

Piezoelectric Coefficient and Permittivity Changes in Piezoelectric Material ZnO as Functions of Applied Electric Field

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Abstract

The piezoelectric coefficient and permittivity of a piezoelectric material depend on the crystal structure which can be modified by an external electrical field. In this research, we aim to find out a relationship between external electrical field and the piezoelectric and permittivity properties of ZnO. The numerical analysis, finite element analysis, and experimental measurements are to be addressed in this paper. The result of this work can be a good source for the study of piezoelectric material.

1 Introduction

The piezoelectric effect was first discovered by Pierre Curie and Jacques in 1880s [1]. This effect means converting mechanical energy into electrical energy and vice versa. The piezoelectric materials are available in natural form, and can also be artificially synthesized. Quartz, Rochelle salt, and tourmaline are examples of the natural piezoelectric materials. Some piezoelectric materials such as Lead Zirconium Titanate (PZT), Lead Lanthanum Zirconate Titanate (PLZT), Aluminum Nitride (ALN), Polyvinylidene Fluoride (PVDF), and Zinc Oxide (ZnO) belong to man-made piezoelectrical materials [2]. Piezoelectric property is related to the material's non-centrosymmetric crystal structure. The non-centrosymmetric crystal structure of Quartz is shown in Figure 1. The polarization happens when external force is applied on the quartz and at the same an electrical displacement is exhibited within the material [3].

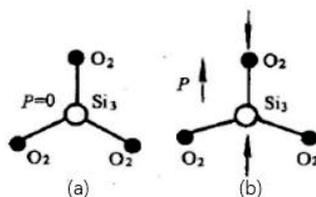


Figure 1 (a) Non-centrosymmetric crystal structure of quartz with no external force, (b) Polarization happens when applying force on the quartz.

Similar to the change when applying force on a piezoelectrical material, when an electrical field is applied on piezoelectrical material, the crystal structure will change as well, which leads to the change of piezoelectrical coefficient and dielectric constant [2]. A reduction of the value of piezoelectric coefficient of PZT was reported when applying DC bias [4]. This is critical for the applications of piezoelectrical material since the piezoelectric coefficient and dielectric constant mainly determine the applicability of a piezoelectric material as an actuator or a sensor. With the variations of piezoelectric coefficient and dielectric constant, the piezoelectric devices are not able to work as expected. ZnO is a very commonly used piezoelectric material for vibration sensing and energy harvesting because it has a high piezoelectric efficiency and that ZnO devices are easy to fabricate [5][6]. However, there is no work shows the characterization of piezoelectric coefficient and dielectric constant under the influence of external electric field. Thus, the piezoelectric coefficient and permittivity of ZnO change as a function of electrical field will be discussed in detail in this paper.

2 Numerical Analysis

Equation (1) gives the relation between internal electric field, electric permittivity, external mechanical stress, piezoelectric charge constant, and electric displacement of a piezoelectric material. D , d , T , ϵ , and E are the electric displacement, piezoelectric constant, external mechanical stress, electrical permittivity, and internal electric field. From the equation, we know that when the piezoelectric material is forced by external mechanical stress, electric displacement is equal to the external mechanical stress times piezoelectric constant plus internal electric field times electric permittivity.

$$D = dT + \epsilon E \quad (1)$$

Equation (2) is a matrix form of equation (1). For the external mechanical stress, we use subscript 1, 2, and 3 to define the directions along X, Y, and Z axis, respectively. Subscript 4, 5, and 6 show the shear directions of X, Y, and Z axis, respectively.

$$\begin{bmatrix} D_1 \\ D_2 \\ D_3 \end{bmatrix} = \begin{bmatrix} d_{11} & \dots & d_{16} \\ \vdots & \ddots & \vdots \\ d_{31} & \dots & d_{36} \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} + \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix} \quad (2)$$

The piezoelectric effect is a reversible process. Equation (3) describes the relation of strain, elastic compliance, stress, piezoelectric constant, and external electrical field. The abbreviation s , S , T , d , and E are the strain, elastic compliance, stress, piezoelectric constant, and external electrical field, respectively.

$$s = ST + dE \quad (3)$$

Equation (4) denotes the matrix form of equation (3).

$$\begin{bmatrix} s_1 \\ s_2 \\ s_3 \\ s_4 \\ s_5 \\ s_6 \end{bmatrix} = \begin{bmatrix} S_{11} & \dots & S_{16} \\ \vdots & \ddots & \vdots \\ S_{61} & \dots & S_{66} \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} + \begin{bmatrix} d_{11} & \dots & d_{31} \\ \vdots & \ddots & \vdots \\ d_{16} & \dots & d_{36} \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix} \quad (4)$$

In order to measure the piezoelectric coefficients d_{33} and d_{31} , this work applies the Capacitance-Voltage (CV) characteristics to extract the piezoelectric coefficients through the change in capacitance. As shown in Figure 2, A is the top and bottom surface area, ΔA is the variation in area, T is the disk thickness, and ΔT is the variation in thickness.

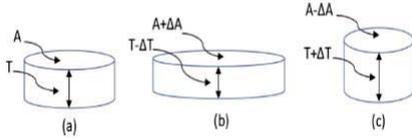


Figure 2 (a) piezoelectric ZnO disk with no bias, (b) piezoelectric ZnO disk with anti-parallel bias, (c) piezoelectric ZnO disk with parallel bias.

The capacitance between the parallel plates can be expressed as:

$$C = \epsilon A / T \quad (5)$$

C , ϵ , A , T are the capacitance, dielectric constant, surface area, and thickness, respectively. Due to the piezoelectric effect, the surface area and thickness of the disk will change which leads to the change of the capacitance. Applying electrical field opposite to the polled field will result in the contraction of the thickness and expansion in the area, hence the capacitance is expressed:

$$C1 = \epsilon(A + \Delta A) / (T - \Delta T) \quad (6)$$

$C1$ is the capacitance when applying electrical field opposite to the polled field. Applying electrical field parallel to the polled field will result in the expansion of the thickness and contraction in the area.

$C2$ is the capacitance when applying electrical field parallel to the polled field.

$$C2 = \epsilon(A - \Delta A) / (T + \Delta T) \quad (7)$$

Dividing (6) over (7), we get:

$$Cr(T - \Delta T) / (T + \Delta T) = (A + \Delta A) \quad (8)$$

Where $Cr = C1 / C2$. Reference [7] gave the solution to this equation as:

$$d_{31} = (-Cr + 1) + \sqrt{Cr^2 + 2.5Cr + 0.5} / E \quad (9)$$

From this equation we know that d_{31} is independent of A and T . To calculate d_{31} , all we need to do is to measure the capacitance change ratio Cr and the external electric field.

The above numerical model ignores the change of dielectric constant which is very small. We will conduct experiment to measure the dielectric constant first and then determine what equations can be applied.

3 Simulation and Experimental Measurements

We will conduct the measurements following the above CV measurement method and use finite element analysis tool, COMSOL simulator, to verify the results. The difference between the experiment and simulation results may be caused by the temperature, sample size, and degree of polarization of ZnO.

4 Results and Discussion

We will present analysis, measurement, and simulation results and draw our conclusions in the final version and at the Symposium presentation.

5 Conclusion

Analysis and simulation of piezoelectric shows that applying electric field to the material has the effect of changing its permittivity and the piezoelectric coefficient. These result from changes in the crystal structure as a result of applying the electric field. Measurements will verify the simulated results. Applications of these properties lead to controlled low-loss phase-shifting of RF signals propagating across the piezoelectric material. The resulting phase shifts are frequency dependent according to the permittivity changes.

6 Acknowledgement

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7 References

- [1] R. Hinchet, U. Khan, C. Falconi, and S.-W. Kim, "Piezoelectric properties in two-dimensional materials: Simulations and experiments," *Materials Today*, vol. 21, no. 6, pp. 611–630, 2018.
- [2] Sukesha, R. Vig, and N. Kumar, "Effect of Electric Field and Temperature on Dielectric Constant and Piezoelectric Coefficient of Piezoelectric Materials: A Review," *Integrated Ferroelectrics*, vol. 167, no. 1, pp. 154–175, 2015.
- [3] Y. Zhou, "Design and Simulation of SAW-Driven Drug Delivery Device." Order No. 28086984, The George Washington University, Ann Arbor, 2020.
- [4] J. Masys, W. Ren, G. Yang, and B. K. Mukherjee, "Piezoelectric strain in lead zirconate titanate ceramics as a function of electric field, frequency, and dc bias," *Journal of Applied Physics*, vol. 94, no. 2, pp. 1155–1162, 2003.
- [5] S. Joshi, M. M. Nayak, and K. Rajanna, "Evaluation of Transverse Piezoelectric Coefficient of ZnO Thin Films Deposited on Different Flexible Substrates: A Comparative Study on the Vibration Sensing Performance," *ACS Applied Materials & Interfaces*, vol. 6, no. 10, pp. 7108–7116, 2014.
- [6] Q. Shi, T. Wang, and C. Lee, "MEMS Based Broadband Piezoelectric Ultrasonic Energy Harvester (PUEH) for Enabling Self-Powered Implantable Biomedical Devices," *Scientific Reports*, vol. 6, no. 1, 2016.
- [7] M. A. Ahmad and A. Allataifeh, "Electrical extraction of piezoelectric constants," *Heliyon*, vol. 4, no. 11, 2018.

[4]

[5]