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Quantized acoustic-phonon shear horizontal modes in an unbounded hexagonal nitride-based piezoelectric nanostructure

M. Mazouchi[a,*], M. Dutta[a,b], M.A. Stroscio[a,b,c]

[a] *Department of Electrical and Computer Engineering, University of Illinois at Chicago, Chicago 60607, USA*
[b] *Department of Physics, University of Illinois at Chicago, Chicago 60607, USA*
[c] *Department of Bioengineering, University of Illinois at Chicago, Chicago 60607, USA*

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ABSTRACT

For the first time a quantum mechanics based theoretical description of acoustic-phonon shear horizontal modes in a class of piezoelectric media is proposed. The quantized acoustic modes that are needed in the transition from the microscale to the nanoscale are derived for a resonator with geometries of interest in optoelectronics and nanoelectronics. The acoustic-phonon frequency dispersion relations are obtained quantum mechanically for odd and even symmetry shear horizontal modes. It is shown that the derived dispersion relations are identical to the previously reported dispersion relations obtained classically as is expected. For each symmetry, the phonon-mode amplitude is derived in terms of the energy of the quantized vibrational mode, which is of great importance for modelling carrier-acoustic phonon interactions. Moreover, the product of quality factor and frequency ($\boldsymbol{Q}.\boldsymbol{f}$) have been estimated for AlN and GaN resonators by using the anharmonic phonon scattering theory. Furthermore, the electrical surface perturbation in the piezoelectric nanoresonator is studied and the resulting resonance frequency shift is determined.

1. Introduction

During the past decade, the use of nanoelectromechanical systems (NEMS) has been explored extensively for a vast range of applications including high frequency filtering, sensing, wireless components, signal processing and data storage [1–4]. The resonance frequency in mechanical resonators increases as device dimensions shrink from the microscale to the nanoscale due to the reduction of the effective mass [5–7]. In transitioning from microelectromechanical systems (MEMS) to NEMS through shrinking the dimensions of the systems from micrometers down into the nanometer range many advances and interesting applications ranging from quantum measurement to biotechnology can be expected [8]. Recent developments in nanotechnology and MEMS have extended the scope of biomedical applications using NEMS [9]. In general, as the device dimensions shrinking the device physical properties become more susceptible to the external perturbations. This ultrasensitivity of NEMS is offering a wide range of unprecedented functionalities for applications such as a superior methodology for proteomics, mass spectrometry and pressure assisted switches [8,10,11]. This new branch of electronic systems uses the integrated-circuits (ICs) manufacturing methodology to fabricate the fully integrated on-chip, miniature actuators and sensors, with a fast-growing range of applications. From the previous literatures, scaling down from MEMS to NEMS not only enhance the resonance frequency of the system but also it will lead to the lower energy consumption, higher integration densities, and thus much smaller footprint [12].

Thus, to obtain high resonance frequencies of the order of sub-terahertz, minimizing the size of the resonator down to a few nanometers, while maintaining a sufficiently high quality factor of the resonance is required [13].

To design high frequency nanomechanical resonators, it is of great importance to gain an understanding of the phononic behavior of these nanoscale structures, as phonon properties in nanostructures generally differ significantly from those in microstructures.

In particular, acoustic nanoresonators are of significant interest for providing extremely high resonance frequencies while preserving a relatively high resonance quality factor (Q) sufficient for high frequency applications [1,14]. The effect of size reduction when scaling from the microscale to the nanoscale to achieve high resonance frequencies of the order of a terahertz, on the acoustic response of the nanoresonators has attracted considerable attention.

In recent years, enormous advances in nanotechnology have enabled the fabrication of nanostructures and increased the feasibility of acoustic wave confinement [15]. As a result of their smaller dimensions, these structures portend applications at higher frequencies than those for

* Correspondence to: University of Illinois at Chicago, Department of Electrical and Computer Engineering, 851 S Morgan St, Chicago, IL 60607, USA.
E-mail address: mmazou2@uic.edu (M. Mazouchi).

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microscale structures. In addition, nanofabrication offers access to resonant frequencies reaching the sub-terahertz range, which can be used in single-chip or monolithic RF signal processing systems. Despite of these wide applications of acoustic-phonon confinement, only a few analytical attempts have been made to study the properties of confined acoustic phonons in nanoresonators [16–19].

To the best of our knowledge, this paper is the first to report on the quantized acoustic shear horizontal modes that are required in the transition from the microscale to the nanoscale. This paper, for the first time, provides the quantized acoustic shear horizontal (SH) modes for a piezoelectric nanoresonators which is of importance for modelling and understanding charge carrier-acoustic phonon interactions. Due to the piezoelectric coupling, the charge carrier-acoustic phonon interaction has a non-zero contribution from both transverse acoustic (TA) phonons and longitudinal acoustic (LA) phonons [20]. Piezoelectric crystal plates are of significant interest, due to the low required actuation voltages for the excitation and therefore have been studied extensively in the literature [21]. In this study, the theory of the thickness mode piezoelectric nanoresonator is developed by quantizing the general un-quantized classical equations given and used by Auld [22] in microscale application and modified where needed to make the results meaningful and usable on the nanoscale. Shear horizontal mode propagation in an X-cut hexagonal elastic plate is analyzed to provide an analytical solution for general quantized acoustic nanoresonators.

In the following sections, first the formulations for the particle displacement is provided. Then, the Christoffel equations and the SH wave solutions are derived. Then, the elastic continuum mechanics model along with a suitable quantization procedure are used to determine the quantized acoustic-phonon modes of the desired structure. The $Q.f$ product of AlN and GaN are calculated and presented, and finally the electrical surface perturbation in the nanoresonator which has the significant interest for sensing application is studied and the resulting resonance frequency shift, is derived and calculated.

2. Theory and formulation

As depicted in Fig. 1, a piezoelectric X-cut hexagonal plate of a 6 mm crystal of infinite length in a z direction having a small thickness of b in the y direction, with a x-directed infinite width, which has two perfectly conducting electrodes separated from both surfaces of the plate by a small gap of thickness, h, including the coordinate system to be used is considered. The surfaces of the plate are stress free and the plate has a relatively small enough thickness for the quasi-static approximation to be valid. In this problem only the x-polarized particle displacement is considered due to the fact that it is the only component that is electrically coupled to the produced potential [22]. Considering the boundary conditions, the un-quantized acoustic SH displacement wave solutions propagating in the y direction are calculated as [19,22]:

$$U_x = \begin{cases} A_s \cos(ky), & \nu=0,\ 2,\ 4,\ \dots \\ A_s \sin(ky), & \nu=1,\ 3,\ 5,\ \dots \end{cases} \tag{1}$$

where $k = \frac{\nu\pi}{b}$ is the wave vector, and A_s is the unknown wave amplitude.

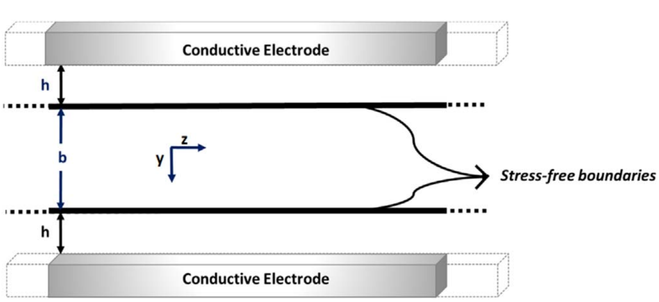

Fig. 1. (Colour online) Infinite piezoelectric X-cut hexagonal crystal (class 6 mm) resonator considered for quantization of acoustic SH modes.

To find the propagation constants and the modal field distributions, the governing equations of the problem along with the associated boundary conditions, based on Auld's [22] notations are formulated as follows:

(i) Maxwell's electromagnetic equations for a lossless medium with no source, where $J_e=0, \rho_e=0$

$$-\nabla \times E = \frac{\partial B}{\partial t}, \tag{2}$$

$$\nabla \times H = \partial D/\partial t, \tag{3}$$

where E is the electric field, B is the magnetic field, H is the magnetic field strength, and D is the electric displacement field;

(ii) Acoustic equations

$$\nabla.\quad T = \frac{\partial P}{\partial t} - F, \tag{4}$$

where T, is the stress tensor field, P is the particle momentum field, and F is the body force distribution;

(iii) Constitutive equations for an anisotropic hexagonal piezoelectric crystal (class 6 mm) [23]

$$B = \mu_0 H, \tag{5}$$

$$D = \epsilon_{xx}^{s} \bullet E + e_{x5} : S, \tag{6}$$

$$T = -e_{x5} \bullet E + c_{44}^{E} : S, \tag{7}$$

where μ_0 is the vacuum magnetic permeability constant, $S=\nabla_s u$ is the strain tensor, $\epsilon_{xx}^{s}, e_{x5}$, and c_{44}^{E} are the dielectric strain constant, piezoelectric stress constant, and elastic stiffness constant under constant electric intensity, respectively. For a piezoelectric medium with no body force sources ($F = 0$), Christoffel equations can be derived by manipulating the governing equations,

$$\nabla.\ c_{44}^{E} : \nabla s.\ U \quad = \rho \frac{\partial^2 U}{\partial t^2} + \nabla.\ e_{x5}.\ E \tag{8}$$

$$-\nabla \times \nabla \times E = \mu_0 \epsilon_{xx}^{s} \left(\frac{\partial^2 E}{\partial t^2} \right) + \mu_0 e_{x5} : \nabla s.\ \frac{\partial^2 U}{\partial t^2} \tag{9}$$

In this problem, in the presence of two conductive electrodes, the elastic stiffness increases from c_{44}^{E} to $\overline{c_{44}} = c_{44}^{E} + \frac{e_{x5}^2}{\epsilon_{xx}^{s}}$, due to the piezoelectric stiffness phenomenon [23,24].

By substituting the quasi-static approximation result, $\nabla \times E=0$, into the Christoffel equations, while considering the source free medium ($\rho_e=0$), where $\nabla.\ D = 0$ in (6), the SH wave solutions within the plate are derived as follows,

$$\varphi_{SH} = \frac{e_{x5}}{\epsilon_{xx}^{s}} U_x \tag{10}$$

$$(T_{xy})_{SH} = -ikA_s \left(c_{44}^{E} + \frac{e_{x5}^2}{\epsilon_{xx}^{s}} \right) e^{-iky} \tag{11}$$

$$(D_y)_{SH} = 0 \tag{12}$$

while the electrostatic wave solutions within the plate, are as follows,

$$\varphi_e = A_e y + B_e, \tag{13}$$

$$(T_{xy})_e = e_{x5} A_e, \tag{14}$$

$$(D_y)_e = -\epsilon_{xx}^{s} A_e, \tag{15}$$

where A_e and B_e are the unknown wave amplitudes.

Outside the plate, where $U = 0$ and $\nabla.\ \nabla.\ \varphi = 0$, the electrical potential solutions are represented by,