Supporting Information

Electric Field Stiffening Effect in C-Oriented Aluminum Nitride Piezoelectric Thin Film

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Mathematical derivation for the electromechanical equivalent model of thin film bulk acoustic resonator

Here we provide an analytical method to calculate the resonance frequency of the nano thin film bulk acoustic resonator. For a piezoelectric material, the constitutive equations for elastic stress T and electric field E (the fourth type of piezoelectric equations) are

$$T_j = c_{ji}^D x_i - h_{mj} D_m \tag{1}$$

$$E_n = -h_{ni} x_i + \beta_{nm}^x D_m \tag{2}$$

where x_i are the components of strain, D_m are the components of electric displacement, c_{ji}^D denote the equivalent stiffness components at constant electric displacement, h_{mj} denote the piezoelectric constants, h_{ni} are the components of transpose of tensor $\boldsymbol{h}$, β_{nm}^x denote the dielectric isolation constants at constant strain. Here i,j=1,2,3,4,5,6 and m,n=1,2,3. When an aluminum nitride piezoelectric thin film vibrates thickness extension mode, there is only strain along thickness direction that needs to be taken into consideration, which means $x_1=x_2=x_4=x_5=x_6=0$, $x_3 \neq 0$. Besides, considering the electric field is parallel to the thickness direction, the electric displacements satisfy: $D_1=D_2=0$, $D_3 \neq 0$. Therefore, the constitutive equations can be simplified to

$$T_3 = c_{33}^D x_3 - h_{33} D_3 \tag{3}$$

$$E_3 = -h_{33} x_3 + \beta_{33}^x D_3 \tag{4}$$

Electrical state

Since there is no free charge in aluminum nitride piezoelectric thin film which indicates $\partial D_3/\partial z=0$ exists. Here z represents the thickness direction of piezoelectric thin film. Considering the definition of strain in the direction of z-axis, i.e., $x_3=\partial\xi/\partial z$, the following formula can be deduced by taking derivatives with z on both sides of Eq. (4)

$$\frac{\partial E_3}{\partial z}=-h_{33}\frac{\partial^2\xi}{\partial z^2} \tag{5}$$

where ξ is the displacement of vibration. Then by setting up an integral over z we obtain

$$E_3=-h_{33}\frac{\partial\xi}{\partial z}+a \tag{6}$$

where a is the constant term produced by the integral. The voltage across the piezoelectric thin film is given by

$$V=\int_0^d E_3 dz \tag{7}$$

where d is the thickness of aluminum nitride piezoelectric thin film. Substituting Eq. (6) into Eq. (7) , the constant term a is calculated by

$$a=\frac{V}{d}-\frac{h_{33}}{d}\left(\xi_1+\xi_2\right) \tag{8}$$

where V is excitation voltage applied on piezoelectric thin film, ξ_1, ξ_2 are the displacement at lower surface (z=0) and upper surface (z=d), respectively. Substituting Eq. (8) into Eq. (6), the electric field can be derived as

$$E_3=-h_{33}\frac{\partial\xi}{\partial z}+\frac{V}{d}-\frac{h_{33}}{d}\left(\xi_1+\xi_2\right) \tag{9}$$

Substituting Eq. (9) into Eq. (4), we obtain the electric displacement

$$D_3=\frac{1}{\beta_{33}^x d}V-\frac{h_{33}}{\beta_{33}^x d}\left(\xi_1+\xi_2\right) \tag{10}$$

Considering the conversion relationships between the several types of piezoelectric constants, i.e. $\beta_{33}^{x}=1/\varepsilon_{33}^{x}$, $h_{33}=e_{33}/\varepsilon_{33}^{x}$, the displacement current in the piezoelectric film can be expressed by

$$I=i\omega D_3 S=i\omega C_0 V-n\left(\dot{\xi}_1+\dot{\xi}_2\right) \tag{11}$$

where ω=2πf is the angular frequency, S is the area of piezoelectric thin film and, $C_0=\left(\varepsilon_{33}^{x}S\right)/d$ is the electrostatic capacitor, $n=h_{33}C_0=e_{33}/\varepsilon_{33}^{x}\cdot C_0$ is the electromechanical transformation factor.

Mechanical state

For thickness extension mode, the vibration equation can be expressed by

$$\rho\frac{\partial^2\xi}{\partial t^2}=\frac{\partial T_3}{\partial z} \tag{12}$$

where ρ and t represent density and time respectively. Substituting Eq. (3) into Eq. (12), we obtain

$$\rho\frac{\partial^2\xi}{\partial t^2}=c_{33}^{D}\frac{\partial^2\xi}{\partial z^2} \tag{13}$$

Let $\upsilon=\sqrt{c_{33}^{D}/\rho}$ representing the acoustic velocity of piezoelectric thin film in the z direction. Eq. (13) can be simplified to

$$\frac{\partial^2\xi}{\partial t^2}=\upsilon^2\frac{\partial^2\xi}{\partial z^2} \tag{14}$$

For a harmonic excitation $\xi(t)=\xi e^{i\omega t}$, Eq. (14) can be deduced to

$$\frac{\partial^2\xi}{\partial z^2}+k^2\xi=0 \tag{15}$$

where $k=\omega/v$ is the wave number, $\omega=2\pi f$ is the angular frequency. The solution of Eq. (4) is

$$\xi=A\sin\left(kz\right)+B\cos\left(kz\right) \tag{16}$$

where A and B are two constant terms produced in solution process. Utilizing boundary conditions: $\xi|_{z=0} = \xi_1$, $\xi|_{z=t_1} = -\xi_2$, we get the expression of displacement

$$\xi = \frac{\xi_1 \sin\left[k\left(d-z\right)\right] - \xi_2 \sin\left(kz\right)}{\sin\left(kd\right)} \tag{17}$$

On the other hand, the force of both surfaces of piezoelectric film should be balanced with external force, that means

$$-F_1 = c_{33}\left(\frac{\partial \xi}{\partial z}\right)\bigg|_{z=0} S - h_{33} D_3 S \tag{18}$$

$$-F_2 = c_{33}\left(\frac{\partial \xi}{\partial z}\right)\bigg|_{z=t_1} S - h_{33} D_3 S \tag{19}$$

From Eq. (4) the following can be deduced

$$h_{33} D_3 S = nV - \frac{n^2}{i\omega C_0}\left(\dot{\xi}_1 + \dot{\xi}_2\right) \tag{20}$$

Substituting Eq. (17) and Eq. (20) into Eq. (18) and Eq. (19), the forces on both surfaces of piezoelectric thin film can be obtained as

$$F_1 = \left(\frac{\rho \upsilon S}{i \sin\left(kd\right)} - \frac{n^2}{i\omega C_0}\right)\left(\dot{\xi}_1 + \dot{\xi}_2\right) + i\rho\upsilon S \tan\left(\frac{kd}{2}\right)\dot{\xi}_1 + nV \tag{21}$$

$$F_2 = \left(\frac{\rho \upsilon S}{i \sin\left(kd\right)} - \frac{n^2}{i\omega C_0}\right)\left(\dot{\xi}_1 + \dot{\xi}_2\right) + i\rho\upsilon S \tan\left(\frac{kd}{2}\right)\dot{\xi}_2 + nV \tag{22}$$

where F_1, F_2, $\dot{\xi}_1$, $\dot{\xi}_2$ are the forces on the surfaces of piezoelectric film and vibration velocities of the surfaces, respectively.

Equivalent electromechanical circuit

Based on Eq. (11), Eq. (21) and Eq. (22), both the electrical state and mechanical state of aluminum nitride piezoelectric thin film can be presented in a single equivalent electromechanical circuit, as shown in Figure S1.

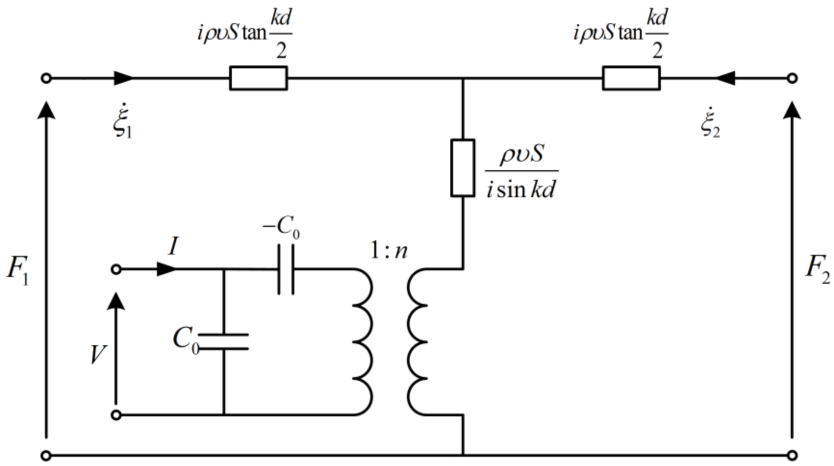

Figure S1. Equivalent electromechanical model for aluminum nitride piezoelectric thin film

For common acoustic layer without piezoelectric effect, the acoustic transmission line model is as depicted in Figure S2.

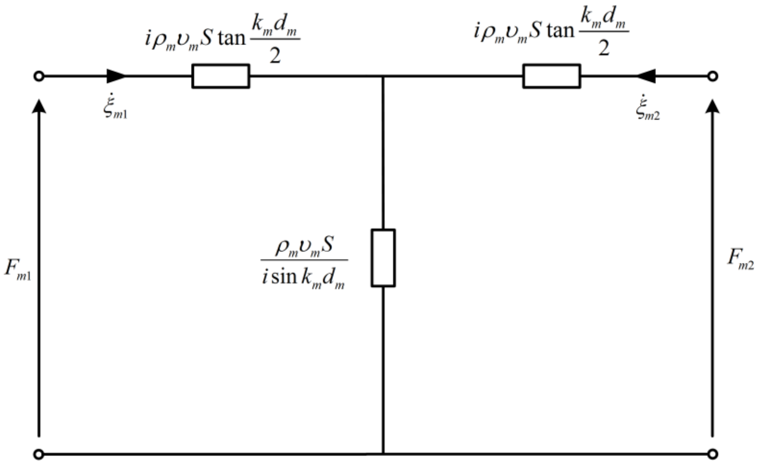

Figure S2. Equivalent model for common acoustic layer

where ρ_m, υ_m, k_m, d_m, F_{m1} and F_{m2} represent density, acoustic velocity, wave number, thickness, the force on upper surface and the force on bottom surface of material 'm', respectively.

In order to simplify the expression, we do the following definition

$$
\begin{cases}
a_m = i\rho_m v_m S \tan\left(\dfrac{k_m d_m}{2}\right) \\
b_m = \dfrac{\rho_m v_m S}{i\sin\left(k_m d_m\right)} \\
v_m = \sqrt{c_m/\rho_m} \\
k_m = \omega/v_m = 2\pi f/v_m
\end{cases}
, m = 1,2,3,4,5 \tag{23}
$$

where the subscript m=1,2,3,4,5 denote Al, AlN, Pt, Ti and SiO_2 respectively, a_m and b_m represent acoustic impedance of each layer, v_m is the acoustic velocity of each layer, k_m is the wave number of each layer.

Therefore, according to transmission line theory, the equivalent electromechanical model for the five-layer nano thin film bulk acoustic resonator can be obtained, as shown in Figure S3.

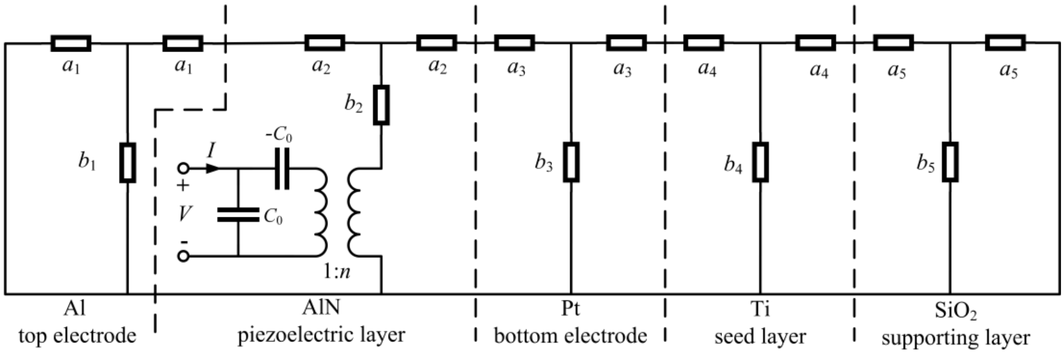

Figure S3 Electromechanical equivalent model for five-layer film bulk acoustic resonator. Here parameters a_m and b_m (m=1,2,3,4,5) represent acoustic impedance of each layer given by Eq. (23).

The flowchart for extraction of equivalent stiffness

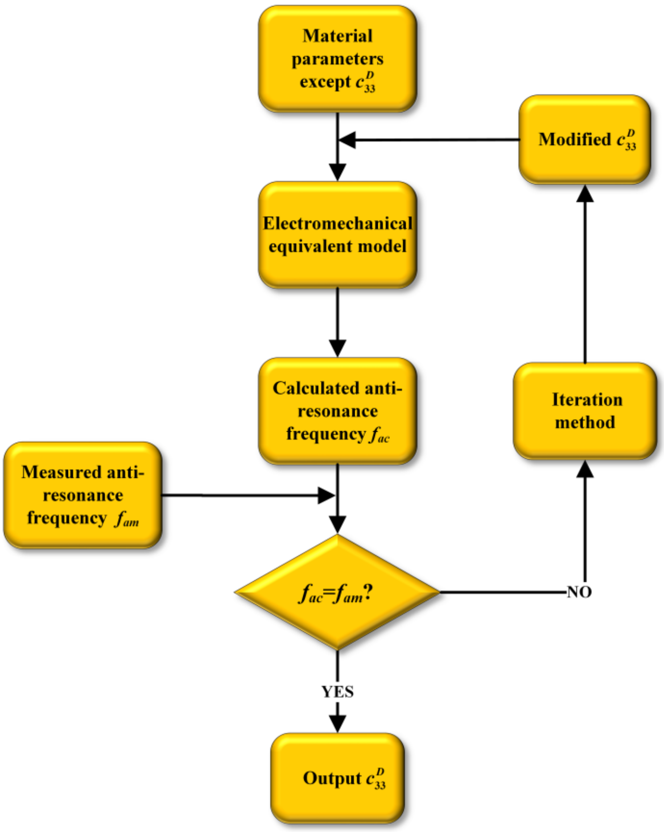

Figure S4. The flowchart for extraction of equivalent stiffness constant in aluminum nitride piezoelectric thin film.

Experimental setup

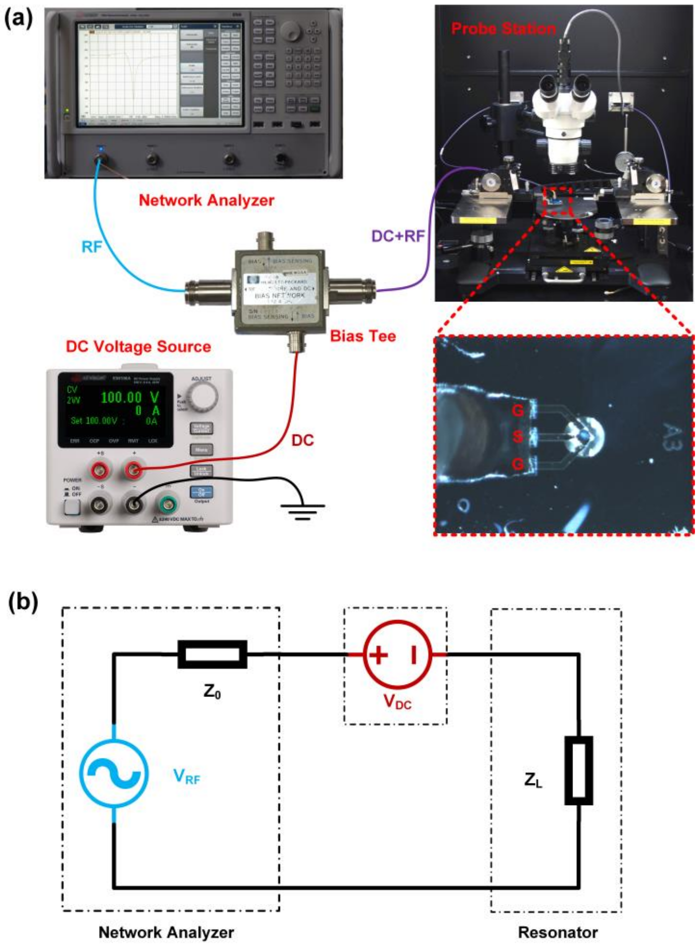

Figure S5. (a)The schematic of experimental setup. (b) The equivalent circuit of experimental setup.