-optical elements

Nano-optical elements combine functionality of micro and diffractive optical elements with the optical properties of nanophotonic structures like photonic crystals. NOEs can enhance performance of devices by providing a means to circumvent fundamental limitations imposed by conventional materials. Concept diagrams of several nano-optical elements are provided in Figure 1. An example simulation is depicted in Figure 2 where a lens has been formed inside a photonic crystal. When light within the photonic band gap is applied, it is completely reflected. When light from outside the band gap is applied, it is transmitted and focused by the lens. In this manner, multiple functions have been multiplexed into a single device.

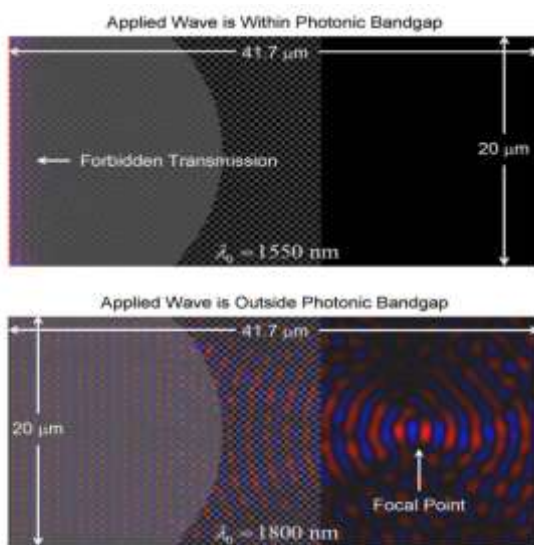


Figure 2: Multifunctional Nano-Optical Element

II. SIGNIFICANCE OF NANO-OPTICAL ELEMENTS

Photonic crystals and other nanophotonic structures hold great promise for many applications, and the research community is beginning to integrate them into higher level systems like NOEs. NOEs should find a host of applications multiplexing and demultiplexing signals due to inherent spectral filtering properties of photonic crystals. This could include wavelength division multiplexing (WDM) in fiber optic systems, color filtering in imaging systems, and more. Devices based on NOEs could be an enabling technology for system miniaturization. Dimensions of optical integrated circuits may be reduced through more efficient routing of waveguides using tighter bends and improved crossing. Imaging systems can be made more compact by replacing complex multi-element lens systems with single element NOEs. Reducing size and number of components in a system can also lead to improved reliability and lower cost. Display technology may benefit as well. Due to the porous nature of photonic crystals, they can be backfilled with a number of materials with tunable optical properties. Liquid crystals could tune the index contrast, moving the band gap, and effectively changing color. Sensor technology can exploit highly sensitive optical resonances to detect many things. Chemical sensors could be formed by backfilling with chemically sensitive materials. Highly sensitive acoustic, seismic, pressure, stress, strain, and vibration sensors could be made by detecting small deformations of the lattice. Imaging systems are likely to benefit from the ability to engineer optical materials. Properties such as negative refractive index could be designed into imaging optics to reduce aberrations. This issue is particularly severe in ultra-miniaturized systems. When more is known about NOEs other applications should become apparent. These may include beam steering, bio-photonics, adaptive optics, and more.

III. IMPACT OF FABRICATION ON OPTICAL BEHAVIOR

Mechanisms causing nano-optical elements to deviate from their “perfect” geometry fall into two categories. First, random distortions arise from random fluctuations in size, alignment, surface roughness, and other volumetric inhomogeneities. Random distortions are difficult to predict and quantify because simulations are often very large and statistics of the fluctuations must be understood. Second, deterministic distortions produce similar effects, but repeat throughout the element. Deterministic distortions tend to affect optical behavior most severely because the same electromagnetic disturbances are encountered many times throughout the entire structure. Fortunately, these can be predicted by modeling fabrication. Despite this, random distortions remain the most heavily studied. As nano-optical elements move from theory to practice, understanding both mechanisms will be critical. For random distortions, the most commonly studied photonic crystal is the stacked-bar, or woodpile, structure [23, 24]. Two-

dimensional arrays of cylinders [25] and inverse opals [8] have also been studied among others [17]. Width of the photonic band gap seems to be the dominant figure of merit to assess how resilient a photonic crystal is to fluctuations in its geometry. Virtually no work can be found on how distortions affect the dispersive behavior of photonic crystals. Most literature concludes that fluctuations on the order of 10% to 15% of the lattice constant lead to a 40% to 50% reduction in width of the photonic band gap. A notable exception is the inverse opal, where the band gap resides at much higher frequencies between the 8th and 9th bands. For inverse opals, the band gap was found to completely close if fluctuations exceeded just 2%. Two-dimensional photonic crystals were found to be more sensitive to size fluctuations than variations in alignment. As may be expected, transverse magnetic (TM) modes were shown to be more sensitive than transverse electric (TE) modes. Very little work investigating deterministic distortion can be found in the literature. Deformations arising in an autocloning process were addressed in Ref. [19]. This dissertation has contributed to studies on holographic lithography, NFNP, and more [1-7]. It was shown that optical absorption during holographic exposure leads to photonic crystals where fill factor varies with depth. For negative photoresists like Epon® SU-8 [4], photonic crystals become thinner with depth leading to chirped lattices with broadened spectral response. High contrast exposures were shown to be quite robust to reflections and standing waves during exposure. A face centered-cubic photonic crystal was able to tolerate 20% reflection from a substrate while maintaining similar optical performance. It was shown that performing multiple exposures can superimpose different lattices forming hybrids with optical properties of both. Figure 3 compares severity of random and deterministic distortion for one specific photonic crystal. The lattice is a 2D array of air cylinders in a dielectric medium with $\epsilon_r=12$. The leftmost diagram in Figure 3(a) shows the “perfect” photonic crystal with uniform holes, its Brillouin zone, and the photonic band structure for both TE and TM modes. Bands are symmetric about Γ because the lattice is symmetric through a rotation of 90° . In Figure 3(b) and (c), the lattice is distorted leading to altered band structures. Distorted bands, represented by solid lines, are compared to bands of the “perfect” photonic crystal, indicated by dashed lines. In Figure 3(b), deterministic distortion is introduced by increasing hole size by 10% of the lattice constant. Bands of the distorted lattice retain their symmetry, but are offset in frequency with increasing severity at higher frequencies. A band gap has opened for the TE modes between the first and second bands. The TM band gap has shifted by around 30% to higher frequencies and is wider. In Figure 3(c), random distortion is introduced by randomly varying hole size by 20% of the lattice constant. It is immediately obvious how less the bands are affected by random fluctuations. This is partially due to overall average refractive index remaining the same. For purely random

variations, bands should retain their symmetry. The small degree of asymmetry observed in this example is attributed to a slight anisotropy of the supercell used in the calculation, so it is a purely numerical artifact. It should be noted that while random distortion is visually most dramatic, it is the more subtle deterministic distortion that is most serious. For this reason, it is important to predict optical behavior of nano-optical elements based on realistic geometry.

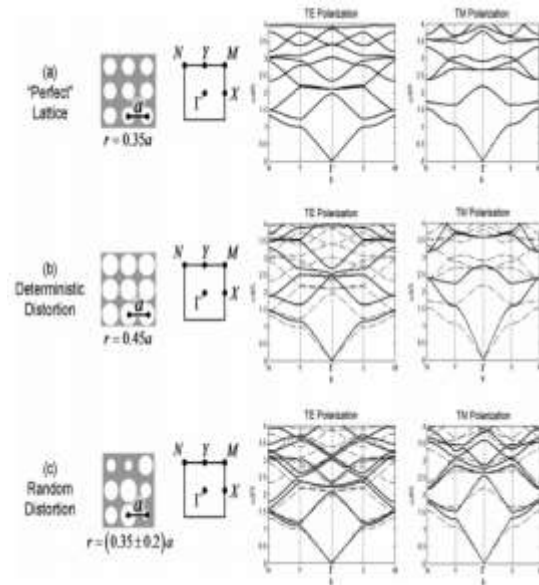


Figure 3: Comparison between random and deterministic distortion

To demonstrate the impact of realistic geometry on a real structure, reflection from two face-centered-cubic photonic crystals are compared in Figure 4. A depiction of the unit cells are shown at the left side of the diagram. The “perfect” geometry is rendered in blue, while a more realistic geometry resulting from holographic lithography is rendered in red. Reflection from a ten layer slab from both lattices are compared at the right side of the diagram. Width of the band gap is slightly wider for the realistic case and red-shifted to a longer wavelength. Peak reflection of the realistic structure is lower. A kink observed in the spectrum of the realistic photonic crystal suggests there is interesting dispersive behavior that is completely missed when perfect geometry is assumed.

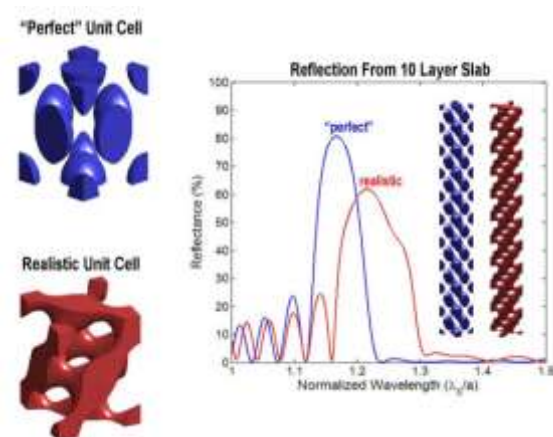


Figure 4: Comparison of “perfect” and realistic FCC photonic crystal

IV. GENERAL CONSIDERATIONS FOR NUMERICAL MODELING

To predict geometry of NOEs, key steps in fabrication must be identified and modeled accurately. A background in suitable numerical methods is helpful. It is best to seek techniques capable of handling large scale problems with high volumetric complexity since realistic devices are rarely comprised of perfect geometric patterns and can be quite large in terms of the optical wavelengths of interest. For electromagnetic simulations, finite-element methods [10] and finite-difference methods [11-17] are attractive, particularly when metals are incorporated. For 2D simulations, the finite-difference frequency-domain (FDFD) method is accurate, simple to implement, and excellent for modeling complex structures of finite size [5, 6]. The transfer matrix method [2, 8] is popular for 2D and 3D structures, especially when they contain metals. For layered and periodic dielectric devices with moderate to low index contrast, rigorous coupled-wave analysis (RCWA) [9-12] is very fast and efficient. Finite-difference time-domain (FDTD) [3, 4] remains a very powerful tool for modeling finite sized devices, large scale structures, and characterizing devices over very broad frequency range. FDTD has difficulty resolving sharp resonances or any abrupt change in spectral response, but it is exceptionally capable of identifying if resonances are present and locating their position in frequency

Figure 5 compares theoretical results obtained in Ref. [13] to benchmark simulations for all electromagnetic simulation tools outlined in this dissertation. Numerical resolution, spectral resolution, and simulation time is summarized in this figure. A close-up of the simulated resonances is provided in the bottom right diagram. Numerical dispersion has shifted the resonance peaks to slightly longer wavelengths in the models employing finite-differences. Etching, developing, and deposition processes can be modeled by tracking progression of a surface. There are four popular approaches found in literature. These are string methods [9, 4, 5], cell volume methods [3, 6-10], level set methods (LSM) [1-3], and fast marching methods (FMM) [13]. String, or marker particle, methods resolve the surface with a number of discrete points. During simulation, position of each point is updated based on position of surrounding points and a local rate function. These methods are very fast and efficient when surface topology is simple, smooth, and continuous. This is the case for much of grayscale lithography and analog devices. When structures are complex with detached surfaces and sharp bends, the method can become unstable and is difficult to implement. For these reasons, the string method is mostly limited to 2D problems. Cell volume methods represent bulk materials as an array of cube shaped cells. Each cell is assigned a fictitious volume that is adjusted as the surface progresses. Cells with zero volume represent points where the bulk material does not exist. Cells where the volume is filled represent points where the bulk material is present. Cells with partially filled volumes interpolate position of the surface. The main trick implementing these methods is modifying how cell volume is reduced based on the direction the surface is moving through the cell. This is a difficult calculation in the cell volume framework and fine grids are needed to obtain accurate results. For this reason, cell volume methods require large amounts of memory and run slower than string methods, but are able to handle arbitrarily complex surfaces and extend well to three dimensions. Of all techniques, LSM and FMM seem to offer the greatest compromise between speed, flexibility, and efficiency while being able handle very complex geometries. Level set methods may be the most generalized and most rigorous technique for modeling evolution of surfaces. They are best tailored for modeling etching and deposition due to the bidirectional nature of the surface and surface dependent growth rates encountered in the process. Fast marching methods are incredibly fast and accurate algorithms best suited to model processes like developing where surfaces progress in only one direction and rate depends only on position. Both LSM and FMM offer much simpler means of calculating geometric properties of the surface such as surface normal and curvature.

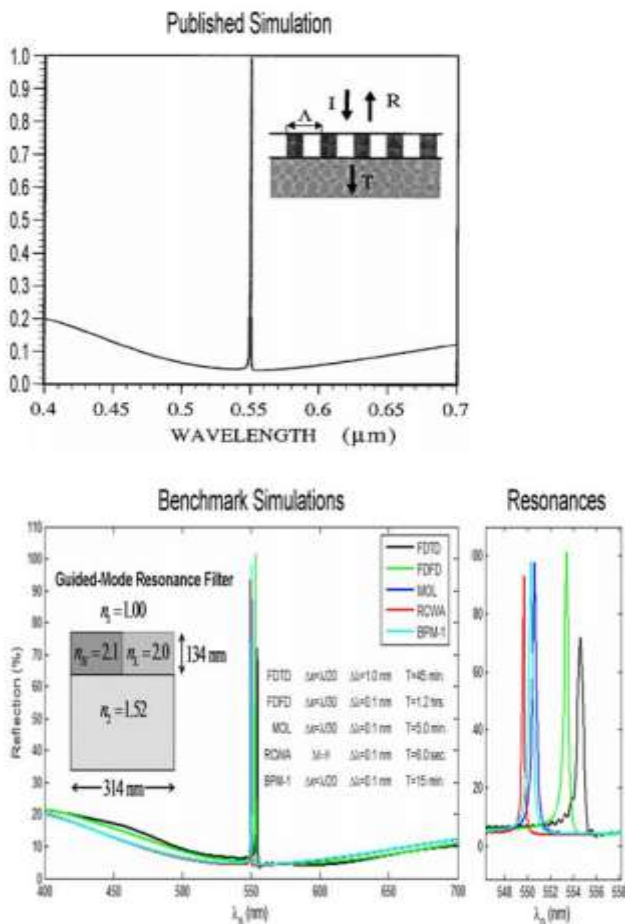


Figure 5: Benchmark Simulations for EM Simulation Tools

V. MAXWELL'S EQUATIONS AND THEOREMS

Maxwell's equations are the fundamental laws that govern behavior of all electromagnetic energy. They are based on a macroscopic view of how waves interact with matter and may

take many forms. To understand optical behavior in nano-optical elements, it is necessary to have an understanding of Maxwell's

Table 1: Maxwell's Equations

Integral Form	Differential Form	Description	
$\oiint_S \vec{D}(t) \cdot d\vec{S} = \int_V \rho_v(t) dv$	$\nabla \cdot \vec{D}(t) = \rho_v(t)$	Gauss' law	Time-Domain
$\oiint_S \vec{B}(t) \cdot d\vec{S} = 0$	$\nabla \cdot \vec{B}(t) = 0$	No magnetic charge	
$\oint_L \vec{E}(t) \cdot d\vec{l} = -\frac{\partial}{\partial t} \iint_S \vec{B}(t) \cdot d\vec{S}$	$\nabla \times \vec{E}(t) = -\frac{\partial \vec{B}(t)}{\partial t}$	Faraday's law	
$\oint_L \vec{H}(t) \cdot d\vec{l} = \iint_S \left[\vec{J}(t) + \frac{\partial \vec{D}(t)}{\partial t} \right] \cdot d\vec{S}$	$\nabla \times \vec{H}(t) = \vec{J}(t) + \frac{\partial \vec{D}(t)}{\partial t}$	Ampere's circuit law	
$\vec{D}(t) = \vec{\epsilon}(t) \cdot \vec{E}(t)$		$\vec{B}(t) = \vec{\mu}(t) \cdot \vec{H}(t)$	
$\oiint_S \vec{D} \cdot d\vec{S} = \int_V \rho_v dv$	$\nabla \cdot \vec{D} = \rho_v$	Gauss' law	Frequency-Domain
$\oiint_S \vec{B} \cdot d\vec{S} = 0$	$\nabla \cdot \vec{B} = 0$	No magnetic charge	
$\oint_L \vec{E} \cdot d\vec{l} = -j\omega \iint_S \vec{B} \cdot d\vec{S}$	$\nabla \times \vec{E} = -j\omega \vec{B}$	Faraday's law	
$\oint_L \vec{H} \cdot d\vec{l} = \iint_S (\vec{J} + j\omega \vec{D}) \cdot d\vec{S}$	$\nabla \times \vec{H} = \vec{J} + j\omega \vec{D}$	Ampere's circuit law	
$\vec{D} = \vec{\epsilon} \vec{E}$		$\vec{B} = \vec{\mu} \vec{H}$	

equations and how they are applied. A summary of Maxwell's equations is provided in Table 1.

A. Time-Domain Form

The most widely used form of Maxwell's equations are differential equations, as opposed to integral equations. In time-domain form [24], these are:

$$\nabla \cdot \vec{D}(t) = \rho_v(t) \tag{1}$$

$$\nabla \cdot \vec{B}(t) = 0 \tag{2}$$

$$\nabla \times \vec{E}(t) = -\frac{\partial \vec{B}(t)}{\partial t} \tag{3}$$

$$\nabla \times \vec{H}(t) = \vec{J} + \frac{\partial \vec{D}(t)}{\partial t} \tag{4}$$

The field parameters $\vec{D}, \vec{B}, \vec{E}$ and \vec{H} represent electric flux density (C/m²), electric field intensity (V/m), magnetic flux

density (W/m²), and magnetic field intensity (A/m) respectively. Electric charge density ρ_v (C/m³) and electric current density \vec{J} (A/m²) represent sources that can induce electromagnetic fields or be induced by the fields. All materials are comprised of charged particles that are displaced in the presence of an applied electric field. Accelerating charges radiate fields that combine out of phase with the applied wave. The overall effect is to modify propagation so waves behave differently than they would in a vacuum. To incorporate these effects in a simplified manner, they are treated macroscopically through the constitutive parameters $\vec{\epsilon}(t), \vec{\mu}(t)$, and sometimes $\sigma(t)$. In general, these are time-varying tensor quantities that relate to the fields through the following equations that involve convolutions.

$$\vec{D}(t) = \vec{\epsilon}(t) * \vec{E}(t) \tag{5}$$

$$\bar{B}(t) = \bar{\mu}(t) * \bar{H}(t) \quad (6)$$

$$\bar{J}(t) = \bar{\sigma}(t) * \bar{E}(t) \quad (7)$$

The dielectric permittivity $\bar{\epsilon}$ characterizes how well a material can store energy imposed by an electric field. Permeability $\bar{\mu}$ quantifies how efficiently energy is stored due to an applied magnetic field. The conductivity $\bar{\sigma}$ arises from free charges that form electrical currents in the presence of an applied electric field.

B. Frequency-Domain Form

Transforming Eqs. (1) - (7) to the frequency-domain simplifies the mathematical framework by reducing convolutions to simple products.

$$\nabla \cdot \bar{D} = \rho_v \quad (8)$$

$$\nabla \cdot \bar{B} = 0 \quad (9)$$

$$\nabla \times \bar{E} = -j\omega \bar{B} \quad (10)$$

$$\nabla \times \bar{H} = \bar{J} + j\omega \bar{D} \quad (11)$$

$$\bar{D} = \bar{\epsilon} \bar{E} \quad (12)$$

$$\bar{B} = \bar{\mu} \bar{H} \quad (13)$$

$$\bar{J} = \bar{\sigma} \bar{E} \quad (14)$$

In this form, it is possible to eliminate the terms \bar{D} , \bar{B} and \bar{J} from Maxwell's equations.

$$\nabla \cdot (\bar{\epsilon} \bar{E}) = q \quad (15)$$

$$\nabla \cdot (\bar{\mu} \bar{H}) = 0 \quad (16)$$

$$\nabla \times \bar{E} = -j\omega \bar{\mu} \bar{H} \quad (17)$$

$$\nabla \times \bar{H} = \bar{\sigma} \bar{E} + j\omega \bar{\epsilon} \bar{E} \quad (18)$$

Most often permittivity and permeability are not tensor quantities. In addition, charge ρ_v is usually ignored and conductivity is incorporated into a complex permittivity term. Under these conditions, Maxwell's equations assume their most familiar form.

$$\nabla \cdot (\bar{\epsilon} \bar{E}) = 0 \quad (19)$$

$$\nabla \cdot (\bar{\mu} \bar{H}) = 0 \quad (20)$$

$$\nabla \times \bar{E} = -j\omega \bar{\mu} \bar{H} \quad (21)$$

$$\nabla \times \bar{H} = j\omega \bar{\epsilon} \bar{E} \quad (22)$$

C. Wave Equations

Perhaps the most significant aspect of Maxwell's equations is that they predict propagating waves. The curl equations show that time changing electric fields induce curling, or circulating, magnetic fields in the immediate vicinity. Likewise, time changing magnetic fields induce circulating electric fields. In this manner, oscillating fields continue to induce other oscillating fields and a wave is formed. To better understand the wave phenomenon, it makes sense to combine Maxwell's curl equations since it is the interaction of these two equations that

predicts propagation. The combined equation is called a "wave equation" and it is possible to derive it in terms of just the magnetic field or just the electric field. Wave equations enable fully rigorous analysis of electromagnetic problems using a single equation while incorporating all information from both of Maxwell's curl equations. To begin deriving full vector wave equations, Eqs. (21) and (22) are written as

$$(1/\mu) \nabla \times \bar{E} = -j\omega \bar{H} \quad (23)$$

$$(1/\epsilon) \nabla \times \bar{H} = j\omega \bar{E} \quad (24)$$

Taking the curl of these equations leads to:

$$\nabla \times (1/\mu) \nabla \times \bar{E} = -j\omega (\nabla \times \bar{H}) \quad (25)$$

$$\nabla \times (1/\epsilon) \nabla \times \bar{H} = j\omega (\nabla \times \bar{E}) \quad (26)$$

The curl operations on the right side of these equations can be replaced using the original curl equations. This leads to the full vector wave equations.

$$\nabla \times \frac{1}{\mu} \nabla \times \bar{E} = \omega^2 \epsilon \bar{E} \quad (27)$$

$$\nabla \times \frac{1}{\epsilon} \nabla \times \bar{H} = \omega^2 \mu \bar{H} \quad (28)$$

The wave equations can be written in terms of the free space wave number k_0 , where $k_0 = \omega/c$.

$$\nabla \times \frac{1}{\mu_r} \nabla \times \bar{E} = k_0^2 \epsilon_r \bar{E} \quad (29)$$

$$\nabla \times \frac{1}{\epsilon_r} \nabla \times \bar{H} = k_0^2 \mu_r \bar{H} \quad (30)$$

VI. CONCLUSION

This manuscript designed and optimized several nano-optical elements by considering how fabrication affects their optical behavior. Background was given to understand device theory. Numerical tools were discussed and detailed formulations were provided for each along with block diagrams

summarizing their implementation. To better understand electromagnetic theory of nano-optical elements and concepts used to develop numerical models, background information was provided to introduce Maxwell's equations from which wave equations were derived. These were used to explain scaling theories and introduce the concept of left-handed materials. Microscopic models of the response of materials were presented in the form of the Lorentz oscillator model for dielectrics and the Drude model to metals. From these, basic properties of bulk optical materials were identified and described.

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