Modeling of Micro- and Nanostructures Made of Films and Crystals/Fibers Arrays

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Introduction. Currently, the development of nanotechnologies produces a wide range of nanomaterials, including well-known materials, such as nanoshells and nanosprings (single-walled and multi-walled nanotubes, etc.) with particular properties.
These helical-like structures have a number of attractive properties for various applications. For example, the high flexibility, piezoelectric characteristics, and other principal particularities make these structures suitable for creation of the nanosensors, nanoswitches, propulsion systems and other nanoelectromechanical systems (NEMS). The modeling of the above described structures can significantly influence the development of nanotechnology in the area of using shell-like helical structures and their assemblies.

Problem Definition

The construction a complete model of helical nanostructures and to open new opportunities for their applications in practice with development of the modern nanotechnologies.

Objectives

The aim of this work is the complex research of the behavior of a multilayer structure which has a chiral geometry on the joint of multiphysics in the field of coupled tasks. The multiphysics statement consists in the consideration of mechanical action, electric response and two-way interaction between fluid and structure.

Cooperation

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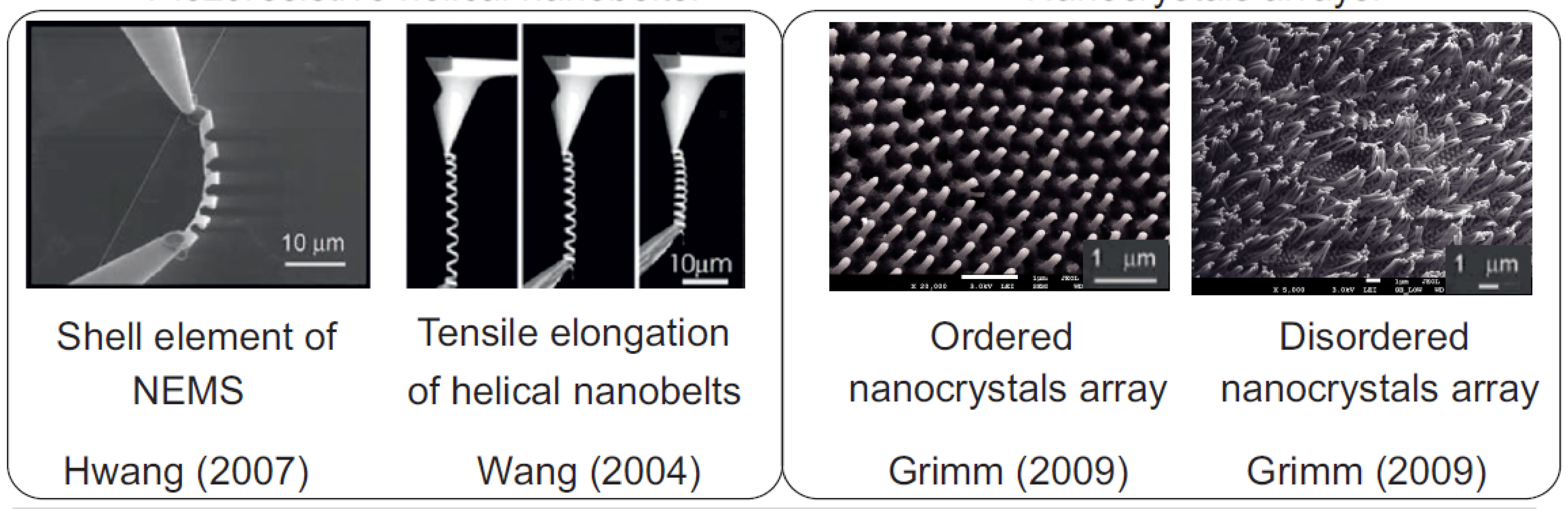


Figure 1. Examples of Investigated Nanostructures

Steps of Investigation

✓Interaction of a helical shell with a non-linear viscous fluid

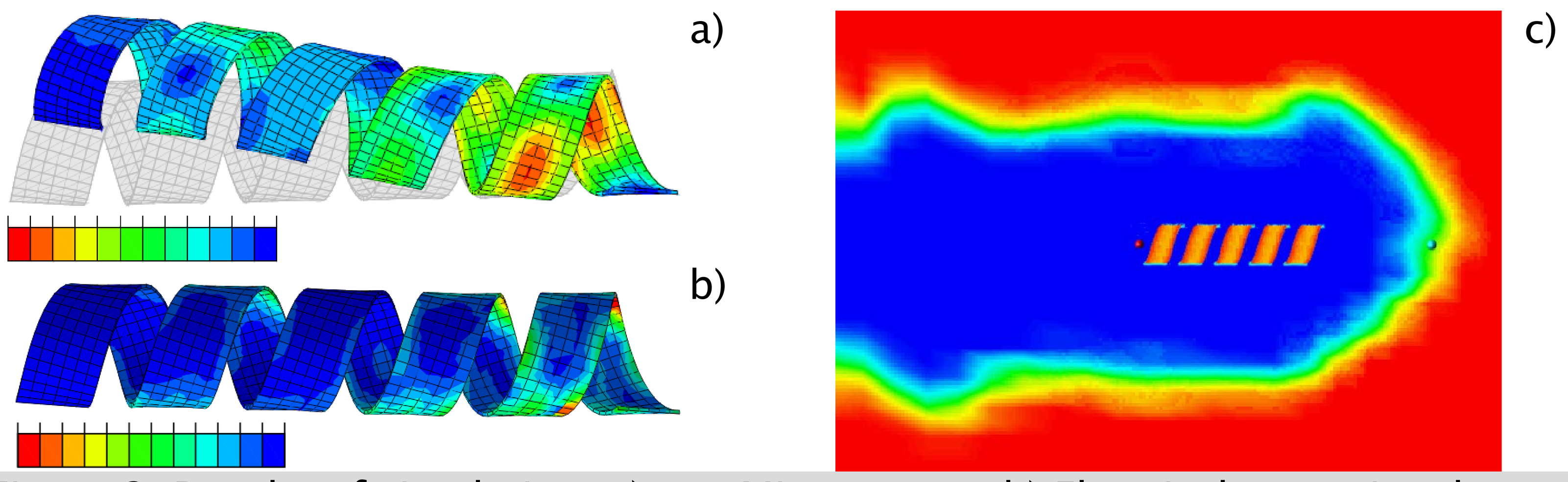


Figure 2. Results of simulation: a) von Mises stress; b) Electrical potentional gradient; c) Distribution of fluid viscosity

✓Instability of a piezoelectric helical shell under electrical field action

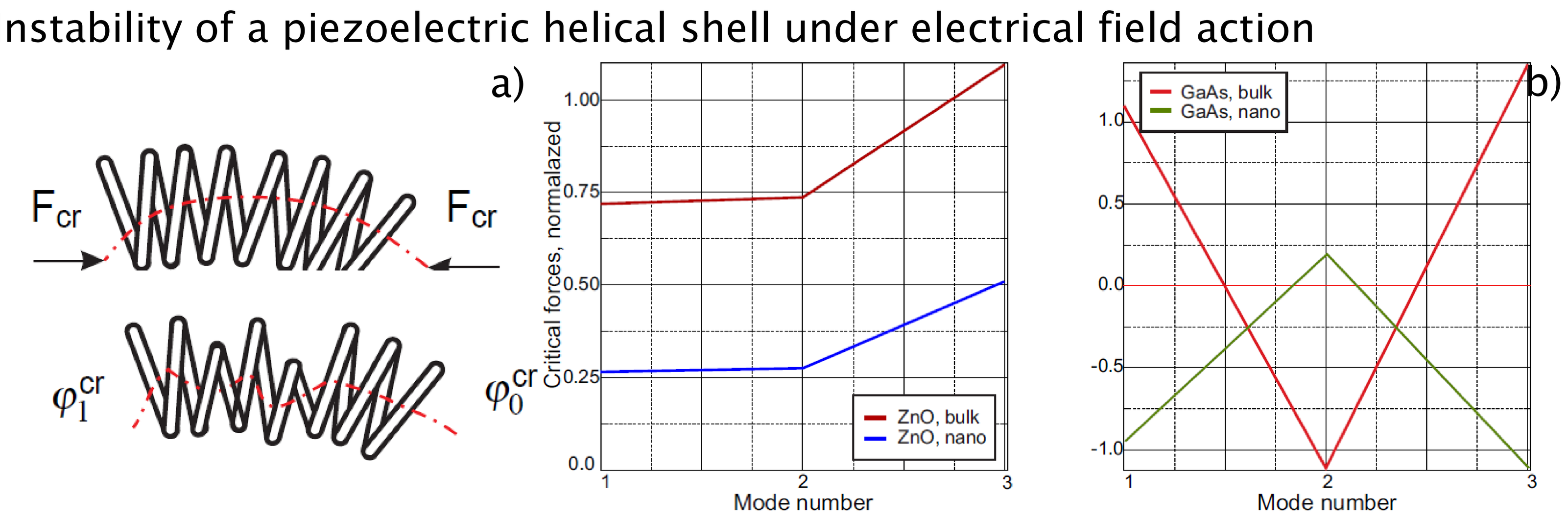


Figure 3. Results of simulation: a) Simplified view of apparent effect by the buckling collapse; b) Influence of the Size Law on the Different Materials

✓Investigation of metamaterials with chiral elements

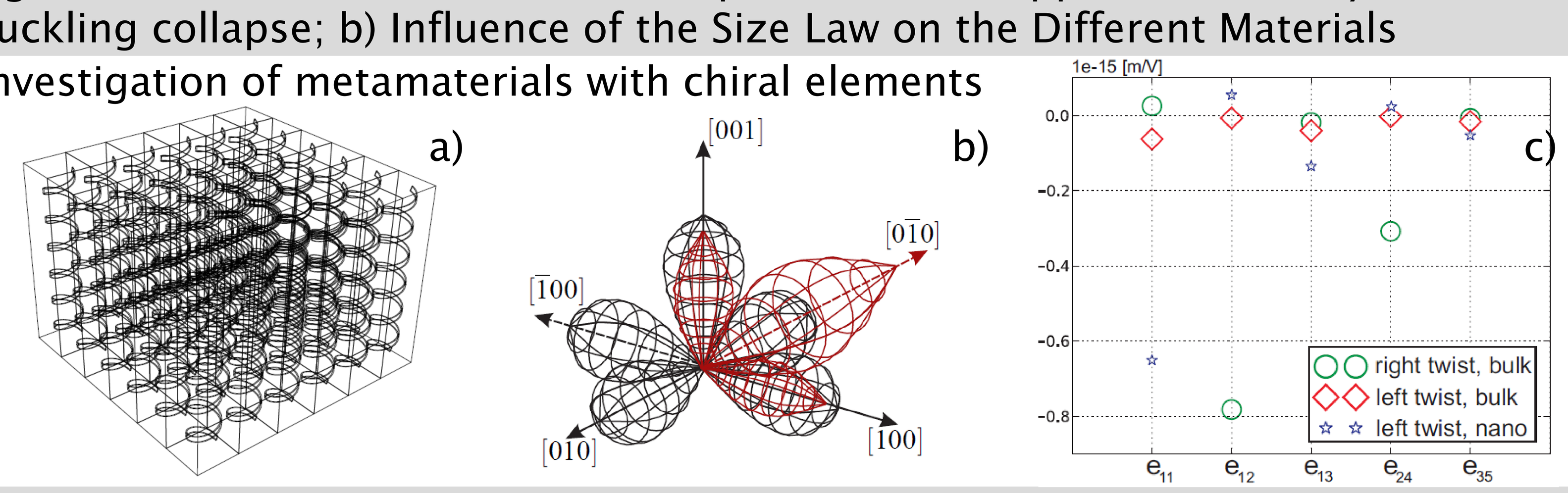


Figure 4. Results of simulation: a) Structure of chiral material; b),c) Piezoelectric modulus distribution by taking into account nanosize effect influence

Analytical Description

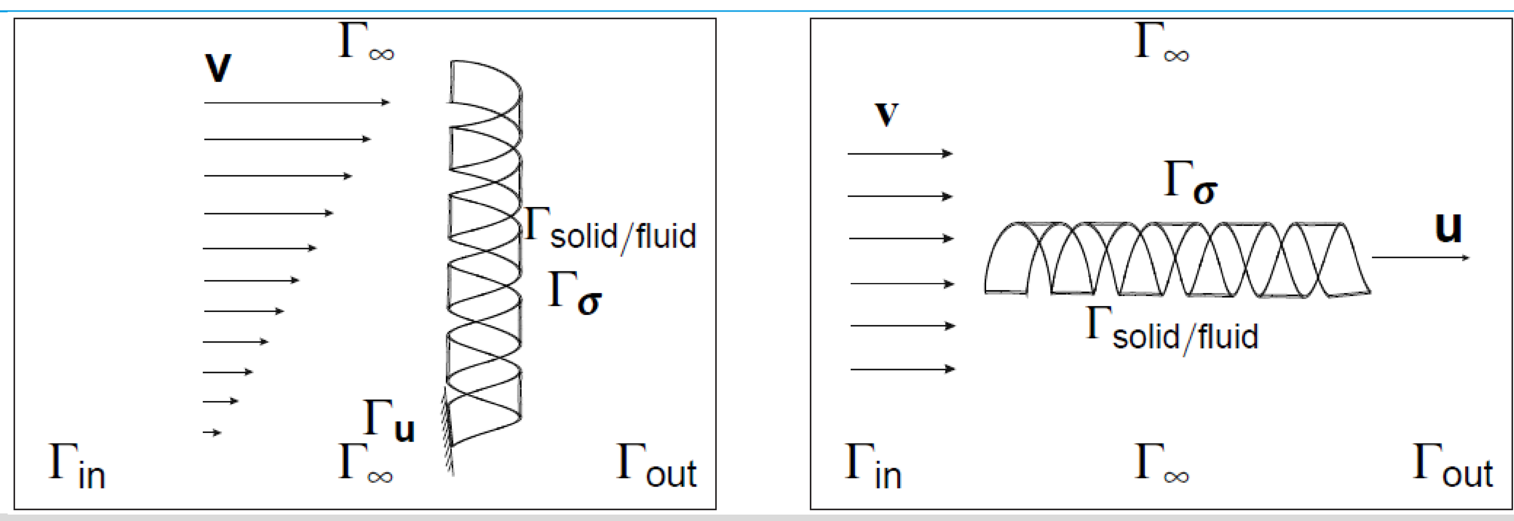


Figure 5. Problem Statement of the Fluid-Structure Interaction Task

✓Electrodynamics

$$\rho \ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{F},\ \nabla \cdot \mathbf{D} = 0,$$

$$\boldsymbol{\sigma} = \mathbf{C} \cdot\cdot\, \boldsymbol{\varepsilon} - \mathbf{e} \cdot \mathbf{E},\ \mathbf{D} = \mathbf{e} \cdot \boldsymbol{\varepsilon} + \mathbf{d} \cdot \mathbf{E},$$

$$\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^\top),\ \mathbf{E} = \nabla \varphi;$$

✓Fluid dynamics

$$\rho_f \left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v}\right] = -\nabla p + \mu \nabla \cdot (\nabla \mathbf{v}) + \nabla \mu \cdot \nabla \mathbf{v} + \mathbf{f}_m$$

Rheological model

$$\mu = k \|\mathbf{J}\|^{\frac{n-1}{2}},\ \boldsymbol{\sigma}_f = -p\mathbf{I} + 2\mu(\mathbf{J})\mathbf{J},\ \mathbf{J} = \tfrac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$$

✓Boundary conditions

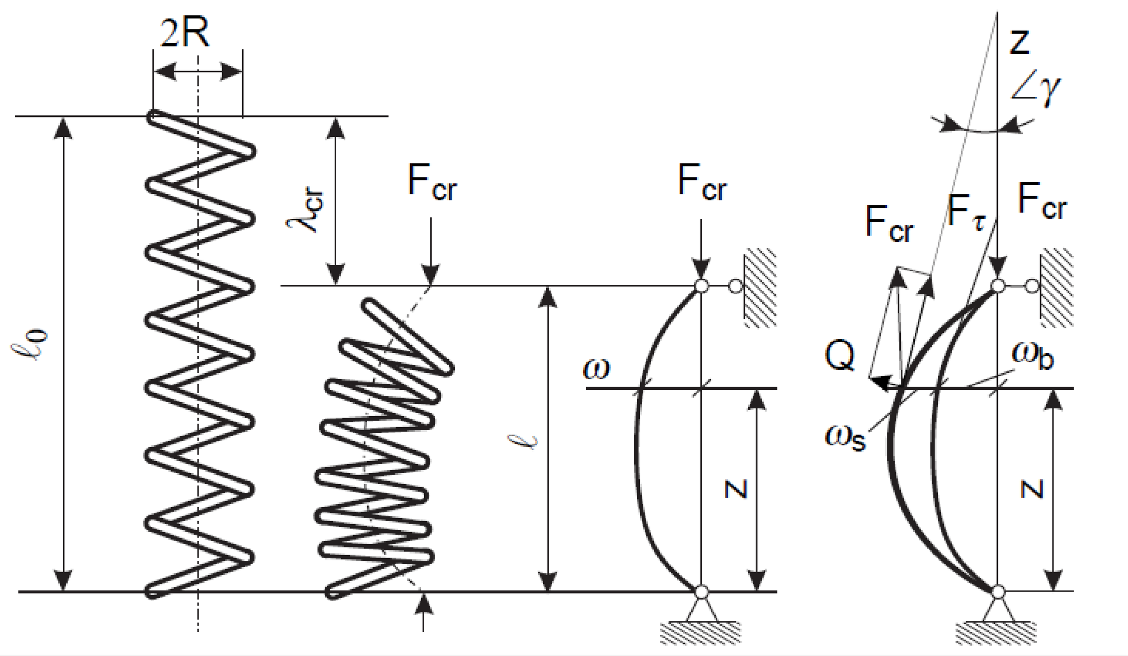
Solid

$$\mathbf{u}|_{\Gamma_\mathbf{u}} = u_0,\ \mathbf{n} \cdot \boldsymbol{\sigma}|_{\Gamma_\sigma} = \mathbf{p}$$
$$\mathbf{n} \cdot \boldsymbol{\sigma}|_{\Gamma_{solid/fluid}} = \mathbf{n} \cdot \boldsymbol{\sigma}_f = \mathbf{F}$$
$$\mathbf{v}|_{\Gamma_{solid/fluid}} = \dot{\mathbf{u}}$$
$$\varphi|_{\Gamma_\varphi^1} = \varphi_1,\ \varphi|_{\Gamma_\varphi^2} = \varphi_2$$
$$-\mathbf{n} \cdot \mathbf{D}|_{\Gamma_q} = q$$

Fluid

$$\mathbf{v_n}|_{\Gamma_\infty} = 0$$
$$\mathbf{v}_\tau|_{\Gamma_\infty} = 0,\ \text{or } \mathbf{v}_\tau|_{\Gamma_\infty} = \mathbf{v}_{wall}$$
$$(\mathbf{v}, \mathbf{n})|_{\Gamma_{in}} = \mathbf{v_n}$$
$$\begin{cases} \nabla(\mathbf{v}, \mathbf{n})|_{\Gamma_{out}} = \mathbf{0}, (\mathbf{v}, \mathbf{n}) \le 0 \\ (\mathbf{v}, \boldsymbol{\tau})|_{\Gamma_{out}} = v_\tau, (\mathbf{v}, \mathbf{n}) > 0 \\ p|_{\Gamma_{out}} = 0 \end{cases}$$

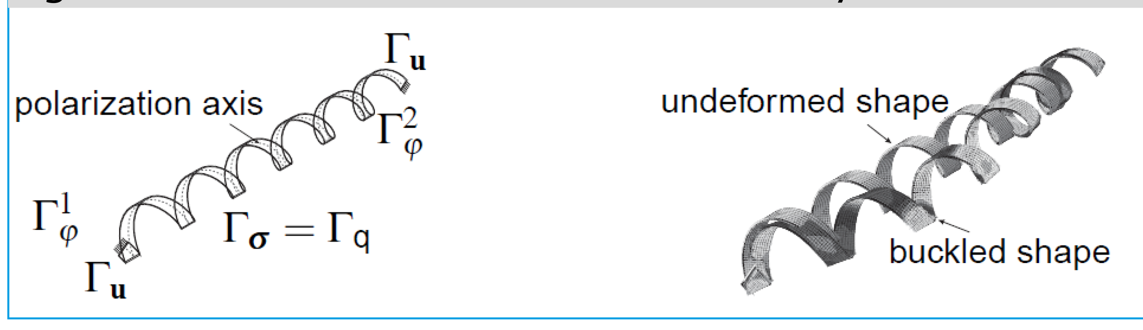
Theoretical approach of investigation buckling collapce for tape helixes



✓Limit value

$$\left(\frac{\ell_0}{2R}\right)_\infty = \sqrt{\pi^2 \frac{2 - C/B_b}{1 + C/B_n}}$$

Figure 6. Mechanical Model of the Stability Loss Problem



✓Buckling possibilities

$$\frac{\ell_0}{2R} \geq \left(\frac{\ell_0}{2R}\right)_\infty$$

Results and Discussion

Done solutions:
✓Interaction of PE shell with environment (offers the possibility of contactless control by IPE)
✓Stability loss problem under influence of electric field (shown, that the buckling under electrical fields cannot be modeled by effective mechanical loads and significant influence of size effect)
✓Investigation of the chiral materials (offers the new possibilities to produce chiral material with desired properties)

Conclusions

The set of the problems solved in the present work, allows to construct a complete model of helical nanostructures and to open new opportunities for their application in practice with development of the modern nanotechnologies.

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