Travelling Wave Solutions of Integro-Differential Equation Arising in Nano-Structures

G. Agranovich

Department of Electrical and Electronic Engineering, Ariel University Center of Samaria, Ariel, Israel
E-mail: agr@ariel.ac.il

E. Litsyn

Department of Mathematics, Ben-Gurion University of the Negev Beer-Sheva, Beer-Sheva, Israel
E-mail: elena.litsyn@weizmann.ac.il

A. Slavova

Institute of Mathematics, Bulgarian Academy of Sciences, Sofia, Bulgaria
E-mail: slavova@math.bas.bg

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 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.

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. 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])

$$\begin{aligned} c_{44}^N \Delta u_3^N + e_{15}^N \Delta u_4^N - \rho^N u_{3,tt} = 0, \\ e_{15}^N \Delta u_3^N - \varepsilon_{15}^N \Delta u_4^N = 0, \end{aligned} \tag{1}$$

where $x = (x_1, x_2)$, $\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}$ 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 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 and boundary conditions on S are

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

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 Section 2 we shall construct CNN model for the BVP (1), (2). In section 3 we shall find travelling wave solutions of this model and we shall provide validation.

2 Cellular Nonlinear Network (CNN) Model of the BVP

In [1] fundamental solutions of the BVP (1), (2) are found using the Fourier transform. Then using the Gauss theorem and proceeding as in [1] from the BVP a system of integro-differential equations (IDE) is obtained for the unknowns $u_{3,4}$ on S. This system has the following general form

$$\frac{\partial u}{\partial t} = D\,\frac{\partial^2 u}{\partial x^2} - C_1 \int\limits_S f(u(t,x))\,dt, \quad t \in [0,1], \tag{3}$$

where C_1 is a constant depending on the ρ^M, $c_{44}^M > 0$, $e_{15}^M \neq 0$ and $\varepsilon_{11}^M > 0$, D is diffusion coefficient.

Then the CNN model [4] for the IDE (3) can be written as

$$\frac{du_{ij}}{dt} = DA_1 * u_{ij} - C_1 \int\limits_S f(u_{ij}(t))\,dt, \quad 1 \le i \le n, \quad j = 3, 4, \tag{4}$$

where A_1 is 1-dimensional discretized Laplacian template, $*$ is convolution operator.

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

$$y(u_{ij}) = au_{ij} + b\big(|u_{ij} - V_p| - |u_{ij} - V_v|\big) - b\big(|u_{ij} + V_p| - |u_{ij} + V_v|\big) = N(u_{ij}), \quad j = 3, 4, \tag{5}$$

where $a > 0$, $b < 0$ are constants, V_p, $V_v (0 < V_p < V_v)$ are the peak and valley voltages of the 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 1 below.

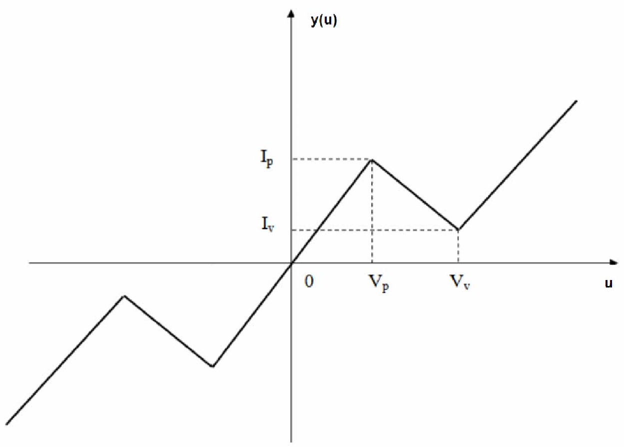

Figure 1. Graph of the output function (5) for the CNN model.

3 Travelling Wave Solutions of IDE CNN Model

We shall study traveling wave solutions of IDE CNN model (4) of the form

$$u_i = \Phi(i - ct), \tag{6}$$

for some continuous function $\Phi : \mathbf{R}^1 \to \mathbf{R}^1$ and some unknown real number c. Let us denote $s = i - ct$. Let us substitute (6) in the IDE CNN model (4). Therefore $\Phi(s, c)$ and c satisfy the equation of the form

$$-c\Phi^{'}(s,c) = \Phi(s-1,c) - 2\Phi(s,c) + \Phi(s+1,c) - C_1 \int\limits_S f(\Phi(s,c))\,dt. \tag{7}$$

Our aim in this note is to study traveling wave solution of the IDE CNN model (4). We consider solution of equation (7). The following theorem about travelling wave solution of our IDE CNN model holds.

Theorem 1. *Let $\Phi(s, c)$ be a solution of (7) satisfying the following conditions*

$$\lim_{s\to-\infty} \Phi(s,c) = 0, \quad \lim_{s\to\infty} \Phi(s,c) = 1.$$

Then

(i) *If $c = c^* < 0$, $\Phi(s, c)$ is a stable travelling wave solution of IDE CNN model.*

(ii) *If $c = c_* > 2$, $\Phi(s, c)$ is unstable travelling wave solution.*

We shall skip the proof due to the lack of space.

Traveling wave solution for our IDE CNN model (4) is given on Figure 2. We use the following parameter set for the numerical simulation.Material parameters of the matrix are for transversely isotropic piezoelectric material PZT4 are: elastic stiffness: $c^M_{44} = 2.56 \times 10^{10}\, N/m^2$; piezoelectric constant: $e^M_{15} = 12.7\, C/m^2$; dielectric constant: $\varepsilon^M_{11} = 64.6 \times 10^{-10}\, C/Vm$; density: $\rho^M = 7.5 \times 10^3\, kg/m^3$.

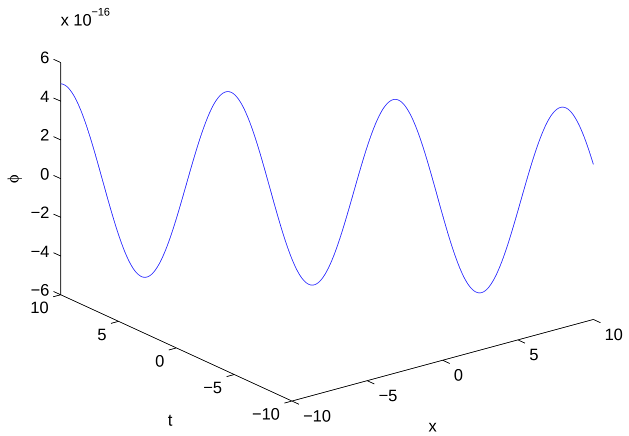

Figure 2. Traveling wave solution of IDE CNN model (4).

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

$$\sigma = -\sigma_{13}\sin(\varphi) + \sigma_{23}\cos(\varphi), \tag{8}$$

where φ is the polar angle of the observed point, σ_{ji} is the stress (2) near S. 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 $D_0 = k\,\frac{\varepsilon_{11}^M}{e_{15}^M}\,\sigma_0$.

The validation of our model is provided below on Figure 3 for the parameter sets given above.

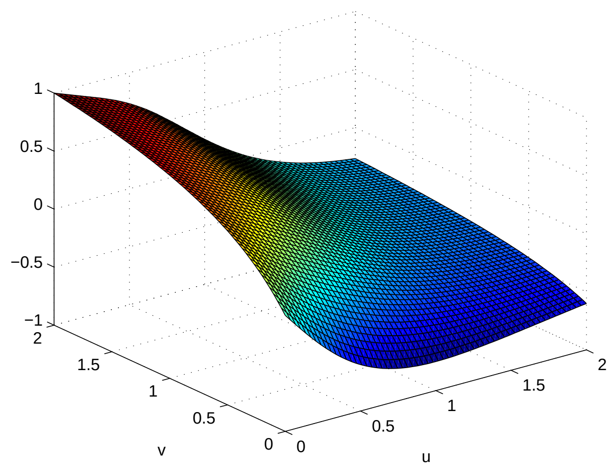

Figure 3. Validation – dynamic SCF at observed point.

Acknowledgements

This paper is performed in the frames of working program on the Bilateral Res. Project between Bulgarian Academy of Sciences and Israel Academy of Sciences. This paper is supported by the project DFNI-I 02/12.

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