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Electrical and Quantal Analysis of Photonic Crystals

The novel coupled potential equations and the Schrodinger equation were employed to analyze the light scattering, quantum quality of crystal structures. Compared with other related researches, quantum effects were directly involved in this paper. The finite-difference time-domain (FDTD) was applied to discretize the coupled equations.

INTRODUCTION

Recent technology developments in quantum regions have opened a way to control quantum states of electrons, atoms, molecules, and nano-scale objects[1]. These studies have attracted great attention over the past 20 years since they seem to have the ability to control photochemical reactions with high efficiency. But this pioneering technology needs to design external laser pulses to the target systems, which are not that simple to figure out through the basic quantum theories[2]. Hence, optical control of states through computational algorithm has been a growing interest in recent years. These have prompted demand for new analysis technique for electrical structures in nano-scale where quantum effects have to be considered so as to cut down time and cost of researches.

Since the Maxwell's and Schrodinger's equations are both time- and spatial-domain differential, finite difference time domain (FDTD) method and its variants have been proved to be the most efficient, concise and employed[3, 4]. However, some of these seem to rely on the assumption that the electromagnetic fields near the atoms would not be disturbed by atoms excitation or the disturbance can be negligibly tiny to be ignored [5].

NUMERICAL MODEL

Computational electromagnetics is aimed at solving Maxwell's equations numerically. A variety of techniques like FDTD and finite element method (FEM) have been developed over the last few decades to solve scattering problems, antenna designs, wave propagation and so on[6, 7]. With Maxwell's equations being still valid in both macro- and nano- scale, coupling it with Schrodinger's equation is the most straightforward and strict way to solve multi-physics studies.

The quantization of the electromagnetic field can be done more expediently with the vector and scalar potential rather than with electronic and magnetic fields. The vector and scalar potential formulation are quite convenient to both quantum theory and classical electromagnetic simulations. The rapid development in quantum optics applications calls for new numerical solutions which can bridge the multi-scale systems. Furthermore, the equations neither exhibit the low-frequency catastrophe nor the frequency imbalance observed in the traditional formulation using E-H fields, in our earlier study[8].

The coupled equations of our frame can be writes as

$$\frac{\partial^2}{\partial t^2}\varepsilon\vec{A}+\frac{\partial}{\partial t}\sigma\vec{A}+\frac{\partial}{\partial t}\varepsilon\nabla\Phi+\nabla\times\mu^{-1}\nabla\times\vec{A}+\sigma\nabla\Phi=0 \qquad (1)$$

$$\frac{\partial}{\partial t}\nabla\cdot\varepsilon\vec{A}+\nabla\cdot\varepsilon\nabla\Phi=-\rho \tag{2}$$

The coupled discretized equations should be justified for the anisotropic medium, compared with our early work. If Maxwell equations are still involved in the system, the extra steps will be energy-cost and slow to solve electromagnetic fields into pre-requisite potentials. And the cost will be more than doubled in anisotropic medium with sensor drawn into. The dielectric sensor of many crystals can be symmetrical, as shown in (3).

$$\vec{\vec{\varepsilon}}=\begin{bmatrix}\varepsilon_x & 0 & 0\\ 0 & \varepsilon_y & 0\\ 0 & 0 & \varepsilon_z\end{bmatrix} \tag{3}$$

(3) is substituted in to (2), and the discretized vector updated equation is given as follows,

$$\begin{aligned}&A_v^{n+1}(\mathrm{i,j,k})=2A_v^{n}(\mathrm{i,j,k})-A_v^{n-1}(\mathrm{i,j,k})\\&-\{\Delta t^2\vec{\vec{\varepsilon}}^{-1}[\sigma\nabla\Phi+\nabla\times\mu^{-1}\nabla\times\vec{A}-I_3\vec{\vec{\varepsilon}}\nabla\mu^{-1}\vec{\vec{\varepsilon}}^{-2}\nabla\cdot\vec{\vec{\varepsilon}}\vec{A}-\vec{J}_{in}]\}_v\end{aligned} \tag{4}$$

where $v=x,y,z$ means the v-component of the term, $I_3=\begin{bmatrix}1 & 1 & 1\end{bmatrix}^T$ flattens the tensor to vector scale.

For the sake of brevity, only the most difficult term is minutely discussed, i.e. $\Delta t^2\vec{\vec{\varepsilon}}^{-1}[I_3\vec{\vec{\varepsilon}}\nabla\mu^{-1}\vec{\vec{\varepsilon}}^{-2}\nabla\cdot\vec{\vec{\varepsilon}}\vec{A}]$, as follows.

To start with, we suggest dealing with div part,

$$\begin{aligned}&f_1=\nabla\cdot\vec{\vec{\varepsilon}}\vec{A}=\\&\frac{\varepsilon_x\left(i+\frac{1}{2},j,k\right)A_x\left(i+\frac{1}{2},j,k\right)-\varepsilon_x\left(i-\frac{1}{2},j,k\right)A_x\left(i-\frac{1}{2},j,k\right)}{\Delta x}\\&+\frac{\varepsilon_y\left(i,j+\frac{1}{2},k\right)A_y\left(i,j+\frac{1}{2},k\right)-\varepsilon_y\left(i,j-\frac{1}{2},k\right)A_y\left(i,j-\frac{1}{2},k\right)}{\Delta y}\\&+\frac{\varepsilon_z\left(i,j,k-\frac{1}{2}\right)A_z\left(i,j,k-\frac{1}{2}\right)-\varepsilon_z\left(i,j,k-\frac{1}{2}\right)A_z\left(i,j,k-\frac{1}{2}\right)}{\Delta z}\end{aligned} \tag{5}$$

The gradient term can be discretized as,

$$f_2=\nabla\vec{\vec{\varepsilon}}^{-2}\mu^{-1}f=\begin{bmatrix}\nabla\frac{f}{\varepsilon_x^2\mu} & 0 & 0\\ 0 & \nabla\frac{f}{\varepsilon_y^2\mu} & 0\\ 0 & 0 & \nabla\frac{f}{\varepsilon_z^2\mu}\end{bmatrix} \tag{6}$$

For the above term, only the first component is shown because the components in the other two rows are analogous.

$$
\begin{aligned}
fx_3 &= \nabla \frac{f}{\varepsilon_x^2 \mu} = \\
&\left[\frac{f\left(i+\frac{1}{2},j,k\right)}{\varepsilon_x^2\left(i+\frac{1}{2},j,k\right)\mu\left(i+\frac{1}{2},j,k\right)} - \frac{f\left(i-\frac{1}{2},j,k\right)}{\varepsilon_x^2\left(i-\frac{1}{2},j,k\right)\mu\left(i-\frac{1}{2},j,k\right)}\right] \\
&+\left[\frac{f\left(i,j+\frac{1}{2},k\right)}{\varepsilon_x^2\left(i,j+\frac{1}{2},k\right)\mu\left(i,j+\frac{1}{2},k\right)} - \frac{f\left(i-\frac{1}{2},j,k\right)}{\varepsilon_x^2\left(i-\frac{1}{2},j,k\right)\mu\left(i-\frac{1}{2},j,k\right)}\right] \\
&+\left[\frac{f\left(i,j,k+\frac{1}{2}\right)}{\varepsilon_x^2\left(i,j,k+\frac{1}{2}\right)\mu\left(i,j,k+\frac{1}{2}\right)} - \frac{f\left(i,j,k-\frac{1}{2}\right)}{\varepsilon_x^2\left(i,j,k-\frac{1}{2}\right)\mu\left(i,j,k-\frac{1}{2}\right)}\right]
\end{aligned} \tag{7}
$$

With the help of (5), (6) and (7), the complicated term can be discretized eventually,

$$
\begin{aligned}
&\Delta t^2 \vec{\vec{\varepsilon}}^{-1}[I_3 \vec{\vec{\varepsilon}} \nabla \mu^{-1} \vec{\vec{\varepsilon}}^{-2} \nabla \cdot \vec{\vec{\varepsilon}} \vec{A}] = \\
&\left[\Delta t^2 \varepsilon_x(i,j,k)([fx_3]_x + [fy_3]_x + [fz_3]_x)\right. \\
&+\left[\Delta t^2 \varepsilon_y(i,j,k)([fx_3]_y + [fy_3]_y + [fz_3]_y)\right. \\
&+\left[\Delta t^2 \varepsilon_z(i,j,k)([fx_3]_z + [fy_3]_z + [fz_3]_z)\right.
\end{aligned} \tag{8}
$$

When the length scales of simulations are shrunk to nano-scales, the sizes of the objects may be much smaller compared to wavelengths of incident waves[9]. The solution in this paper is to employ magnetic vector potential and electric scalar potential rather than electromagnetic fields when dealing with sensor calculation and anisotropic medium. And the coupled equations are of great benefits to reducing computational cost and simulation time.

COUPLED SCHRODINGER SYSTEM

The length gauge can transform the Schrodinger equation into one with the fields directly involved. However, the gauge will be inaccurate when the wavelength of the source becomes shorter or almost near the size of structures[10, 11].

In the presence of electromagnetic fields, the time-dependent Schrodinger equation for a particle can be modified by including vector and scalar potentials terms, respectively, as follows[1]:

$$
i\hbar \frac{\partial}{\partial t}\Psi(\vec{r},t) = \frac{1}{2m}\{[-i\hbar\nabla - q\vec{A}(\vec{r},t)]^2 + q\Phi(\vec{r},t) + V\}\Psi(\vec{r},t) \tag{9}
$$

where $\hbar$ denotes Planck's constant, Ψ represents the wave function, m is the effective mass of the particle, q represents the charge of the particle, V is the confinement potential.

RESULTS AND DISCUSSIONS

Through model-solid theory and effective mass approximation, the energy band of the numerical PhCs can be obtained. Strain contributions are taken into account.

The strained InGaAs conduction band edge $E_{c\_InGaAs\_s}$ can be given by the following equation,

$$
E_{c\_InGaAs\_s} = E_{c\_InGaAs} + E_g + P_c \tag{10}
$$

with E_{c_InGaAs} , E_g and P_c as the unstrained energy of InGaAs, the energy gap and the strained-induced energy shifts.

A schematic of the simple crystals model is shown in Fig .1.

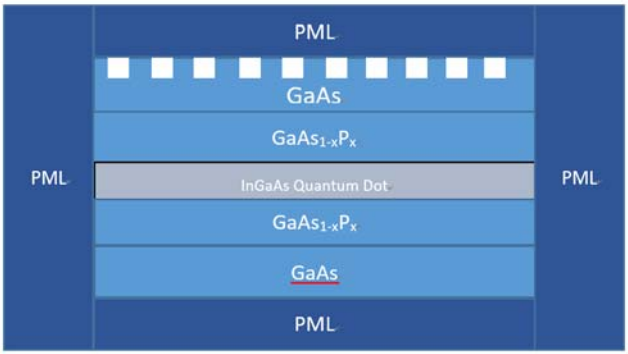

Fig .1 The simulation domain

The thickness of the substrate of GaAs is 4.5nm, thinner than usual experiment. This is because the wavefunctions of the priticles are zero in these layers. By reducing the thickness of unneeded, the cost of simulation is cut down. The time step of the simulation is 0.1fs, the spatial is 0.05nm. The PML will absorb any radiation that reashes the edges of the simulation domain, and about 20 units thickness PML can effectively eliminate any reflection at the boundaries that interferes with the simulation. The filling factor and depth of PhCs are 0.035 and 1nm, respectively.

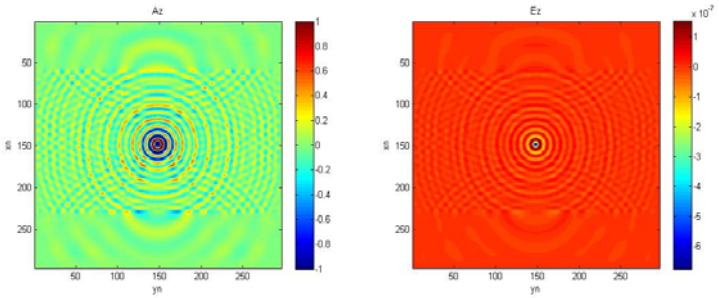

Fig .2 vector potential v.s. conventional electric filed

As illustrated in the results, our method can get right simulation results as same as the conventional FDTD method. And the time cost is 40 percent smaller than Maxwell system.

CONCLUSIONS

A novel algorithm is proposed to simulate the electrical and quantal characteristics of PhCs in this paper.

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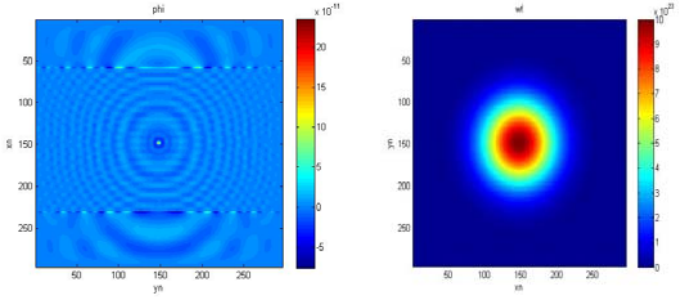

Fig .2 scalar potential and the possibility

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