From micro to nano. Problems of modeling of nanoelectromechanical sensors

M A Barulina*, S A Galkina, O V Markelova and O V Golikova

Laboratory of Analysis and Synthesis of Dynamic Systems in Precision Mechanics, Institute of Problems of Precision Mechanics and Control of the Russian Academy of Sciences, ul. Rabochnaya, 24, Saratov, 410028, Russia

*Corresponding author: marina@barulina.ru

Abstract. Microelectromechanical (MEMS) sensors are a class of devices that appeared relatively recently, only 50-60 years ago but are widely used in various fields of science and technology due to such characteristics as small sizes, low power consumption, and sufficient accuracy. The next step in miniaturization led to the creation of nanoelectromechanical sensors (NEMS) – measuring instruments that combine electronic and mechanical components that do not exceed 100 nm in size. On the one hand, the development and manufacture of NEMS require a high level of nanotechnologies. On the other hand, the development and manufacture of NEMS lead to the development of new materials with new effects such as surface and quantum effects. At the same time, the range of tasks that can be solved with using NEMS is quite wide – it’s expecting that the mass implementations of NEMS sensors and devices on their base can significantly improve the quality of people’s life, expand their physical capabilities, or compensate disadvantages. For NEMS, as well as for MEMS, such issues as temperature influence, electronic and mechanical noises, the possibility of chaotic outside signal appearance, and so on are relevant. However, because of the small sizes of NEMS, classical approaches may not be fully applicable to solving these issues. Besides that, during the NEMS design, the bunch of specific problems that not relevant for MEMS has appeared. The article provides a brief review of the state of developments in the area of NEMS sensors and problems that significant for NEMS due to their small size.

1. Introduction

Microelectromechanical (MEMS) sensors have appeared relatively recently and now widely used in various science and applied fields from the military industry to civilian electronics [1-10]. The advantages of MEMS are small size, low power consumption, and sufficient accuracy for non-precision devices. Moreover, some types of electronic devices could not be developed without the use of MEMS devices. These devices include, for example, smartphones, virtual reality helmets, drones, etc. [11,12].

Currently, MEMS sensors and their components are relatively well studied in frames of classical mechanics of deformable bodies, as well as in frames of solid-state physics and with the involvement of such theories as a theory of oscillations, theory of thermoelasticity and thermoelectricity, theory of deterministic chaos, and others [13-18].

One of the directions of MEMS development is the further miniaturization of their components, which led to the emergence of a new class of devices - NEMS. Nanoscales, new materials, and new NEMS sensors assembly capabilities have predetermined a wide range of their possible applications.
In the format of nanosensors sensitive sensors could be created, for example – bio-detectors, chemical sensors, motion sensors, and life parameters sensors, including human activity [19-21]. Thus, prototypes of so-called “wearable” NEMS sensors have already been created, which can, for example, monitor the blood pressure and breathing of a person (Figure 1), measure temperature, determine the movement of an object, etc. [20]. Potential applications of NEMS sensors range from medicine and civilian electronics to the military and space industry. At the same time, it is expected that the mass implementation of NEMS sensors and devices based on them can significantly improve the quality of people’s life and expand their physical capabilities and compensate disadvantages [22-25].

**Figure 1.** Manufacturing process (a) pressure sensor made of carbonized silk nanofiber membrane; demonstration of transparency (b) and flexibility (c) of the sensor; photography of sensor in scale 100 μm (d) and 1 μm (e); heart rate sensor response when installed on the wrist (h) and the neck (i).

NEMS resonators were used to study characteristics of quantum liquid – superfluid helium-4 [26]. For this purpose, rigidly fixed from both ends nanobeams with a width of 200 nm, a thickness of 130 nm, and a length of 30 and 150 microns were used (Figure 2a). The self-frequency of the beams was 11.6 and 1.6 MHz, quality factor $Q > 10^6$. The temperature was from 1K to several parts of K in order to be able to study the various mechanisms of dissipation.

The device is driven by a network analyzer through 80 dB of attenuation distributed over several temperature stages of the cryostat. At the output, two 40-dB low-noise amplifiers are used at room temperature to improve the signal-to-noise ratio.

The performed experiment (Figure 2b) showed an excellent agreement of experiment results and the model that takes into account acoustic emission and interaction with ballistic phonons and rotons at the low temperature. Nanobeams have proven to be a convenient, customizable, and fairly accurate tool for the determination of the environmental properties with high accuracy.
The development and design of NEMS sensors require an interdisciplinary approach, since the classical approaches to studying the dynamics and functioning process that are used in MEMS, can not be applicable for NEMS due to the nanoscales dimensions of their components and ultra-small (to 20-30 nm) gaps between components, which leads to the necessity for accounting, for example, of quantum effects. Therefore, such miniaturization requires a revision of classical theories and the creation of new ones. Thus, also need to understand that NEMS sensors are a very wide class of sensors that differ significantly in size, operating principles, and used materials.

This paper considered NEMS sensors that combine electronic and mechanical components whose dimensions do not exceed 100 nm and the far-reaching range of problems that should be taken into account in their numerical and mathematical models.

2. Dimensional effects and material anisotropy

In works [27-31] was shown that size effects play an important role in microstructures (microbeam, crystals, plates). For example, in [32] was experimentally proved that dimensionless self-frequencies increase about 2.1 times when the beam thickness decrease from 15 to 2.1 microns. A number of papers have been published on the influence of dimensional effects on the dynamics of nanosensor sensing elements [32-36]. The results obtained in these works relate either to beams or to isotropic plates. But in many cases, the performance characteristics of NEMS are affected by anisotropy of its components, which must be taken into account when modeling.

Chen W. J. made a great contribution to the study of anisotropic plates with dimensional effects [37, 38]. In [39], he proposed a new modified theory of stress pairs for anisotropic elasticity, which contains three parameters of the material length scale. The main relations between stresses and deformations, according to this theory, have the form:

\[
\begin{align*}
\sigma_{ij} &= \hat{C}_{ijkl} \varepsilon_{kl} , \\
m_{ij} &= l_i^2 G_i \chi_{ij} + l_j^2 G_j \chi_{ji} , \\
\varepsilon_{ij} &= \frac{1}{2} (u_{ij} + u_{ji}) , \\
\chi_{ij} &= \omega_{i,j} , \\
\omega_i &= \frac{1}{2} e_{ijk} u_{k,j} ,
\end{align*}
\]

where \(l_i\) - size-dependent material parameter; \(\hat{C}_{ijkl}\), \(G_i\) – elastic constants; \(\sigma, \varepsilon\) – stress and strain tensor; \(\chi\) - the curvature tensor (gradient of the rotation); \(m\) - the tensor of moments of the pair of voltages; \(u\) – movements; \(e\) - permutation symbol (Levi-Civita Symbol).
Based on this theory, a size-dependent model of the bending of a composite multilayer Kirchhoff plate was developed [39]. Some simulations result for a free supported multilayer square plate under a cylindrical bending load \( q_0 = 1 \text{N}/(\mu \text{m})^2 \) are shown in Figure 3. The length of each side of the plate is \( L = 200 \mu \text{m} \) and thickness \( h = 25 \mu \text{m} \).

![Figure 3](image-url)

**Figure 3.** Size-depend effects. a - the deflection of the plate \([0, 90, 0]\) at \( y = 0.5L \); b - natural frequency.

In [40] the next step was taken and the equations of motion of NEMS sensing element as an anisotropic rectangular nanoscale plate were constructed. In case of small deformation and when the coordinate system is combined with the median plane of the plate, with the center of coordinate located in the center of the edge, the axis \( x_3 \) is vertically down, these equations have the form:

\[
\begin{align*}
N_{11,1} + N_{12,2} + X_u &= I_0 \ddot{u}_0 + J_1 \ddot{\phi}_1 - c_1 I_3 \ddot{w}_{0,1}, \\
N_{22,2} + N_{12,1} + X_v &= I_0 \ddot{v}_0 + J_1 \ddot{\phi}_2 - c_1 I_3 \ddot{w}_{0,2}, \\
(N_{13} - c_2 R_{13} )_{1} + (N_{23} - c_2 R_{23} )_{2} + c_1 (P_{11,11} + 2P_{12,12} + P_{22,22}) + q + X_w &= I_0 \ddot{w}_0 + c_1 I_3 (\ddot{u}_{0,1} + \ddot{v}_{0,2}) + c_1 J_4 (\ddot{\phi}_{1,1} + \ddot{\phi}_{2,2}) - c_1^2 I_6 (\ddot{w}_{0,12} + \ddot{w}_{0,22}), \\
(M_{11} - c_1 P_{11})_{1} + (M_{12} - c_1 P_{12})_{2} - (N_{13} - c_2 R_{13}) + X_{\phi_1} &= J_1 \ddot{\phi}_1 - c_1 J_4 \ddot{w}_{0,1}, \\
(M_{22} - c_1 P_{22})_{2} + (M_{12} - c_1 P_{12})_{1} - (N_{23} - c_2 R_{23}) + X_{\phi_2} &= J_1 \ddot{\phi}_2 - c_1 J_4 \ddot{w}_{0,2},
\end{align*}
\]

where \( X_u, X_v, X_w, X_{\phi_1}, X_{\phi_2} \) - terms that distinguish the equation obtained in this paper from the “classical” equation of the third-order plate bending theory, for example, in [41].

Equations (2) were obtained using a dynamic version of the virtual displacement principle, a modified theory of paired stresses, and the theory of layered composite plates and shells of the third order.

### 3. The possibility of chaotic movement of the NEMS component.

Another problem that occupies the attention of researchers is the problem of the occurrence of chaotic signals in NEMS sensors [42 - 45]. The probability of occurrence of chaotic signals in NEMS sensors is high due to the significant non-linearity of the system under consideration, for example, due to non-linear relations for determining the physical and mechanical properties of the nano-element manufacturing material, mid-plane stretching, squeezing film damping, and nonlinear coupling between electrostatic force and resonator displacement. This non-linearity can lead to effects such as frequency response bending, jump phenomenon, and chaotic motion [46].

The effect of the deterministic chaos phenomenon can be useful in some cases and can be used for highly sensitive sensors measuring certain parameters [47, 48]. Detecting the changes in the shapes of strange attractors was used to measure experimentally the small variation in the mass of cantilever [49]. The effect of the phenomenon of deterministic chaos can be useful in some cases and can be used for
highly sensitive sensors measuring certain parameters. In most cases, the occurrence of chaotic movements of NEMS components leads to a violation of the functionality of the device.

Thus, at the design stage of the MEMS sensor is necessary to forecast conditions when chaotic movements may occur in the sensor. To now, a large number of papers have been published on this problem and a large number of numerical and semi-analytical methods have been proposed for forecasting the occurrence of chaotic movements in both NEMS and MEMS structures. For modeling the chaotic motion of MEMS and NEMS oscillators, it is most widely used a version of the Mathieu equation and the Melnikov method was used to derive an inequality expression describing the region in the parameter space where the chaos exists [50]. At the same time, experiments have shown that the Melnikov conditions describe quite well the conditions under which MEMS oscillators randomly move [46].

To illustrate the above, consider a doubly clamped nanobeam under electrostatic actuation (Figure 4) [51]. The movable nanobeam is of length $L$, width $b$, and thickness $h$, and is surrounded by a surface layer. Two electrodes are placed on top and underneath of the nanobeam. The initial gap between the nanobeam and the electrodes is $g_0$, and the applied electrostatic voltages through the lower and upper electrodes are denoted by $V_l$ and $V_u$, respectively. The applied voltage via the lower electrode is assumed to be a combination of a DC bias voltage, $V_{DC}$, and an AC voltage with amplitude $V_{AC}$ and frequency $\Omega$, and the voltage applied through the upper electrode is a pure DC load, equal to the DC component of the lower electrode. As illustrated in Figure 4, the $xyz$ inertial coordinate system passes through the neutral axis of the undeformed beam and is located at the left clamped end of the nanobeam. The horizontal and vertical displacements of any material point located on the centroidal axis of the beam in $x$ and $z$-directions are represented by $u(x,t)$ and $w(x,t)$, respectively [51].

![Figure 4. Schematic diagram of a clamped–clamped nanobeam with double-sided electrostatic actuation.](image)

The distributed interatomic forces induce an attractive force between the movable electrode and the two stationary electrodes. Two interaction regimes consist of van der Waals and Casimir forces ($F_{vdW}$ and $F_{cas}$, respectively) can be considered. Expressions for these forces can be formulated as:

$$F_{vdW} = \frac{A_h b}{6\pi} \left( \frac{1}{(g_0 - w(x,t))^3} - \frac{1}{(g_0 + w(x,t))^3} \right),$$

$$F_{cas} = \frac{\pi^2 h c b}{240} \left( \frac{1}{(g_0 - w(x,t))^4} - \frac{1}{(g_0 + w(x,t))^4} \right),$$

where $A_h$ is the Hamaker constant with values in the range of $[0.4 - 4] \times 10^{-19}$ J, $\hbar = 1.055 \times 10^{-34}$ - denotes the Planck’s constant divided by $2\pi$, and $c = 2.998 \times 10^8$ m/s is the speed of light [51].

The distributed electrostatic force can be written as:

$$F_{elec} = \frac{\varepsilon_0 b V_{dc}^2}{2(g_0 - w(x,t))^2} \left( 1 + 0.65 \frac{g_0 - w(x,t)}{b} \right) - \frac{\varepsilon_0 b V_{ac}^2}{2(g_0 + w(x,t))^2} \left( 1 + 0.65 \frac{g_0 + w(x,t)}{b} \right)$$
Taking into account the above expressions for the Van Der Waals forces, Casimir forces, and distributed electrostatic force, in [51] we obtained and investigated the equation of motion for the system under consideration using the principle of virtual displacements and the consistent couple stress theory. The results of the study are shown in Figure 5 and Figure 6 with the following parameters \( \beta_3 = \frac{\varepsilon_0 b l_4 v_{DC}^2}{2 g_0(R)_{eq}} \)

830 and excitation frequency of \( \Omega \), equal 2 or 3, \( R = \frac{V_{AC}}{V_{DC}} \).

![Figure 5. Bifurcation diagram with varying actuation amplitude. (a) – \( \Omega = 2 \) and \( \beta_3 = 830 \); (b) – \( \Omega = 3 \) and \( \beta_3 = 830 \).]

![Figure 6. Poincaré portrait for \( R=0.0125 \). a) – \( \Omega = 2 \) and \( \beta_3 = 830 \); (b) – \( \Omega = 3 \) and \( \beta_3 = 830 \).]

As can be seen from the above figures, the system under consideration becomes dynamically unstable when the excitation frequency or the DC voltage amplitude increases.

4. Quantum effects

NEMS can be components of some quantum device and perform certain functions in it. The range of quantum systems interacting with NEMS includes single-electron transistors, quantum point contacts, trapped ions, quantum dots, electron spins, Bose-Einstein condensates of cold atoms, superconducting structures such as phase, charge, and fluxoid qubits, and microwave planar resonators [52,53].

Besides, when the size of the NEMS sensor component is 30 nm or less, quantum effects begin to appear in full, and the properties of its material, such as electrical conductivity, in this case, will be determined by the quantum mechanical interference of electronic waves. Figure 7 shows the significant effect of Casimir forces on the static deflection of the midline point of the nanobeam [51], discussed in section 3.
In general, quantum effects have such a significant impact on the dynamics of MEMS sensors that highly sensitive NEMS sensors can be constructed on their basis as a principle of operation [54]. Such effects include, for example, the effect of quantum compression. In [54], zero-point displacement uncertainty and quantum squeezing effects in strained multilayer graphene NEMS were investigated as a function of the film dimensions, temperature, applied voltage, and strain applied to the film. And the authors concluded that such an effect can be the basis for creating high-sensitivity graphene-based nano-transducers.

5. Conclusion
The article provides a brief and far from an exhaustive overview of the problems that need to be solved when developing MEMS sensors and creating their digital models. The small size of NEMS does not allow us to consider them as homogeneous solids, since the discrete structure of the material, in this case, can no longer be ignored, so it is necessary to use size-dependent elasticity theories. Also, the nano-size and small distances between the components of the device lead to a significant increase in the influence of quantum effects, which directly affects their performance. The significant non-linearity of the equations describing the dynamics of NEMS determines the possibility of a chaotic signal, which is confirmed by experiments. Combinations of NEMS parameters and operating conditions that are likely to cause chaos should be identified at the NEMS design stage and methods developed to prevent it.

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