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CNN MODELLING OF NANO-INCLUSIONS*

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Piezoelectrical material with heterogeneities of nano-inclusions is considered in the case when it is subjected to time harmonic electro-mechanical load. The model is defined by the system of two partial differential equations and the boundary conditions for the generalized stress. On the exterior boundary, boundary conditions prescribe traction on the part of the boundary and prescribe displacement on the complemented part. We construct Cellular Nonlinear/Nanoscale Network (CNN) architecture for the boundary value problem. The dynamics of the obtained CNN model is studied via harmonic balance method. Traveling wave solutions are obtained numerically. The simulations are provided which illustrate the theoretical results. The obtained results are applicable in the field of non-destructive testing and fracture mechanics of multi-functional materials and structural elements based on them.

1. Introduction

The demand for smaller and faster devices has encouraged technological advances resulting in the ability to manipulate matter at nanoscales that have enabled the fabrication of nanoscale electromechanical systems. With the advances in materials synthesis and device processing capabilities, the importance of developing and

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understanding nanoscale engineering devices has dramatically increased over the past decade. Computational Nanotechnology has become an indispensable tool not only in predicting, but also in engineering the properties of multi-functional nano-structured materials. The presence of nano-inclusions in these materials affects or disturbs their elastic field at the local and the global scale and thus greatly influences their mechanical properties. In this paper we shall look for a solution of 2D dynamic coupled problem in multifunctional nano-heterogeneous piezoelectric and magnitopiezoelectric composites. More in detail, we shall present first modeling and solution of two-dimensional anti-plane (SH) wave propagation problem in piezoelectric/magnitopiezoelectric anisotropic solids containing multiple nano-inclusions. The model is based on the principles of elastodynamics, wave propagation theory and surface/interface elasticity theory. Nano-heterogeneities are considered in two aspects as wave scatters provoking scattered and diffraction wave fields and also as stress concentrators creating local stress concentrations in the considered solid. In Section 2 we shall state the model of piezoelectric solid with heterogeneities under time-harmonic anti-plane load. Section 3 will deal with the discretization of this model by Cellular Nonlinear/Nanoscale Network (CNN) architecture and dynamic behavior of the obtained CNN model. In Section 4 we shall present simulations and validation for the problem under consideration. Discussions will be provided in the conclusions.

2. Statement of the problem

Let $G \in R^2$ is a bounded piezoelectric domain with a set of inhomogeneities $I = \cup I_k \in G$ (holes, inclusions, nano-holes, nano-inclusions) subjected to time–harmonic load on the boundary ∂G, see Figure 1. Note that heterogeneities are of macro size if their diameter is greater than 10^{-6} m, while heterogeneities are of nano-size if their diameter is less than 10^{-7} m.

The aim is to find the field in every point of $M = G \backslash I$, I and to evaluate stress concentration around the inhomogeneities.

Using the methods of continuum mechanics the problem can be formulated in terms of boundary value problem for a system of 2-nd order differential equations, see [1], Chapter 2.

$$(1) \qquad \left| \begin{array}{l} c_{44}^N \Delta u_3^N + e_{15}^N \Delta u_4^N - \rho^N u_{3,tt} = 0, \\ e_{15}^N \Delta u_3^N - \varepsilon_{15}^N \Delta u_4^N = 0, \end{array} \right.$$

where $x = (x_1, x_2)$, $\Delta = \dfrac{\partial^2}{\partial x_1^2} + \dfrac{\partial^2}{\partial x_2^2}$ is Laplace operator with respect to t, $N = M$ for $x \in M$ and $N = I$ for $x \in I$; u_3^N is mechanical displacement, u_4^N is electric

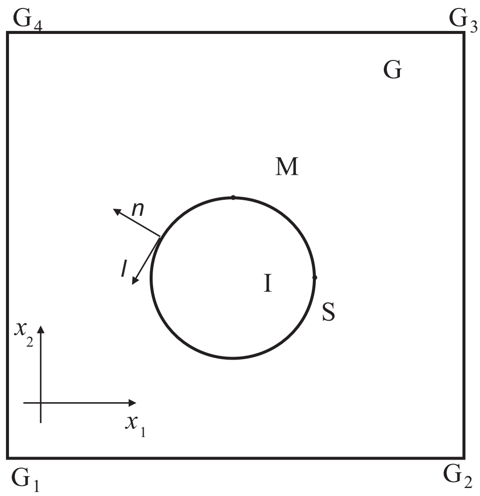

Figure 1: Piezoelectric matrix M with nano-heterogeneities I

potential, ρ^N is the mass density, $c_{44}^N > 0$ is the shear stiffness, $e_{15}^N \neq 0$ is the piezoelectric constant and $\varepsilon_{11}^N > 0$ is the dielectric permittivity.

Assume that the interface between the nano-inclusion I and its surrounding matrix M is regarded as thin material surface S that possesses its own mechanical parameters c_{44}^I, e_{15}^I, ε_{11}^I.

We shall consider the case, when I is a nano-hole, formally we consider that constants in I are $c_{44}^I = 0$, $e_{15}^I = 0$, $\varepsilon_{11}^I = 0$ and boundary conditions on S are

$$t_j^M = \frac{\partial \sigma_{lj}^S}{\partial l} \quad \text{on} \quad S \tag{2}$$

where σ_{lj}^S is generalized stress [1], $j = 3, 4$, l is the tangential vector. Then we shall study boundary value problem (BVP) (1) with boundary conditions (2).

There are no numerical results for dynamic behavior of bounded piezoelectric domain with heterogeneities under anti-plane load. Validation is done in [1] for infinite piezoelectric plane with a hole, in [2] for isotropic bounded domain with holes and inclusions and in [3] for piezoelectric plane with nano-hole or nano-inclusion.

In the next section we shall propose Cellular Nonlinear/Nanoscale Network (CNN) architecture, as a discretized version of the problem (1),(2) and we shall study its dynamics in Section 4.

3. CNN model of boundary value problem

Resonant tunnel diode (RTD) based CNN [4] which represents a class of quantum effect devices, is an excellent candidate for both analog and digital applications because of its structural simplicity, relative ease of fabrication, inherent speed and design flexibility. For this reason we shall apply RTD-based CNN architecture for studying the dynamics of BVP (1), (2). Following [4, 5] we shall write the RTD-based CNN of the BVP which consists of $n = L.L$ cells:

$$\begin{aligned} & c_{44}^N A_1 * u_{3i} + e_{15}^N A_1 * u_{4i} - \rho^N \frac{d^2 u_{3i}}{dt^2} = 0 \\ & e_{15}^N A_1 * u_{3i} - \varepsilon_{11}^N A_1 * u_{4i} = 0, 1 \le i \le n, \end{aligned} \tag{3}$$

where A_1 is 1-dimensional discretized Laplacian template [5], $*$ is convolution operator, $1 \le i \le n$. Boundary conditions (2) can be written in terms of RTD-based CNN architecture are as follows:

$$\begin{aligned} & t_j^M = \frac{\partial \sigma_{lij}^M}{\partial l}, j = 3, 4, \\ & \sigma_{l3i}^M = c_{44}^M \frac{\partial u_{3i}^l}{\partial x_l} + e_{15}^M \frac{\partial u_{4i}^l}{\partial x_l}, \\ & \sigma_{l4i}^M = e_{15}^M \frac{\partial u_{3i}^l}{\partial x_l} - \varepsilon_{11}^M \frac{\partial u_{4i}^l}{\partial x_l}, 1 \le i \le n. \end{aligned} \tag{4}$$

We express from the second equation of (3), $A_1 * u_{4i}$ and substitute in the first equation. So we obtain the following equation for u_{3i}:

$$\tilde{C} A_1 * u_{3i} - \rho^N \frac{d^2 u_{3i}}{dt^2} = 0, \tag{5}$$

where $\tilde{C} = c_{44}^N + \dfrac{(e_{15}^N)^2}{\varepsilon_{11}}$.

We shall take the output of the model (3), (4) as a piecewise linear function [4]:

$$\begin{aligned} y(u_{ji}) = a u_{ji} + b(|u_{ji} - V_p| - |u_{ji} - V_v|) - b(|u_{ji} + V_p| - \\ |u_{ji} + V_v|) = N(u_{ji}), j = 3, 4 \end{aligned} \tag{6}$$

where $a > 0$, $b < 0$ are constants, V_p, V_v $(0 < V_p < V_v)$ are the peak and valley voltages of the RTD-based CNN, and as one can notice the output function is symmetric with respect to the origin. The graph of the output function is given on Figure 2 below:

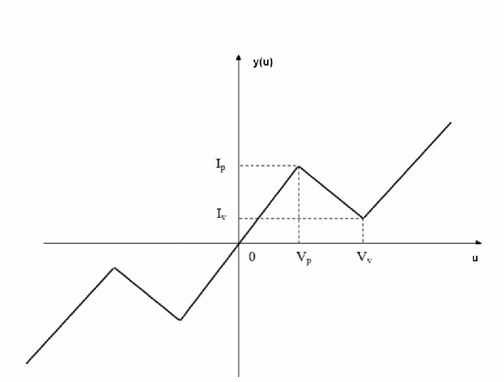

Figure 2: Graph of the output function (6) for the RTD-based CNN model

4. Dynamics of the RTD-CNN model

We shall apply approximative method in order to study the dynamics of our RTD-based CNN model (3), (4). This method is based on a special Fourier transform and is known in electrical engineering as harmonic balance method [5]. Following harmonic balance method we introduce double Fourier transform:

$$F(s,z) = \sum_{k=-\infty}^{k=\infty} z^{-k} \int_{-\infty}^{\infty} f_k(t)\exp(-st)dt. \tag{7}$$

where $z = \exp(I\Omega)$, Ω is continuous spatial frequency, $s = I\omega$, ω is continuous temporal frequency, I is the imaginary identity.

We apply the above transform (7) to (5) and obtain the following transfer function:

$$H(s,z) = \frac{\rho^N s^2}{\tilde{C}(z^{-1}-2+z)}. \tag{8}$$

According to the harmonic balanced method [5] the following proposition hold:

Proposition 1. *RTD-Based CNN model* (3), (4) *consisting of circular array of $n = L.L$ cells has periodic state solutions u_{3i}, u_{4i} with a finite set of spatial frequencies $\Omega = \dfrac{2\pi}{K}$, $0 \leq K \leq n-1$ and minimal period T.*

Proof. We are looking for possible periodic solutions of our CNN model (3), (4) of the form:

$$u_{ji}(t) = \xi(\omega t + i\Omega), j = 3,4 \tag{9}$$

for some function $\xi : \mathbf{R} \to \mathbf{R}$ and for some $0 \le \Omega \le 2\pi$, $\omega = \dfrac{2\pi}{T}$, where $T > 0$ is the minimal period of (9). For the circular array the possible values for Ω can be easily obtained. As $u_{ji}(t)$ is assumed to be periodic, with minimal period T, one has

$$\xi(\omega t + i\Omega) = \xi(\omega t + i\Omega + K\omega T) \tag{10}$$

for any $K \in \mathbf{N}$. One the other hand, the periodic boundary conditions impose that

$$\xi(\omega t) = \xi(\omega t + n\Omega). \tag{11}$$

Combining (10) with $i = 0$ and (11), we get

$$\Omega = \frac{K}{n}\omega T = \frac{2\pi K}{n}, 0 \le K \le n-1, \tag{12}$$

where the range of K is determined by the condition $0 \le \Omega \le 2\pi$.

Now we shall look for the solution of (3), (4) in the form:

$$\begin{aligned} u_{3i} &= U_3 \sin(\omega t + i\Omega), \\ u_{4i} &= U_4 \sin(\omega t + i\Omega), \end{aligned} \tag{13}$$

where U_3, U_4 are amplitudes, $0 \le \Omega \le 2\pi$, $\omega = \dfrac{2\pi}{T}$, T being the minimal period of (9).

We shall express the transfer function (8) in terms of $s = I\omega$ and $z = \exp(I\Omega)$ and we obtain:

$$H_\Omega(\omega) = \frac{-\rho^N \omega^2}{\tilde{C}(2\cos\Omega - 2)}. \tag{14}$$

According harmonic balance method [5] the following constraints hold:

$$\begin{aligned} \mathrm{Re}(H_\Omega(\omega)) &= \frac{U_3}{U_4} \\ \mathrm{Im}(H_\Omega(\omega)) &= 0. \end{aligned} \tag{15}$$

We shall approximate the output of our RTD-based CNN model (3), (4) given by (6) by the fundamental component of its Fourier expansion:

$$y = Y \sin(\omega t + i\Omega) \tag{16}$$

with

$$Y = \frac{1}{\pi}\int_{-\pi}^{\pi} N(u_{ji}\sin\psi)\sin\psi d\psi.$$

Then we substitute real and imaginary part of the transfer function $H_\Omega(\omega)$ (14) in (15) and we obtain the system of algebraic equations for the unknowns (ω, U_3, U_4). We solve this system and find the unknowns. This is the end of the proof. □

Remark. In order to validate the accuracy of the obtained results we apply possible initial conditions from which the network will reach, at steady state, a steady state solution characterized by the desired value of Ω. In our case we propose the initial conditions of the form: $u_{ji}(0) = \sin(\Omega i)$, $j = 3, 4$,$1 \leq i \leq n$.

Consider the square domain $G_1G_2G_3G_4$ given on Figure 1 with a side α, containing a single circular inhomogeneity with a radius $r = \beta\alpha$ and center at the square center. Note that if $\beta < 0.05$ the influence of the exterior boundary G on the solution is expected to be small, while if $\beta > 0.2$ it is expected significant influence. In our case of heterogeneities at nano-scale, material parameters inside I for the hole are 0; for an inclusion are: $c^I_{44} = 0.1c^M_{44}$, $e^I_{15} = 0.1e^M_{15}$, $\varepsilon^I_{11} = 0.1\varepsilon^M_{11}$, $\rho^I = \rho^M$. Spatial frequency is defined as $\Omega = c\sqrt{(\frac{\rho^M}{c^M_{44}})}\omega$. For this parameter set we present below on Figure 3 the obtained solution of our RTD-based CNN model (3), (4).

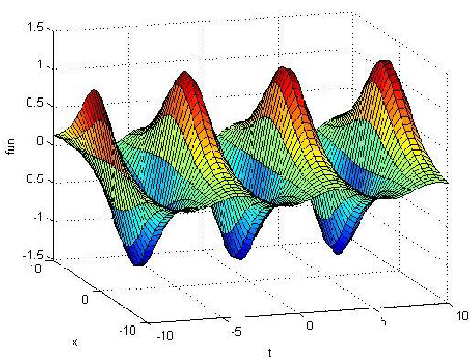

Figure 3: Simulations of RTD-based CNN model (3), (4)

As it can be seen from the above figure we have traveling wave solution of the form:

$$u_{ji} = \Phi(i - ct), j = 3, 4 \tag{17}$$

for for some continuous function $\Phi : \mathbf{R}^1 \to \mathbf{R}^1$ and some unknown real number

c. Let us denote $s = i - ct$, then this solution satisfies:

$$\lim_{s\rightarrow} \Phi(s, c) = 0. \tag{18}$$

Traveling wave solution for our RTD-based CNN model is given on Figure 4. We use the above parameter set for the numerical simulation.

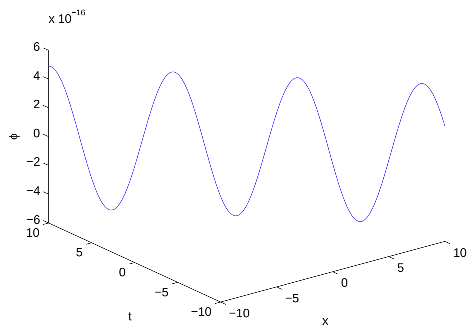

Figure 4: Traveling wave solution of RTD-based CNN model (3), (4)

5. Simulations and validation

The characteristic that is of interest in nano-structures is normalized Stress Concentration Field (SCF) (σ/σ_0) and it is calculated by the following formula:

$$\sigma = -\sigma_{13} \sin(\varphi) + \sigma_{23} \cos(\varphi), \tag{19}$$

where φ is the polar angle of the observed point, σ_{ji} is the stress (2) near S.

Material parameters of the matrix are for transversely isotropic piezoelectric material PZT4 are:

- Elastic stiffness: $c_{44}^M = 2.56 \times 10^{10}$ N/m^2;
- Piezoelectric constant: $e_{15}^M = 12.7$ C/m^2;
- Dielectric constant: $\varepsilon_{11}^M = 64.6 \times 10^{-10}$ C/Vm;
- Density: $\rho^M = 7.5 \times 10^3$ kg/m^3.

The applied load is time harmonic uni-axial along vertical direction uniform mechanical traction with frequency ω and amplitude $\sigma_0 = 400 \times 10^6$ N/m^2 and electrical displacement with amplitude $D_0 = k\frac{\varepsilon_{11}^M}{e_{15}^M}\sigma_0$.This means that the boundary conditions (4) are:

- on $G_1G_2 : t_3^M = -\sigma_0, t_4^M = -D_0$;
- on $G_2G_3 : t_3^M = t_4^M = 0$;
- on $G_3G_4 : t_3^M = {}_0, t_4^M = D_0$;
- on $G_4G_1 : t_3^M = t_4^M = 0$.

The validation of our model is provided below on Figure 5 for the parameter sets given above.

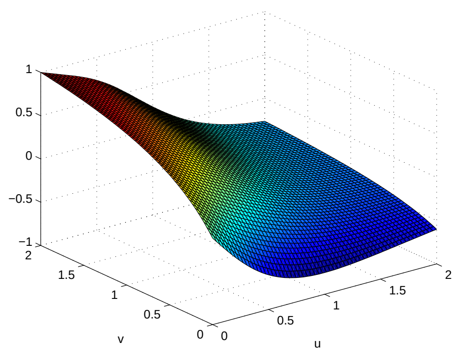

Figure 5: Validation – dynamic SCF at observed point

6. Conclusions

In this paper we consider homogeneous or functional graded piezoelectric material with heterogeneities of different type (hole, crack, inclusion, nano-hole, nano-inclusion) subjected to time-harmonic wave. There is a certain lack of work for solution of 2D ant-plane dynamic problems for piezoelectric and magnetopiezoelectric solids with nanoinclusions or nano-cavities. The reason is that such a goal requires multidisciplinary knowledge and skills.

In this paper we propose RTD-based CNN approach for numerical study of the dynamics of the model (1), (2). We find traveling wave solutions of our CNN model and the simulations illustrate the obtained theoretical results.

Computational nanomechanics has a high priority in Europe, because it concerns the development and creation of new smart materials and devices based on them. The present paper addresses the vital component of accurate description and computation of the wave motions and stress concentrations that are developed in the multifunctional materials with nano-structures.

References

[1] P. Dineva, D. Gross, R. Muller, T. Rangelov. Dynamic Fracture of Piezoelectric Materials. Solutions of Time-harmonic problems via BIEM, Solid Mechanics and its Applications, vol. **212**, Springer Int.Publ., Switzerland, 2014.

[2] X. Q. Fang, J. X. Liu, L. H.Dou, M. Z. Chen. Dynamic strength arround two interactive piezoelectric nano-fibers with surfaces/interfaces in solid under electro-elestic wave. *Thin Solid Films*, **520** (2012), 3587–3592.

[3] M. Jammes, S. G. Mogilevskaya, S. L. Crouch. Multiple circular nano-inhomogeneities and/or nano-pores in one of two joined isotropic half-planes. *Eng. Anal. Bound. Elem.*, **33** (2009), 233–248.

[4] C. H. Hsu, S. Y. Yang. Wave Propagation in RTD-Based Cellular Neural Network. *Journal of Differential Equations*, **204** (2004), 339–379.

[5] A. Slavova. Cellular Neural Networks: Dynamics and Modeling. Kluwer Academic Publishers, 2003.

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