Modeling of Quantum Dot Embedded FRP Smart Composite Structure using Asymptotic Homogenization Method

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ABSTRACT

The exceptional optoelectronic properties of quantum dots (QDs) have stimulated the development of QD based composite materials in recent years. At the nanoscale, the inclusion of QDs strongly influences the overall properties of the macroscopic structure of the composite materials. In the present paper, a micromechanical model is developed for predicting the effective elastic and piezoelectric properties of the QD embedded fiber reinforced composite (FRP) materials. The model is based on modification and application of the multiscale Asymptotic Homogenization technique which has been developed for the periodic composites. The effective elastic and piezoelectric properties of the composite are determined through the solution of the derived local problems formulated on the unit cell of the composite material.

KEYWORDS: quantum dots, Asymptotic Homogenization, effective elastic and piezoelectric properties.

1. INTRODUCTION

Quantum dots are strained zero-dimensional nanostructures which are embedded in a host material with different structural properties. The initial strain is generated due to the lattice mismatch or the thermal expansion difference between the two materials which also induces a piezoelectric field (Pan, 2002). The tuneability of the strain and piezoelectric field of the quantum dot structure is one of the most important features of quantum dots which in turn affect the electrical and optical properties of the QD structure (Wang et al., 2006). Thanks to this unique property, quantum dots have shown significant promise for microelectronics and optoelectronic devices. Recently, For the first time, Fischer et al. (2015) embedded quantum dot-based sensors into fiber-reinforced composite to devise a structural health monitoring (SHM) system where a functional layered quantum dots were integrated into the composite to visualizes mechanical impact by quenching photoluminescence. Fang et al. (2017) labeled quantum dots at the interface between GFRP and matrix to monitor the damage due to the immersion of composite structure into seawater. They demonstrated that quantum dots can detect barely visible seawater immersion damage due to their fluorescence property. Kim et al. (2018) also used aqueous QD solutions for crack monitoring of cement-based materials.

Some theoretical approaches have been developed for the modeling of quantum dot heterostructures. The most common method is the Continuum Elasticity approach based on Eshelby's inclusion theory (Marangati & Sharma, 2007). Green's function method has been proved to be more efficient for calculating strain and piezoelectric field for anisotropic and arbitrarily shaped quantum dot structures (Marangati and

Sharma, 2007). The second approach is the atomistic simulation. A common technique for this approach is to use valence force field (VFF) model with keating potential (Kikuchi et al., 2001). The third approach is the numerical method based on continuum elasticity. This basically utilizes the finite difference and the finite element method whereby geometrical symmetry of the island shapes is assumed, and the strain energy of the structure is minimized (Liu and Jerry, 2002).

In the present paper, the general Asymptotic Homogenization micromechanical model is derived for the quantum dot embedded FRP composite material**.** The derivation is based on the asymptotic homogenization technique developed by Kalamkarov et al. (Kalamkarov, 1992, 2014; Kalamkarov and Kolpakov, 1997; Kalamkarov and Georgiades, 2004). The asymptotic homogenization technique for the periodic smart composite plates with rapidly varying thickness is modified by including nanoscopic scale in the smart structure and considering infinite boundary condition in one direction. The original problem for the regularly non-homogeneous smart QD embedded composite structure with rapidly oscillating thickness reduces to the system of four 'unit cell' local problems that enable the determination of the effective homogenized properties and subsequently the stress and strain fields in the nanocomposite structure.

2. HOMOGENIZED MODEL FOR SMART COMPOSITE STRUCTURES WITH EMBEDDED QUANTUM DOTS

2.1 Problem Formulation

Consider a thin smart layer of periodically arranged quantum dots in the matrix as shown (Figure 1). The periodic structure is obtained by repeating a certain small unit cell Ω_δ in the $x_1 - x_2$ plane (refer to Figure 2). A characteristic dimensionless parameter δ is introduced, where,

$$\delta = \frac{l}{L} \tag{1}$$

Here, L is the global lateral dimension of the structure and l is the local lateral dimension of the unit cell.

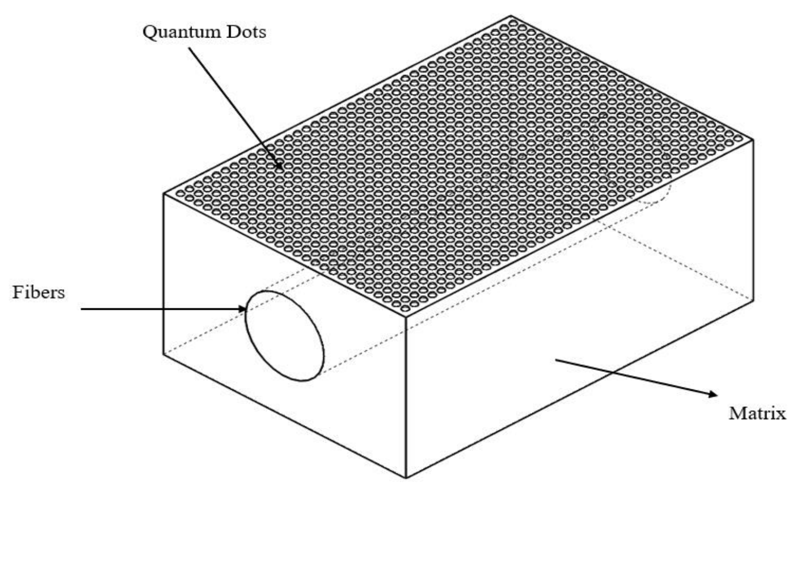

Figure 1: Arbitrarily shaped quantum dots embedded smart FRP composite structure.

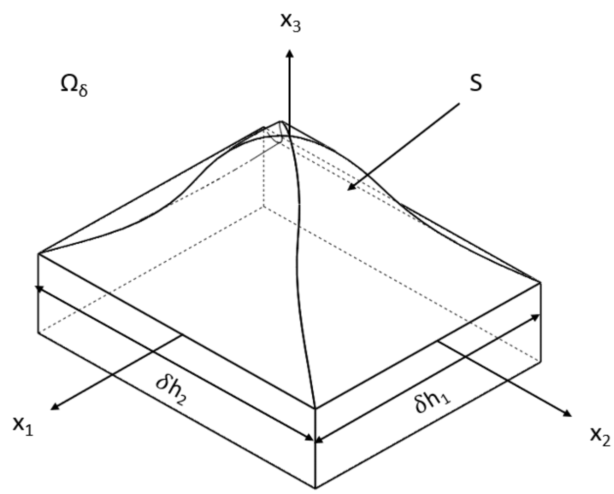

Figure 2: Unit cell (Ω_δ) of the quantum dots embedded smart FRP composite structure.

The unit cell of the problem is defined by the following inequalities, see Figure 2:

$$-\frac{\delta h_1}{2} < x_1 < \frac{\delta h_1}{2}\ ;\ -\frac{\delta h_2}{2} < x_2 < \frac{\delta h_2}{2}\ ;\ -\infty < x_3 < \delta F$$
$$S = \delta F\ \left(\frac{x_1}{\delta h_1}, \frac{x_2}{\delta h_2}\right) \tag{2}$$

Where, δh_1 and δh_2 define the lateral dimensions of the unit cell and F is governed by the profile of the top surface. For the analysis, the thickness of the piezoelectric substrate is considered infinite in the x_3 direction in comparison with the quantum dots dimension embedded on the surface. Moreover, the unit cells are periodic in x_1 and x_2 directions.

If ε^*_{kl} is the lattice mismatch strain or eigenstrain, then

$$\varepsilon^*_{kl} = \frac{a_m - a_{QD}}{a_{QD}} \tag{3}$$

a_m and a_{QD} are the lattice constant for matrix and quantum dot, respectively. The elastic strain is given by subtraction of the eigenstrain from the total strain,

$$\varepsilon^e_{kl} = \varepsilon_{kl} - \varepsilon^*_{kl} \tag{4}$$

The eigenstrain in an elastic material and its representation by the equivalent body force are well-established in classical micromechanics (Mura, 1987; Wang et al., 2006).

$$P_i(x) = -c_{ijkl}\varepsilon^*_{kl,i}(x) \tag{5}$$

The constitutive equation for the stress is defined as,

$$\sigma_{ij} = c_{ijkl}\{(\varepsilon_{k_l}^{e} - \varepsilon_{kl}^{*}) - d_{klm}R_m\} \tag{6}$$

Where,

$$\varepsilon_{kl}^{e} = \frac{1}{2}(u_{k,l} + u_{l,k}) \tag{7}$$

Here, c_{ijkl}, d_{klm} are the tensors of the elastic and piezoelectric coefficient, respectively. R_m is the electric field vector. The governing equation for elastic equilibrium of the structure is finally written as,

$$\sigma_{ij,j} - P_i = 0 \tag{8}$$

The structure in Figure 1 is periodic in the both lateral directions and non-periodic in the transverse direction. The material coefficients in Eq. (6) depend only on the nanoscopic variables y_α, z, (where $\alpha = 1, 2$), whereas the dependent field variables depend on both the nanoscopic and macroscopic variables, y_i ($i = 1, 2, z$) and x_i, respectively. The relation between the nanoscopic and macroscopic variables are as follows,

$$y_1 = \frac{x_1}{\delta h_1}, y_2 = \frac{x_2}{\delta h_2}, z = \frac{x_3}{\delta}\ ;\ \frac{\partial}{\partial x_\alpha} \to \frac{\partial}{\partial x_\alpha} + \frac{1}{\delta h_\alpha}\frac{\partial}{\partial y_\alpha}\ ;\ \frac{\partial}{\partial x_3} = \frac{1}{\delta}\frac{\partial}{\partial z} \tag{9}$$

2.2 Two-scale Asymptotic Expansions

Asymptotic expansion for displacement and stress are as follows:

$$u_i = u_i^{(0)}(x) + \delta u_i^{(1)}(\boldsymbol{x}, \boldsymbol{y}, z) + \delta^2 u_i^{(2)}(\boldsymbol{x}, \boldsymbol{y}, z) + \ \ldots\ldots\ldots \tag{10}$$

$$\sigma_{ij} = \sigma_{ij}^{(0)}(\boldsymbol{x}, \boldsymbol{y}, z) + \delta\sigma_{ij}^{(1)}(\boldsymbol{x}, \boldsymbol{y}, z) + \delta^2\sigma_{ij}^{(2)}(\boldsymbol{x}, \boldsymbol{y}, z) + \ \ldots\ldots\ldots \tag{11}$$

Where all functions are assumed to be periodic in nanoscopic variables y_α.
Boundary conditions,

$$\sigma_{ij}n_j = T_i \ \text{(on top surface z = z}^{+}) \tag{12}$$

Here n_j is the unit normal vector in the outward direction to the top surface.

$$\sigma_{ij} \to 0 \quad (\text{when } z \to -\infty) \tag{13}$$

As a result of asymptotic homogenization procedure, the following relations for the displacements and stresses are derived:

$$u_1 = \delta V_1^{(1)}(x) - z\frac{\partial w}{\partial x_1} + \delta^2\left(U_1^{\alpha\beta}\varepsilon_{\alpha\beta}^{(1)} + V_1^{\alpha\beta}\tau_{\alpha\beta} + U_1^{m}R_m^{(0)} + V_1^{m}R_m^{(1)}\right) \tag{14}$$

$$u_2 = \delta V_2^{(1)}(x) - z\frac{\partial w}{\partial x_1} + \delta^2\left(U_2^{\alpha\beta}\varepsilon_{\alpha\beta}^{(1)} + V_2^{\alpha\beta}\tau_{\alpha\beta} + U_2^{m}R_m^{(0)} + V_2^{m}R_m^{(1)}\right) \tag{15}$$

$$u_3 = w(x) + \delta V_3^{(1)}(x) + \delta^2 \left(U_3^{\alpha\beta} \varepsilon_{\alpha\beta}^{(1)} + V_3^{\alpha\beta} \tau_{\alpha\beta} + U_3^m R_m^{(0)} + V_3^m R_m^{(1)} \right) \qquad (16)$$

$$\sigma_{ij} = \delta\, (b_{ij}^{\alpha\beta} \varepsilon_{\alpha\beta}^{(1)} + \; b_{ij}^{*\alpha\beta}\, \tau_{\alpha\beta} - \; d_{ij}^k R_k^{(0)} - d_{ij}^{*k} R_k^{(1)}) \qquad (17)$$

Here in the text Latin indexes assume values *1,2,3*; Greek indexes assume values *1,2*.

The functions $U_n^{lm}(y_1, y_2, z)$ and $V_n^{lm}(y_1, y_2, z)$ in Eqs. (14) - (17), are periodic in variables y_1, y_2 and are solutions of the unit cell problems which are formulated as follows:

$$\frac{1}{h_\alpha} \frac{\partial}{\partial y_\alpha}\, b_{i\alpha}^{\alpha\beta} + \frac{\partial}{\partial z}\, b_{i3}^{\alpha\beta} = 0$$

$$b_{ij}^{\alpha\beta}\, N_j = 0 \;\text{ at } z = z^+ \qquad (18)$$

$$b_{ij}^{\alpha\beta} \to 0 \quad \text{at } z \to -\infty$$

$$\frac{1}{h_\alpha} \frac{\partial}{\partial y_\alpha}\, b_{i\alpha}^{*\mu\beta} + \frac{\partial}{\partial z}\, b_{i3}^{*\mu\beta} = 0$$

$$b_{ij}^{*\mu\beta}\, N_j = 0 \;\text{ on } z = z^+ \qquad (19)$$

$$b_{ij}^{*\mu\beta} \to 0 \quad \text{at } z \to -\infty$$

$$\frac{1}{h_\alpha} \frac{\partial}{\partial y_\alpha}\, d_{i\alpha}^k + \frac{\partial}{\partial z}\, d_{i3}^k = 0$$

$$d_{ij}^k\, N_j = 0 \;\text{ on } z = z^+ \qquad (20)$$

$$d_{ij}^k \to 0 \quad \text{at } z \to -\infty$$

$$\frac{1}{h_\alpha} \frac{\partial}{\partial y_\alpha}\, d_{i\alpha}^{*k} + \frac{\partial}{\partial z}\, d_{i3}^{*k} = 0$$

$$d_{ij}^{*k}\, N_j = 0 \;\text{ on } z = z^+ \qquad (21)$$

$$d_{ij}^{*k} \to 0 \quad \text{at } z \to -\infty$$

Here the following definitions are used:

$$b_{ij}^{nl} = \frac{1}{h_\beta} c_{ijk\beta} \frac{\partial}{\partial y_\beta} U_k^{nl} + c_{ijk3} \frac{\partial}{\partial z} U_k^{nl} + c_{ijnl}$$

$$b_{ij}^{*nl} = \frac{1}{h_\beta} c_{ijk\beta} \frac{\partial}{\partial y_\beta} V_k^{nl} + c_{ijk3} \frac{\partial}{\partial z} V_k^{nl} + zc_{ijnl}$$

$$d_{ij}^{m} = P_{ijm} - \frac{1}{h_\beta} c_{ijk\beta} \frac{\partial}{\partial y_\beta} U_k^{m} - c_{ijk3} \frac{\partial}{\partial z} U_k^{m} \tag{22}$$

$$d_{ij}^{*m} = z\, P_{ijm} - \frac{1}{h_\beta} c_{ijk\beta} \frac{\partial}{\partial y_\beta} V_k^{m} - c_{ijk3} \frac{\partial}{\partial z} V_k^{m}$$

$$N_j = \left(\frac{1}{h_1} \frac{\partial S}{\partial y_1}, \frac{1}{h_2} \frac{\partial S}{\partial y_2}, 1 \right)$$

The effective properties of the homogenized material are calculated by taking the average of the first four equations of Eq. (22) over the volume of the unit cell **Ω**:

$$< b_{ij}^{nl} > = \int \left(\frac{1}{h_\beta} c_{ijk\beta} \frac{\partial}{\partial y_\beta} U_k^{nl} + c_{ijk3} \frac{\partial}{\partial z} U_k^{nl} + c_{ijnl} \right) dv$$

$$< b_{ij}^{*nl} > = \int \left(\frac{1}{h_\beta} c_{ijk\beta} \frac{\partial}{\partial y_\beta} V_k^{nl} + c_{ijk3} \frac{\partial}{\partial z} V_k^{nl} + zc_{ijnl} \right) dv$$

$$< d_{ij}^{m} > = \int \left(P_{ijm} - \frac{1}{h_\beta} c_{ijk\beta} \frac{\partial}{\partial y_\beta} U_k^{m} - c_{ijk3} \frac{\partial}{\partial z} U_k^{m} \right) dv \tag{23}$$

$$< d_{ij}^{*m} > = \int \left(z\, P_{ijm} - \frac{1}{h_\beta} c_{ijk\beta} \frac{\partial}{\partial y_\beta} V_k^{m} - c_{ijk3} \frac{\partial}{\partial z} V_k^{m} \right) dv$$

By multiplying the unit cell problems by z and applying the Gauss Divergence theorem and periodic boundary conditions it can be shown that (see Kalamkarov and Georgiades, 2004)

$$< b_{i3}^{\mu\beta} > = < b_{i3}^{*\mu\beta} > = < d_{i3}^{m} > = < d_{i3}^{*m} > = 0 \tag{24}$$

The effective properties defined by Eq. (23) enter the global governing homogenized equations as the effective equivalent material properties to find the stresses and displacements of the homogenized structure.

3. CONCLUSIONS

The developed global formulation of the quantum dot embedded fiber reinforced composite model provides the basis for quantifying the average (effective) stress and strain states of the composite structure, with varying geometries of the quantum dots. The set of four 3D local unit cell problems in the nanoscopic scale are derived which are dependent on the periodicity boundary condition in the both lateral directions and the decaying of all functions in the transverse direction as $z \rightarrow -\infty$. The solution of these unit cell problems yields to a set of functions which, when averaged over the volume of the periodicity cell, determine the effective elastic and piezoelectric coefficients of the homogenized quantum dots embedded fiber reinforced smart composite structure. These sets of effective coefficients in turn give the displacement and stress fields by entering them into the governing equations of the system.

The next step will be to apply the developed model for different cases of QD embedded composites and compare the analytical results with numerical results by using Finite Element Method.

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