Novel modeling techniques for photonic devices

(Invited Paper)

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***Abstract*—The combination of purely numerical methods, such as the finite element method, with an analytical treatment can lead to a powerful semi-analytical technique. We present such a technique, which combines the finite element method with a modal approach, with a focus on the modeling three-dimensional photonic structures.**

I. Introduction

Numerical methods such as finite element methods (FEM) can be used to accurately compute Bloch modes over an arbitrary unit cell. But the efficiency of such purely numerical techniques decreases for problems posed over an extended domain consisting of many unit cells. Semi-analytical approaches based on Bloch mode expansion can be very efficient in handling extended domains (including semi-infinite domains) while providing an insight into the physics of the photonic structures. In this talk we a describe powerful modeling technique which result from the combination of numerical and semi-analytical techniques. We focus on the general principles for the accurate and robust FEM solution of full vectorial electromagnetic field problems over two or three-dimensional domains.

II. Numerical stability of vectorial finite element discretization

For a simply connected domain Ω, the gradient, curl and div operators form an exact sequence:

$$H(\text{Grad},\Omega) \overset{\nabla}{\to} H(\text{Curl},\Omega) \overset{\nabla\times}{\to} H(\text{Div},\Omega) \overset{\nabla\cdot}{\to} L(\Omega) \quad (1)$$

i.e., the range of each operator coincides with the kernel of the following one. For the sake of numerical stability [1], FEM approximation spaces must be chosen such that the exact sequence is reproduced at the discrete level. The investigation of the general principles for accurate and stable FEM is an area of active research which combines the fields of numerical analysis, topology and geometry. The understanding of these principles provides theoretical guidance for the construction of stable FEM approximation spaces.

III. Modal formulation of the scattering by a three-dimensional array of cylinders

The conversion efficiency of photovoltaic cells can be increased by using silicon nanowire (SiNW) arrays [2]. The optical conversion efficiency of these devices has been analyzed with general purpose numerical methods such as FEM, plane wave expansions, or the finite-difference time-domain method (FDTD). In order to gain more insight into the absorption mechanism of SiNW, we recently developed a modal formulation for the diffraction and absorption of plane waves by a periodic array of cylinders (see Fig. 1). The fields in the semi-infinite media above and below the cylinder are represented by plane wave expansion. The field within the array of cylinders is represented by an expansion in term of the Bloch modes $\boldsymbol{E}_m(x,y)\exp(i\gamma_m z)$ which have an exponential z-dependence and are quasi-periodic in the (x,y)-plane (with a corresponding wavevector $\boldsymbol{k}_t = (k_x,k_y)$). In the same way as for the modes of conventional z-invariant waveguides, the determination of these Bloch modes reduces

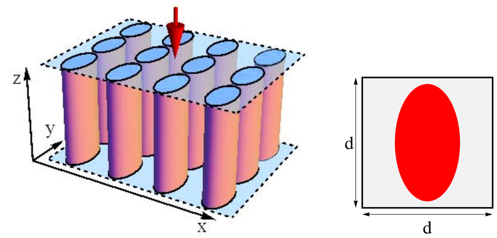

Fig. 1. Left panel: illustration of a square lattice of cylinders; the red arrow represents a plane wave incident from above. Right panel: transverse cross-section of a unit cell.

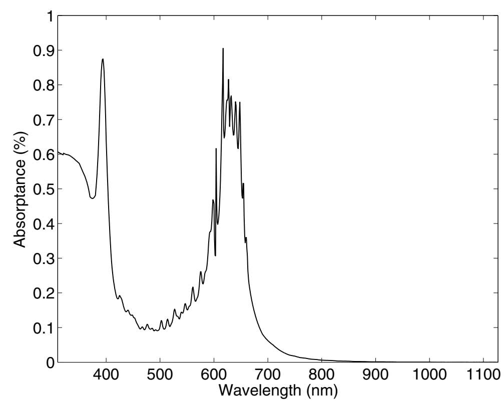

Fig. 2. Absorptance of a dilute SiNW array of circular cylinders.

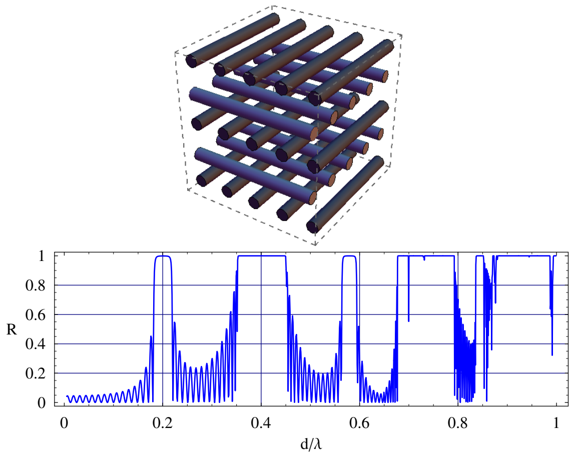

Fig. 3. Upper panel: Schematics of an array of crossed cylinders. Lower panel: Plane wave reflectance curve of a 32-layered crossed-array of circular cylinders under a normal incidence.

to their calculation over the two dimension unit cell shown in the right panel of Fig. 1. We carried out the modal computation using a vectorial FEM code which is an adaptation of a code developed originally for optical fiber modeling [3]. For a given frequency ω and transverse wavevector $\boldsymbol{k}_t$, the problem of finding the propagation constants γ and their associated Bloch modes reduces to a generalized eigenvalue problem with γ^2 as eigenvalue parameter [3]. Since this eigenproblem is not Hermitian (even for lossless media), complex γ^2 can occur and the Bloch modes do not form an orthogonal set. However by introducing an adjoint basis associated with the adjoint quasi-periodicity, we can form biorthogonal bases (see, e.g., [4]) and derive a least squares matching of field expansions at the top and bottom interfaces of the cylinder arrays.

This modal semi-analytic approach allows us to capture the physical origin of the enhancement of solar absorptance by SiNW arrays. For instance, Fig. 2 shows the absorptance spectrum of a dilute SiNW array of circular cylinders (silicon volume fraction approximately 3%). The absorption feature between 600 and 700 nm is absent in bulk silicon and is entirely due to the nanowires. Using our method we have identified some specific Bloch modes which play a key role in this absorption behavior. In our talk, we will demonstrate how this semi-analytic approach can be effectively used to increase absorption in photovoltaic cells.

IV. Analysis of Multilayer Gratings Using a Three Dimensional Finite Element Method

In the context of the FEM for diffraction grating, there are two main formulations to model the radiation into semi-infinite media. The radiation condition can be enforced by applying either the perfectly matched layer (PML) formalism or the plane wave expansion formalism. The PML based formulation leads to a local boundary condition, which is ideal for a computationally efficient FEM implementation; however the use of artificial complex refractive index introduces undesirable numerical loss [5]. While the coupling of FEM with the plane wave expansion formalism leads to non-local boundary conditions, the least square nature of the field matching at the material interfaces naturally preserves the energy conservation property and this is an important consideration when a diffraction grating solver is used for instance to compute the Bloch modes or the band diagram of photonic crystals (see, e.g., Ref. [6]). Thus in this work we have used the latter formulation.

Three dimensional FEM calculation becomes rapidly prohibitive as the ratio of structure size to wavelength increases. Multilayer photonic structures, such as the woodpile photonic crystals shown in Fig. 3, can comprise a large number of layers and the direct application of FEM calculation is not practical. The scattering matrix of multilayer structures can be efficiently computed using recursive expressions such as

$$\mathbf{R} = \mathbf{R}_1 + \mathbf{T'}_1\mathbf{R}_2\left(\mathbf{I} - \mathbf{R'}_1\mathbf{R}_2\right)^{-1}\mathbf{T}_1, \quad (2)$$
$$\mathbf{T} = \mathbf{T}_2\left(\mathbf{I} - \mathbf{R'}_1\mathbf{R}_2\right)^{-1}\mathbf{T}_1. \quad (3)$$

Equations (2) and (3) give the scattering matrix $\mathbf{R}$ and $\mathbf{T}$ of a stack of two layers $\mathcal{L}_1$ and $\mathcal{L}_2$ in term of the scattering matrices $\mathbf{R}_i$, $\mathbf{R'}_i$, $\mathbf{T}_i$, $\mathbf{T'}_i$, for $i = 1, 2$, of each individual layer. In Fig. 3 we show the reflectance of a stack of 32 crossed-cylinder layers obtained by first using FEM to compute the scattering matrices of the two type of cylinder layers, and then by applying the recursion relation 5 times to get the scattering matrices and the reflectance of the 32-layered crossed-array of circular cylinders; the results are in good agreement with results published by other authors.

V. Conclusion

We have presented some applications where the combination of three-dimensional FEM with analytic treatments lead to very powerful semi-analytical techniques. The FEM can play an important role in the development of semi-analytic Bloch mode approaches for 3D structures.

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