3D GL EM and Quantum Mechanical Coupled Modeling for the Nanometer Materials

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Abstract—In this paper, we develop a 3D GL EM and quantum mechanical coupled modeling (GLEMQUAN) for studying nanometer materials. We accumulate the EM field energy, quantum energy, and interaction energy into Lagrangian energy in the nanometer material. The variation equation of the Lagrangian energy is the EM and quantum field coupled equations. We propose the GL modeling to solve the EM and quantum field coupled equations. The nanometer material is divided into set of sub-lattices. In each lattice, the Global EM field and quantum wave function field are successively modified by the local scattering EM and quantum field. When the whole lattice domain is scanned, the GL EM and quantum field solution is obtained. In the GLEMQUAN modeling, there is no big matrix needs to be solved. Also there are no artificial boundary and no error reflection and error dispersion. The synthetic simulations show the GLEMQUAN modeling algorithm is fast, accurate, and very agile. The GLEMQUAN modeling can be used to study optical materials, photosensitivity, photosynthesis, metallography and nanometer materials science and engineering.

DOI: 10.2529/PIERS0060825193447

1. INTRODUCTION

The nanometer materials have important applications in science and engineering. Their mechanical and electromagnetic (EM) properties are active research projects. In this paper, we develop a 3D GLEMQUAN for studying nanometer materials. We use the quantum field to model the micro inhomogeneous variance property of the nanometer materials. The EM field energy, quantum material field energy, and interaction energy are accounted into the total Langrangian. By taking the Euler variation of the Langrangian, we can obtain the EM field and quantum material field coupled equations. By using the GL modeling method [1, 2], we propose the GLEMQUAN method to solve the EM and quantum coupled field equations. The nanometer material is divided into set of lattices. In each lattice, the Global EM field and quantum wave function field are successively modified by the local scattering EM and quantum field. When the whole lattice domain is scanned, the GL EM and quantum field solution is obtained.

The Lagrangian energy method is the important tool to build theory for EM, mechanical, thermal, and flow etc. The Finite Element method (FEM) is a direct numerical Lagrangian energy method. However, the big matrix and artificial boundary condition are cumbersome burden and cost of the FEM and FD method. In particular, in micro Lagrangian model, there is no general constitutive law for variable nanometer materials. The Langrangian energy density is nonstandard and depends variable material experiment and measurement. Therefore, the micro FEM Langrangian energy algorithm and software are often needed to be changed for the different type nanometer materials, it is very inconvenience and cumbersome. In the GLEMQUAN Modeling, there is no big matrix needs to be solved. Also there are no artificial boundary and no error reflection and dispersion. In particular, the GLEMQUAN is very agile to discrete the nonstandard and changeful Lagrangian density for the different type optical materials and nanometer materials. Many simulations show that the GLEMQUAN and GL EMFHS [3] coupled modeling have advantages to overcome the difficulties in FEM Lagrangian modeling.

There are research works to study Lagrangian modeling for optical materials [4]. However, paper [4] only study one dimension case. The 3D Lagrangian modeling for the optical and nanometer materials is lacking. We developed the Macro to Macro, Macro to Micro, and Micro to Micro 3D GLEMQUAN and GLEMHFS coupled modeling.

The GLEMQUAN and GLEMHFS [3] modeling have wide applications in studying optical materials, Bragg grating, photosensitivity, photosynthesis, nanometer materials, metallography, powder metallurgy and metal cast science and engineering.
We arrange the description of the paper as follows. The introduction has been described in Section 1. The Lagrangian EM and quantum energy principle for the nanometer materials is described in Section 2. The variation Euler-Lagrangian equation is described in Section 3. In Section 4, we describe GL EM and nanometer quantum field coupled modeling. The simulation and advantages of the GLEMQUAN modeling is described in Section 5. In Section 6, we conclude this paper.

2. LAGRANGIAN OF THE EM FIELD AND QUANTUM FIELD

We consider interaction phenomena that the high frequency EM field, for example X ray, propagates through the nanometer material. The EM field energy, nanometer quantum field energy, and interaction energy are accounted in the Lagrangian which is integral of the Lagrangian density.

2.1. The Lagrangian Density

The Lagrangian density of the EM field and quantum field energy is as follows.

\[ l_T = l_{EM} + l_{QUAN} + l_{INT}, \]

where \( l_T \) is total Lagrangian energy density, \( l_{EM} \) is the EM field energy density, \( l_{QUAN} \) is the quantum field density, and \( l_{INT} \) is the interaction energy due to the interaction between the EM field and quantum nanometer materials,

\[ l_{EM} = \frac{1}{2} \varepsilon_0 (E \cdot E - c^2 \mu_0^2 H \cdot H), \]

\[ l_{QUAN} = \frac{1}{2} i \hbar \left( \Psi^* \partial \Psi \partial t - \Psi \partial \Psi^* \partial t \right) - \Psi^* \mathcal{H}_Q \Psi, \]

\[ l_{INT} = E \cdot P. \]  

2.2. Langrangian Energy

The Langrangian energy of the EM field and quantum field is as follows

\[ L(E, H, \Psi, t) = \int \Omega l_T (r') \, dr'. \]

3. VARIATION EULER-LAGRANGIAN EQUATION

3.1. Langrangian Function

The Langrangian function is as follows

\[ S(E, H, \Psi) = \int_0^\infty L(E, H, \Psi; t) \, dt. \]

3.2. Euler-Lagrangian Variation

The Euler-Lagrangian variation equation is the following equation,

\[ \delta S(E, H, \Psi) = 0. \]

3.3. EM Field And Quantum Field Coupled Equation

To take variation of the Lagrangian function in (5), we obtain the EM field and quantum field coupled equation.

\[ \nabla \times E = -\mu \frac{\partial H}{\partial t}, \]

\[ \nabla \times H = \varepsilon \frac{\partial E}{\partial t} + J, \]

where

\[ J = -\frac{i \hbar}{2m} A (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) + \sigma (\Psi) E, \]

\[ \sigma \] is the electric quantum conductivity, and quantum wave function \( \Psi \) satisfies the Schrödinger equation with nanometer quantum Hamiltonian \( \mathcal{H}_Q \)

\[ i \hbar \frac{\partial \Psi}{\partial t} = \mathcal{H}_Q \Psi, \]

where \( \mathcal{H}_Q \) is depended on the property of the specific nanometer material and EM filed.
4. GL EM AND NANOMETER QUANTUM FIELD COUPLED MODELING

4.1. The EM and Quantum Field Nonlinear Coupled Equation

The EM field Equation (6), current representation (7) and quantum field Equation (8) couple into EM field and quantum field coupled nonlinear equation. For the nanometer material, we need add the following Macro-Micro constitute nonlinear relation equation,

\[ \sigma = \sigma(e, \Psi), \]
\[ \varepsilon = \varepsilon(e, \Psi), \]
\[ \mu = \mu(e, \Psi). \]  \hspace{1cm} (9)

4.2. Iteration for Solving the Coupled Nonlinear EM and Quantum Field Coupled Equations

We use the following iteration to solve the EM and quantum field coupled equations

\[ \nabla \times \mathbf{E}^{(n)} = -i\omega\mu \left( e^{(n-1)}, \Psi^{(n-1)} \right) \mathbf{H}^{(n)}, \]
\[ \nabla \times \mathbf{H}^{(n)} = i\varepsilon e^{(n-1)} \left( e^{(n-1)}, \Psi^{(n-1)} \right) \mathbf{E}^{(n)} + j \left( e^{(n-1)}, \Psi^{(n-1)} \right), \]  \hspace{1cm} (10)
\[ e^{(n)} \Psi^{(n)} = H_Q \left( \mathbf{E}^{(n)}, \mathbf{H}^{(n)} \right) \Psi^{(n)}. \]  \hspace{1cm} (11)

We solve the linearization Equations (10) and (11) in order to form the \( n \)th circle of the iteration.

4.3. Division of the Domain

The inhomogeneous domain \( \Omega \) is divided into a set of the several lattice domains \( \{ \Omega_k \}, k = 1, 2, \ldots, N \), such that \( \Omega = \bigcup_{k=1}^{N} \Omega_k \). The division is mesh or meshless super lattice.

4.4. GL Modeling for Solving the EM Field Linearization Equation (10)

4.4.1.

In each lattice \( \Omega_k, k = 1, 2, \ldots, N \), we solve the adjoint EM Green’s tensor integral equation of the Equation (10). By the dual curl process, the adjoint Green’s EM field integral equations are reduced into \( 6 \times 6 \) matrix equations. By solving the \( 6 \times 6 \) matrix equations, the Green’s tensor EM field \( \mathbf{E}_k^{M(n)}, \ldots \) and \( \mathbf{H}_k^{M(n)} \) are obtained.

4.4.2.

The global EM field is updated by the following local scattering EM field integral equation

\[ \begin{bmatrix} \mathbf{E}(r) \\ \mathbf{H}(r) \end{bmatrix}^{(n)}_{k} = \begin{bmatrix} \mathbf{E}(r) \\ \mathbf{H}(r) \end{bmatrix}^{(n)}_{k-1} + \int_{\Omega_k} \begin{bmatrix} \mathbf{E}_k^{J(n)}(r', r) & \mathbf{H}_k^{J(n)}(r', r) \\ \mathbf{E}_k^{M(n)}(r', r) & \mathbf{H}_k^{M(n)}(r', r) \end{bmatrix} \begin{bmatrix} D(e^{(n-1)}, \Psi^{(n-1)}) \\ \mathbf{E}(r') \end{bmatrix}^{(n)}_{k-1} dr'. \]  \hspace{1cm} (12)

\( k = 1, 2, \ldots, N \), successively. The \( \begin{bmatrix} \mathbf{E}_N^{(n)}(r), \mathbf{H}_N^{(n)}(r) \end{bmatrix} \) is the GL solution of the 3D GL EM modeling for solving the EM field linearization Equation (10).

4.5. GL Modeling For Solving The Schrödinger Field Linearization Equation (11)

4.5.1.

In each lattice \( \Omega_k, k = 1, 2, \ldots, N \), we solve the adjoint quantum Green’s wave function integral equation of the Schrödinger Equation (11). By the dual process, the adjoint Green’s quantum wave field integral equations are reduced into algebra equation. By solving the algebra equations, the quantum Green’s function tensor \( G_k^{\pm q(n)}(r', r) \) is obtained.

4.5.2.

The Global quantum wave field is updated by the following local scattering quantum wave field integral equation

\[ \Psi_k^{(n)}(r) = \Psi_{k-1}^{(n)}(r) - \frac{2m}{\hbar^2} \int_{\Omega_k} \left( V \left( \mathbf{E}_k^{(n)}, \mathbf{H}_k^{(n)} \right) - V \left( \mathbf{E}_{k-1}^{(n)}, \mathbf{H}_{k-1}^{(n)} \right) \right) G_k^{\pm q(n)}(r', r) \Psi_{k-1}^{(n)}(r') dr', \]  \hspace{1cm} (13)

\( k = 1, 2, \ldots, N \), successively. The \( \Psi_N^{(n)}(r) \) is the GL quantum field solution of the 3D GL quantum field modeling.
5. THE SIMULATION AND ADVANTAGES OF THE GLEMQUAN MODELING

5.1. Simulation

The 20 nm × 20 nm × 20 nm Bragg optical sensor material is embedded into the metal bulk cheap with 5 μm × 5 μm × 5 μm. The X ray propagate through the composite material. The optical material is divided into 1024 lattices. The outside gasket metal bulk is divided into 1024 domains. The initial quantum field is Ψ₀, which satisfies Schrödinger equation with Hamiltonian \( H₀ \). We use the GLEMQUAN modeling to calculate the EM field and quantum wave field function. The \( H_y \) in the transverse section \( Y = 5 \) nm and on surface of the bulk is shown in Figure 1, \( H_y \) is shown in the left graphic, scattering field \( S H_y \) is shown in the right graphic. A quanta wave package is obviously shown in rectangle frame in rear of the scattering wave. The quanta wave package is an EM-quantum coupled effect which is match to the X ray observation. The GLEMQUAN quanta wave package is shown in the Figure 2, it is different from the rear part of macro EM field in which the scattering wave vanished to zero from peak. From the GLEMQUAN EM field and quantum wave field, the quantum fiber strain is calculated. The deformation of the nanometer material crystal due to the quantum fiber strain is shown in the Figure 3. The electric microscope image of the deformation of the nanometer material is shown in Figure 4. The similarity between images in Figure 3 and Figure 4 shows that the GLEMQUAN modeling can obtain high resolution image of the nanometer fiber deformation. The simulations show that the GLEMQUAN modeling is fast and accurate.

Figure 1: \( H_y \) in the transverse section \( Y = 5 \) nm and on surface, \( H_y \) is in the left, scattering field \( S H_y \) is in the right. A quanta is shown in rectangle frame.

Figure 2: GLEMQUAN quanta in the rear of the scattering magnetic field \( H_y \) which is shown in black rectangle frame in Figure 1.

Figure 3: The deformation of the nanometer material crystal due to the quantum fiber strain.

Figure 4: The scan electric microscope SEM image of the deformation of the nanometer material crystal.
5.2. Advantages

The Langrangian principle is very important for sciences. The Langrangian method can be used to model macro and micro mechanics, flow, EM, thermal, and quantum mechanics etc. scientific model. The equivalent between Schrödinger quantum equation and Heisenberg quantum mechanics can be proved by Langrangian principle. The advantage of the Langrangian method is that all macro and micro energy can be written in the Langrangian together. Langrangian method is easy to construct nonstandard modeling. However, its inconvenience is that for each material or process, the Langrangian should be rewritten. The FEM method needs to build and solve big matrix and needs artificial boundary, such that it is very difficult and cumbersome for changeful Langrangian. The GL modeling and inversion method can overcome these difficulties. In the GLEMQUAN modeling, there is no big matrix needs to be solved. There are no artificial boundary and no error reflection and no error dispersion. In particular, the GLEMQUAN is very agile to discrete the nonstandard and changeful Lagrangian density for the different type optical materials and nanometer materials. Using GL method and Langragin principle, we develop GLEMQUAN and GLEMFHS modeling and inversion for macro field to macro material, macro field to micro material, and micro field to micro material [1–3, 5, 6]. The GLEMQUAN and GLEMFHS modeling and inversion is shelf parallelization algorithm.

6. CONCLUSION

The GLEMQUAN EM field and quantum field coupled modeling is proposed and validated in this paper. Many simulations show that the GLEMQUAN and GL EMFHS [3] coupled modelings have advantages to overcome the difficulties in FEM Lagrangian modeling. The GL GLEMQUAN coupled modeling has wide application in optical materials, photosensitivity, photosynthesis, metallography, powder metallurgy, atmosphere chemistry, environment chemistry, nanometer materials sciences and engineering. The patent right of the GLEMQUAN modeling in this paper belongs to the authors of this paper.

REFERENCES