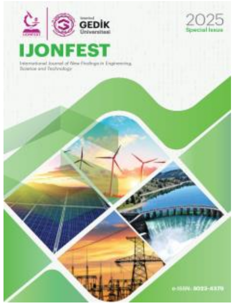
December 2025, Special Issue

International Journal of New Findings in Engineering, Science and Technology

journal homepage: *https://ijonfest.gedik.edu.tr/*



Received:04.07.2025 Accepted:18.07.2025 Published:31.12.2025

Multiphysics Simulation-Based Evaluation of Piezoelectric Materials Using COMSOL: A Study on Stress and Displacement Behaviors

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Abstract

In this study, the performance of piezoelectric materials—Polyvinylidene Fluoride (PVDF), Barium Titanate ($BaTiO_3$), and Zinc Oxide (ZnO)—was investigated through numerical simulations using the COMSOL Multiphysics environment. The aim was to analyze the stress distribution and volumetric displacement behavior of these materials under varying mechanical loads (3,000 Pa, 5,000 Pa, and 10,000 Pa) and electrical potentials (5–25 V) to determine their suitability for flexible sensor applications. PVDF, due to its polymeric and flexible nature, exhibited low stress accumulation but high displacement, making it ideal for large-deformation applications such as wearable electronics. $BaTiO_3$ demonstrated a balanced response with moderate deformation and stress, positioning it as a suitable candidate for hybrid actuator-sensor systems. ZnO, characterized by its rigid crystalline structure, showed the highest stress concentration with minimal deformation, proving its effectiveness in stress-based micro-scale sensors. The simulations confirmed that material selection for piezoelectric systems should be made not solely based on piezoelectric coefficients, but also on comprehensive electromechanical behavior under applied loads. These findings contribute to the design of next-generation smart sensors, energy harvesters, and micro-electromechanical systems (MEMS) by providing comparative insights into the material-specific responses in multiphysical environments.

Keywords: MEMS, Piezoelectric materials, Finite element methods, COMSOL.

1. INTRODUCTION

Energy is not only essential for the continuation of individual life but also plays a critical role in ensuring the sustainability of all industrial processes. The increasing global energy consumption contributes significantly to environmental degradation and climate change, thereby intensifying the interest in renewable and environmentally friendly energy conversion technologies [1]. In this context, the development of alternative energy generation methods capable of meeting the energy demands of low-power electronic devices has become one of the key scientific and technological objectives of our time [2]. In line with this objective, piezoelectric energy harvesting emerges as an effective and sustainable method for directly converting mechanical energy into electrical energy. The piezoelectric effect is based on the principle that applied mechanical stress induces electrical polarization within a material, resulting in an electric potential difference between its two ends [3]. This generated potential is directly proportional to the magnitude of the applied stress. Piezoelectric materials have the capability to generate electricity under physical influences such as pressure, bending, and vibration, without the need for external electrical or magnetic fields [4]. These materials play a critical role in sensor technologies, including pressure sensors, accelerometers, and ultrasonic sensors. Such sensors utilize the piezoelectric effect to convert mechanical energy into electrical signals for the measurement of various physical quantities. This characteristic provides a significant advantage, particularly in applications that require autonomous energy supply, such as wireless sensor networks, wearable systems, and biomedical devices [2], [5-6] .

Among conventional piezoelectric materials, ceramics such as lead zirconate titanate (PZT), barium titanate ($BaTiO_3$), and zinc oxide (ZnO) exhibit high piezoelectric coefficients; however, their rigid and brittle nature limits their applicability in flexible systems. Furthermore, the potential toxic effects of lead-containing materials on the environment and living organisms have raised significant concerns regarding their safety and sustainability. Because of these limitations, piezoelectric polymer materials have emerged as a promising alternative. Organic piezoelectric polymers such as polyvinylidene fluoride (PVDF) are particularly noteworthy due to their advantages including flexibility, light weight, biocompatibility, and high processability. In particular, the

https://doi.org/10.61150/ijonfest.2025030307

β-phase of PVDF exhibits strong piezoelectric performance as a result of its highly oriented crystalline structure, which enables the generation of significant electrical polarization [5], [7]. Additionally, the copolymer P(VDF-TrFE) and hydrogels are widely utilized in various flexible sensor applications owing to their superior physical and chemical properties [2], [8]. Piezoelectric sensors developed for flexible electronic systems serve the function of converting mechanical stimuli from the external environment into electrical signals. These sensors are generally classified into four main categories based on their sensing mechanisms: piezoresistive, capacitive, triboelectric, and piezoelectric. Modern advanced wearable electronic systems require technical features such as high integration, miniaturized structure, and low power consumption [9]. However, piezoresistive and capacitive sensors often fall short of meeting these demands due to their need for external power sources and limited flexibility [10-11]. At this point, piezoelectric sensors stand out as promising solutions for flexible electronics thanks to their superior characteristics, including high power density, high energy conversion efficiency, ultra-thin structures, high sensitivity, rapid response time, stable electrical output, and low susceptibility to electromagnetic interference. Moreover, the performance of polymer-based piezoelectric materials can be significantly enhanced through the incorporation of fillers (e.g., $BaTiO_3$ nanoparticles, carbon nanotubes) and structural modifications. These strategies effectively improve the sensitivity, stability, and applicability of flexible sensors.

The literature reports the widespread use of polymer-based piezoelectric materials such as polyvinylidene fluoride (PVDF) and polydimethylsiloxane (PDMS) in a variety of design and application fields, including C for COVID-19 patients [24], the development of nanotechnological devices [25], and tactile sensor applications [26]. Today, technological advancements are rapidly progressing, particularly toward the miniaturization of electronic systems, which has led to significant breakthroughs in the field of micro- and nano-electromechanical systems (MEMS and NEMS) [12]. It is well known that at these scales, material behavior becomes size-dependent. However, the piezoelectric effect is a linear electromechanical phenomenon and remains independent of size effects. Nevertheless, since only dielectric materials with specific asymmetric crystal structures exhibit piezoelectric properties, the application of this phenomenon in miniaturized systems such as MEMS and NEMS remains limited.

COMSOL Multiphysics is a reliable finite element analysis (FEA) tool developed for multidisciplinary scientific research and incorporates a wide range of multiphysics modules within a comprehensive simulation platform [13]. Due to its flexible modeling infrastructure tailored to various engineering and physical systems, it is widely used, especially in piezoelectric-based applications. In systems involving micro- and nanotechnology, finite element analysis becomes a critical step before proceeding to the production phase. The simulation capabilities offered by COMSOL Multiphysics play a crucial role in the digital modeling of smart sensor system infrastructures. Within the scope of this study, a piezoelectric sensor structure was developed and modeled using various piezoelectric materials, including PVDF, $BaTiO_3$, and ZnO. The relationship between the applied force and the output voltage was examined in detail through comprehensive analysis. The findings obtained from this study provide a significant foundation for the design and development of future smart systems.

2. EXPERIMENTAL SECTION

2.1 Piezoelectric pressure sensor structure

The literature review indicates that a variety of geometries and materials have been employed in the design of piezoelectric pressure sensors. In this study, an analytical investigation was conducted for three different piezoelectric materials, Barium Titanate ($BaTiO_3$), Polyvinylidene Fluoride (PVDF), and Zinc Oxide (ZnO), under varying electrical potentials (5–25 V) and external mechanical loads (3,000, 5,000, and 10,000 Pa). The structural design, illustrated in Fig. 1, and the resulting voltage responses induced by mechanical stress were simulated and analyzed using the COMSOL Multiphysics environment.

The model geometry designed for this study consists of a membrane structure with a thickness of 2 μm and a length of 1 mm, as shown in Figure 1. Along the edges of the main membrane, there is a fixed support region with a width of 0.1 mm. The model geometry is illustrated below.

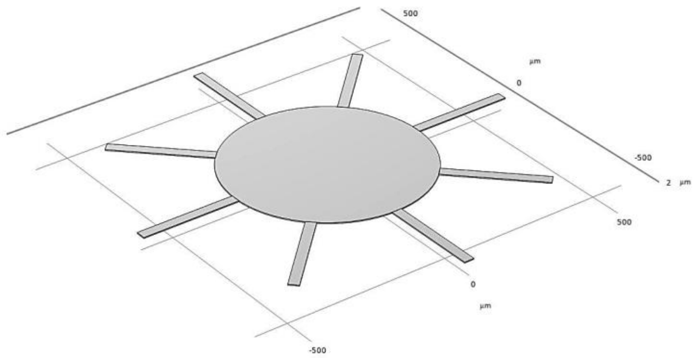

Figure 1. Geometric figure of simulated piezoelectric structure.

2.2 Stress Simulation of Pressure Sensors Using COMSOL Multiphysics

All simulations were designed to include stress and surface deformation. ZnO, $BaTiO_3$, and PVDF materials were evaluated individually under identical conditions. All the analyzed cases are illustrated in the fig.2 fig.3 and fig.4.

Under an applied mechanical load of 10,000 Pa, all three piezoelectric materials exhibited distinct stress distribution behaviors that are closely related to their mechanical properties, particularly stiffness and elasticity.ZnO, known for its high elastic modulus and rigid crystalline structure, demonstrated the highest Von Mises stress concentration among the three materials. The stress was strongly localized near the fixed edges of the membrane structure, with minimal deformation observed throughout the remaining surface. This stress accumulation is indicative of ZnO's inability to dissipate mechanical energy through deformation, instead concentrating it in confined areas. Such behavior is consistent with the expected performance of rigid piezoelectric ceramics and supports its suitability for stress-based sensing applications where high sensitivity is required. $BaTiO_3$, exhibiting intermediate stiffness, responded to the 10,000 Pa load with a more balanced stress distribution. The Von Mises stress was evident near the fixed boundaries but also extended along the mid-section of the cantilever structure. This reflects $BaTiO_3$'s capacity to partially absorb mechanical load via elastic deformation while still maintaining regions of measurable stress concentration. This balance makes it particularly advantageous in hybrid piezoelectric devices that require both mechanical resilience and moderate sensitivity.

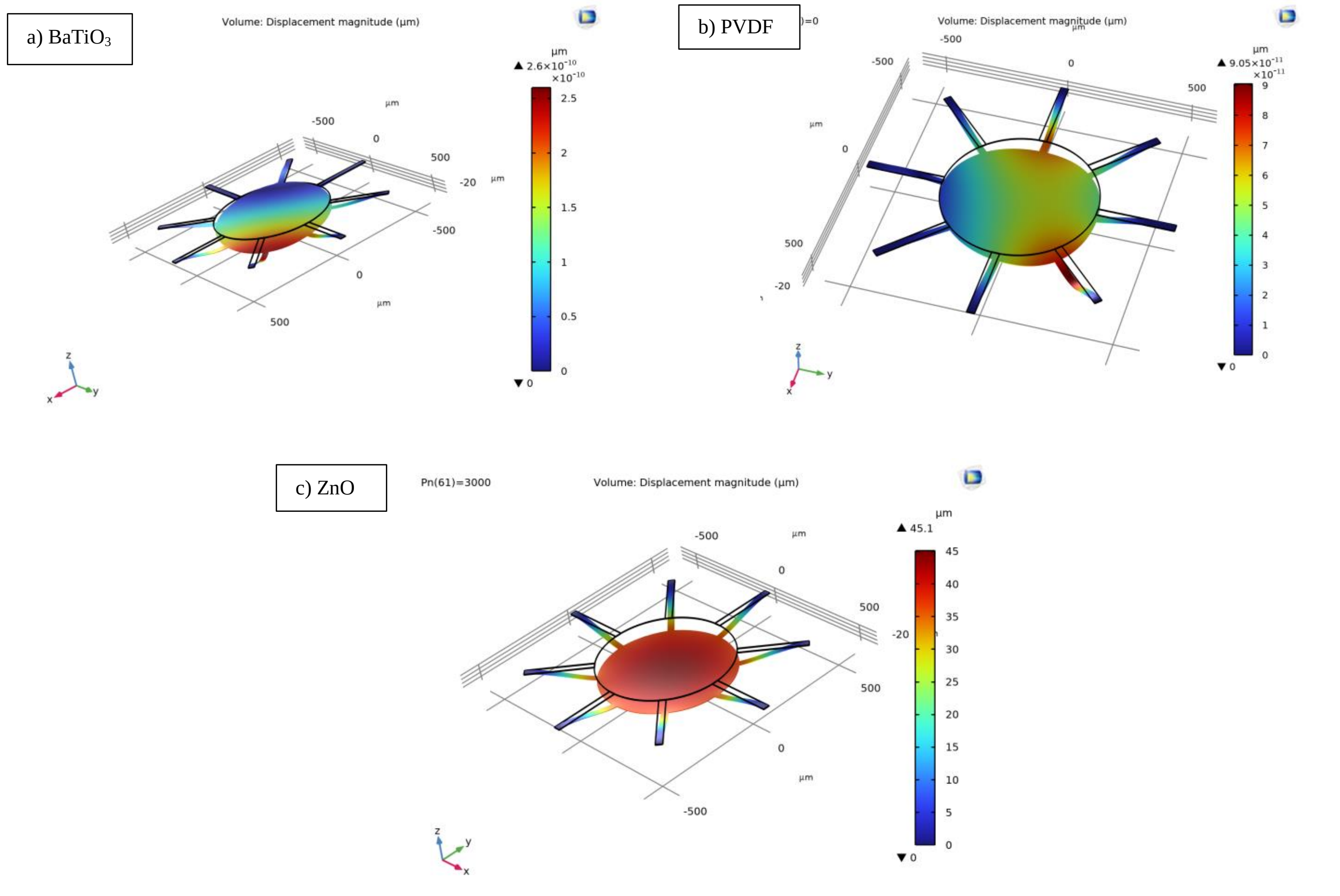

Figure 2. Stress Distribution Analysis of a) $BaTiO_3$, b) PVDF, and c) ZnO under 10,000 Pa mechanical load.

PVDF, as a highly flexible and polymeric material, showed the lowest stress magnitudes under the same loading condition. The stress distribution was diffuse and lacked distinct concentration zones, indicating that PVDF primarily absorbed the applied load through global deformation rather than localized internal stress. This characteristic limits its effectiveness in stress measurement or localization but highlights its potential in applications prioritizing large-scale deformation, such as wearable sensors or low-force actuation systems.

Simulations conducted under a mechanical load of 5,000 Pa revealed that the stress responses of the three piezoelectric materials (ZnO, $BaTiO_3$, and PVDF) differed significantly based on their elastic modulus and structural characteristics.

ZnO, despite its rigid structure, exhibited pronounced Von Mises stress concentrations along the fixed edges and support surfaces. The stress was especially evident in boundary regions and at the junctions between the main membrane and the support arms. This indicates that ZnO accumulates high mechanical stress with minimal deformation, reflecting its ability to respond stably under load despite limited displacement. Such behavior supports its suitability for micro-scale stress sensing applications that require mechanical sensitivity.

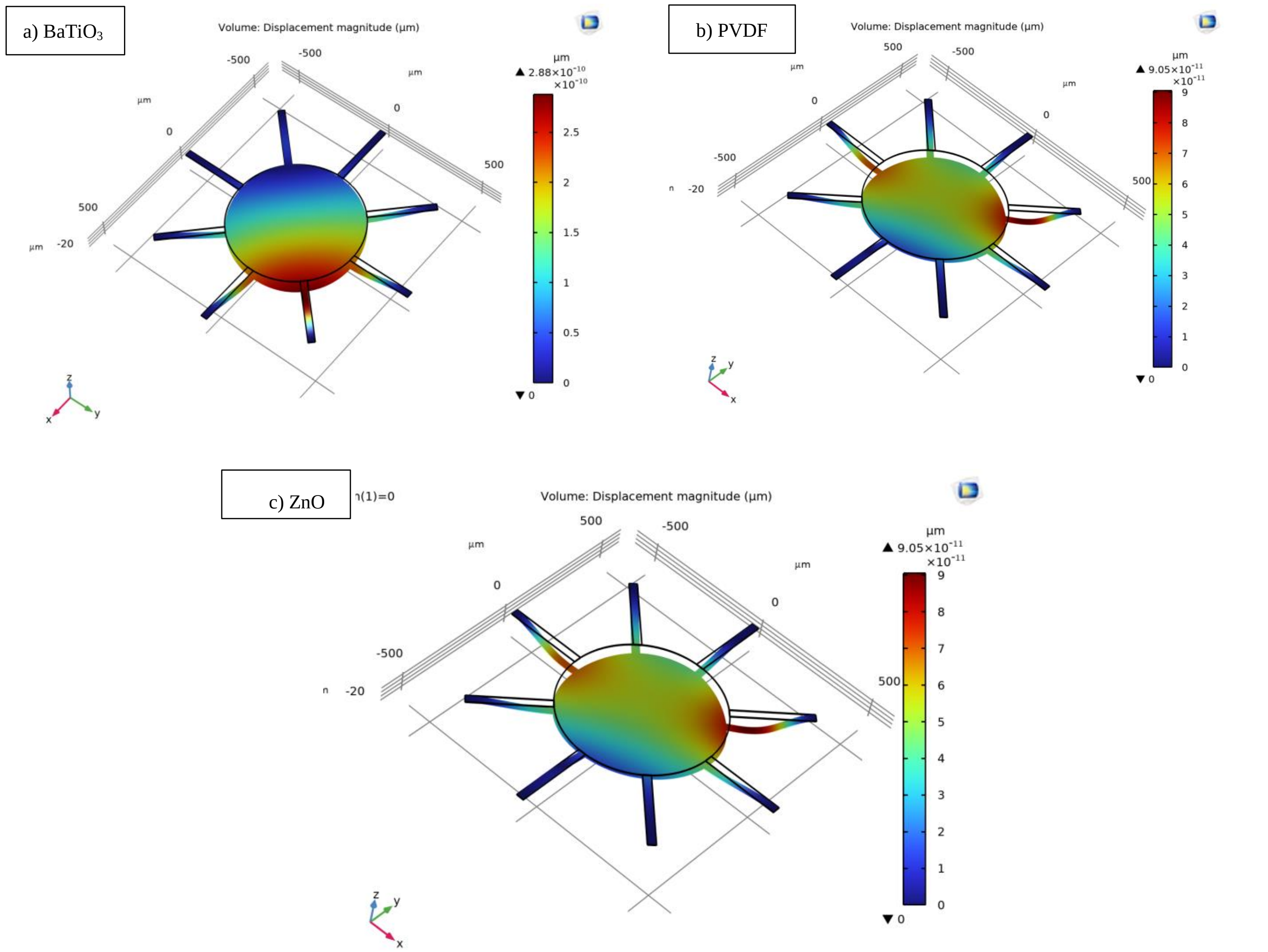

Figure 3. Stress Distribution Analysis of a) $BaTiO_3$, b) PVDF, and c) ZnO under 5000 Pa mechanical load.

$BaTiO_3$ displayed a more balanced and widespread stress distribution under the same loading conditions. Stress levels were evident both at the edges and at the transition points where structural extensions join the central body. As the applied load increased, the stress response scaled proportionally, indicating a stable elastic behavior. $BaTiO_3$'s mechanical characteristics position it as a versatile material for dual-purpose applications involving both actuation and sensing functions.

PVDF, due to its low elastic modulus, absorbed much of the applied load through deformation, resulting in the lowest stress levels among the three materials. The Von Mises stress under 5,000 Pa was distributed uniformly across the surface, without any sharply defined stress concentrations. This behavior highlights PVDF's capacity for large-scale deformation while indicating limited suitability for applications requiring localized stress detection.

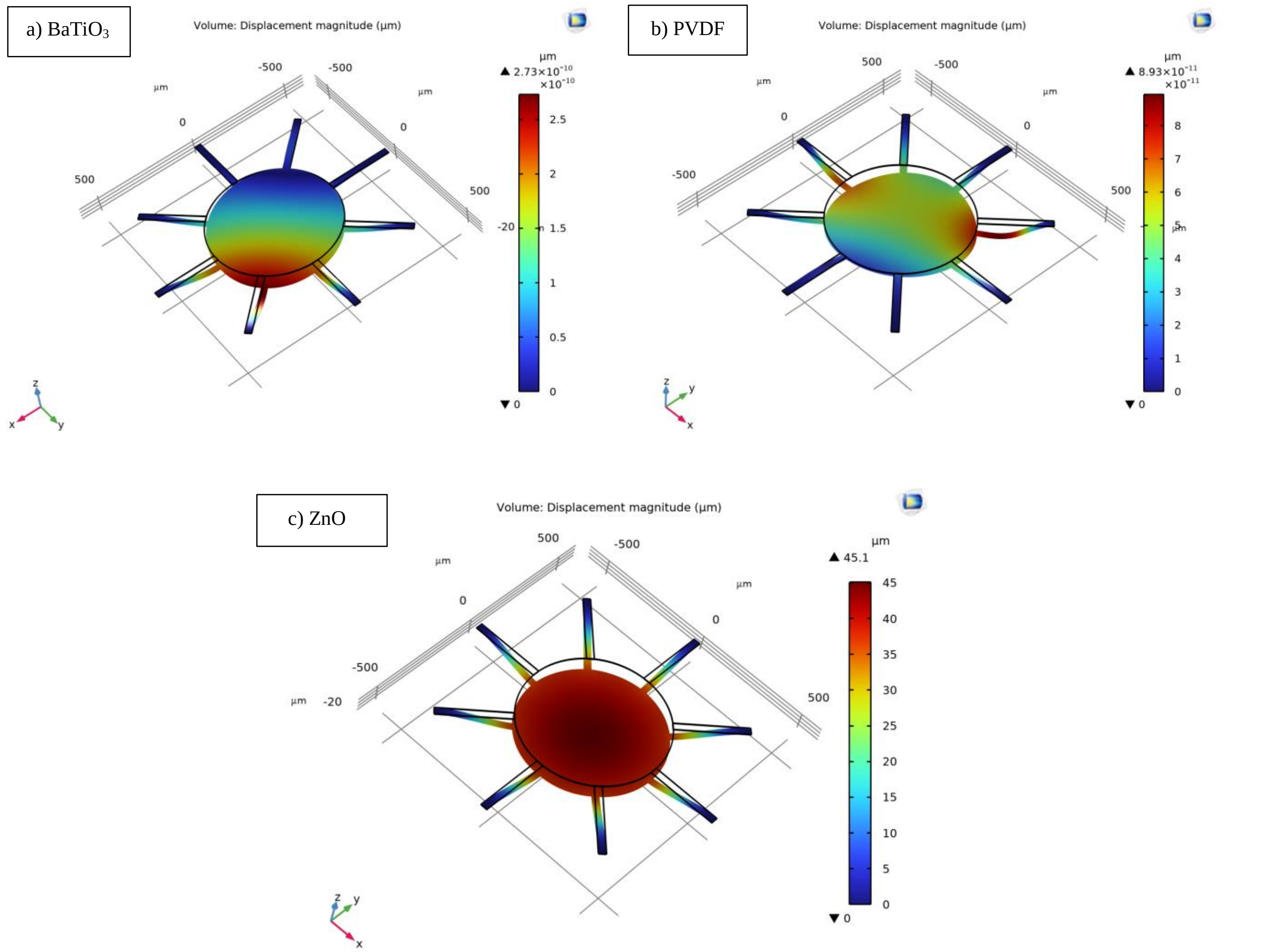

Figure 4. Stress Distribution Analysis of a) $BaTiO_3$, b) PVDF, and c) ZnO Under 3000 Pa mechanical load.

Under a mechanical load of 3000 Pa, the $BaTiO_3$ material generated a noticeable yet broadly distributed Von Mises stress, with moderate accumulation particularly observed along the fixed edge regions. In contrast, ZnO exhibited sharper and more localized stress concentrations under the same load, while PVDF showed almost no significant stress formation, as the load was absorbed through deformation. At this level, $BaTiO_3$ demonstrated both the ability to detect mechanical loading and to maintain controlled structural deformation.

The analyses revealed that the applied mechanical load (3000Pa, 5000Pa, 10000Pa) generally induced a limited level of deformation in the piezoelectric materials. PVDF, due to its flexible structure, exhibited a measurable albeit very small deformation even under low loading conditions. ZnO, despite its rigid crystalline structure, showed low-amplitude yet clearly observable deformation solely under mechanical stress. This behavior indicates that ZnO, while structurally rigid, is responsive to mechanical excitation and may be considered suitable for load-based micro-sensitivity applications. $BaTiO_3$, being neither as rigid as ZnO nor as flexible as PVDF, exhibited minimal deformation under load, reflecting a balanced mechanical response.

2.3 Electric potential-Displacement Simulation of Pressure Sensors Using COMSOL Multiphysics

The relationship between applied electric potential and resulting volumetric displacement was systematically analyzed for all three piezoelectric materials—$BaTiO_3$, PVDF, and ZnO—under mechanical load conditions of 3,000 Pa, 5,000 Pa, and 10,000 Pa. The aim was to evaluate the extent to which external mechanical stress influences the electromechanical deformation behavior of each material, as well as to determine their sensitivity under varying electric field intensities.

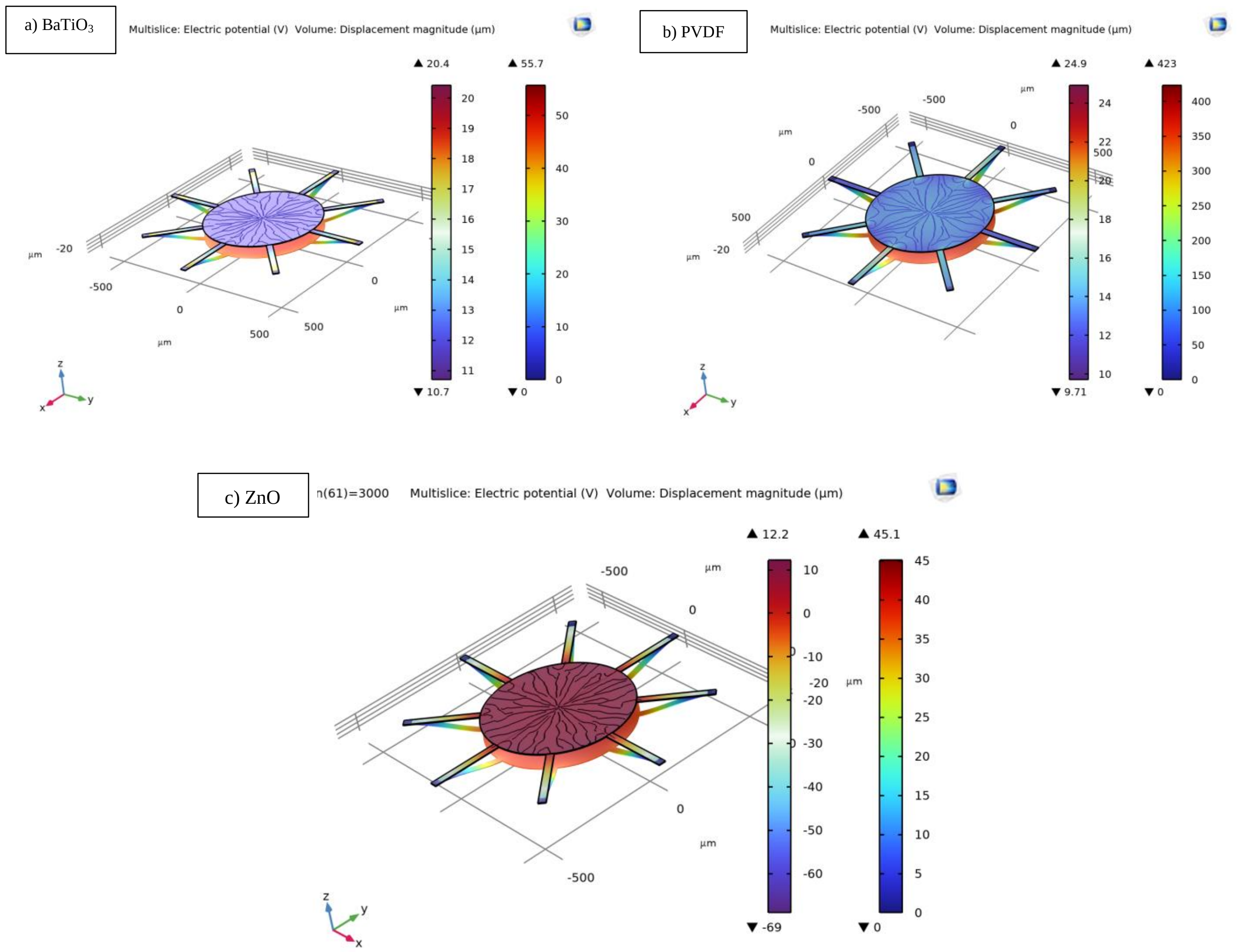

Figure 5. Volumetric Displacement Analysis of a) $BaTiO_3$, b) PVDF, and c) ZnO Under 10000 Pa mechanical load.

Under the highest mechanical loading condition, all three materials showed saturation tendencies in displacement beyond 20 V. PVDF’s response became nonlinear, with deformation rates tapering off, likely due to material softening under high combined electro-mechanical loading. $BaTiO_3$ continued to display a consistent displacement profile, maintaining its structural balance and sensitivity. ZnO's displacement remained the lowest, yet it demonstrated a clear voltage-dependent trend, reinforcing its reliability in systems requiring precision displacement control rather than large deflections.

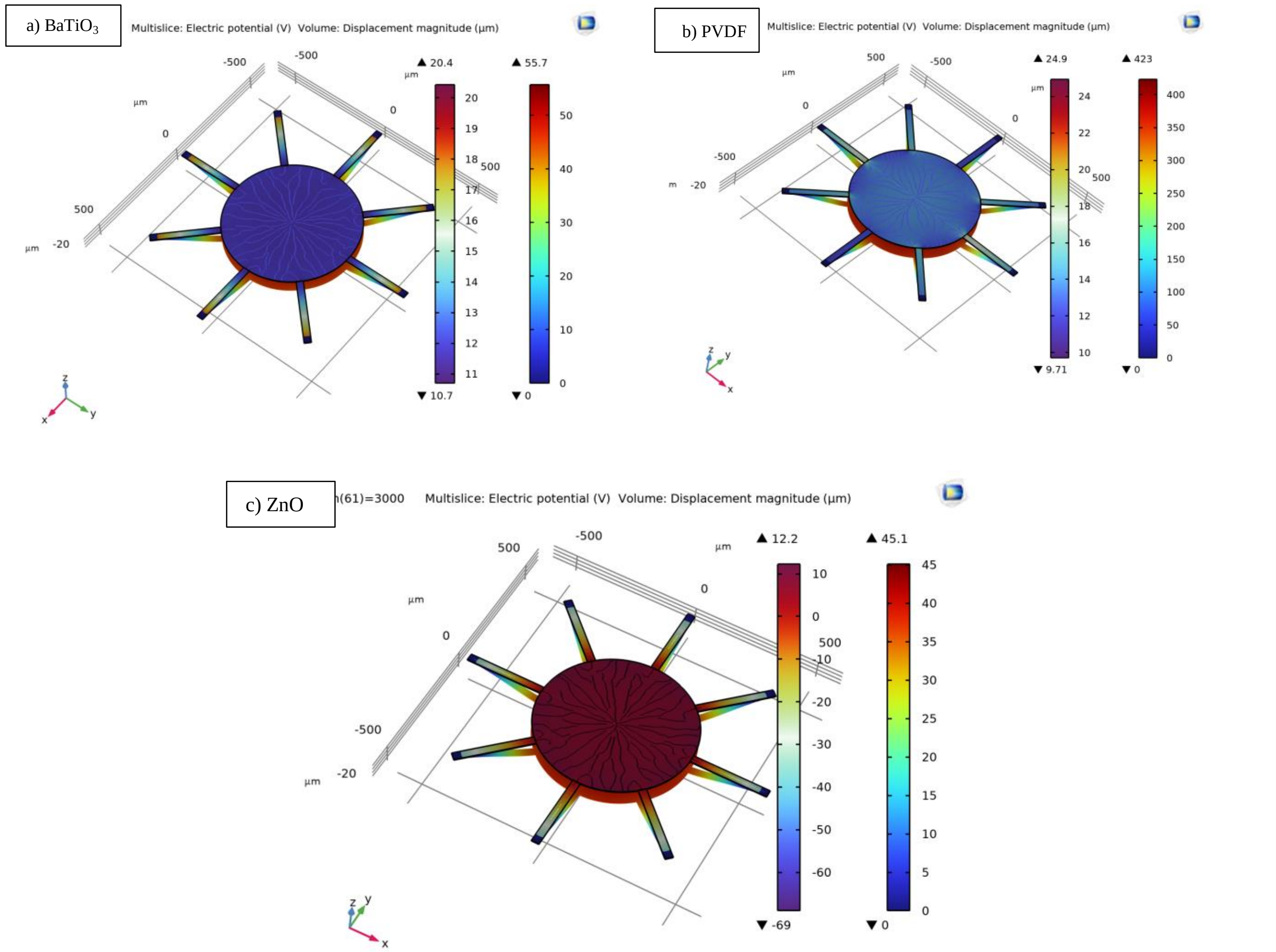

Figure 6. Volumetric Displacement Analysis of a) $BaTiO_3$, b) PVDF, and c) ZnO under 5000 Pa mechanical load.

As the mechanical load increased to 5,000 Pa, the displacement response exhibited a slight but consistent amplification across all materials. PVDF again led in displacement magnitude, with its deformation increasing proportionally with voltage. $BaTiO_3$ demonstrated a stable and scalable electromechanical response, indicating that it can sustain higher loading without compromising structural integrity. ZnO, although rigid, showed a measurable improvement in displacement compared to the 3,000 Pa case, reflecting its capacity to convert mechanical stress into electrical output with minimal geometric change.

Under the lowest applied load, all three materials exhibited minimal but measurable displacement as electric potential increased from 5 V to 25 V. PVDF, due to its low elastic modulus and polymeric flexibility, showed the highest volumetric displacement response among the three. $BaTiO_3$ followed with a moderate level of deformation, while ZnO presented the smallest displacement values. The results suggest that at low mechanical stress, deformation is primarily driven by the piezoelectric effect, with material flexibility playing a dominant role.

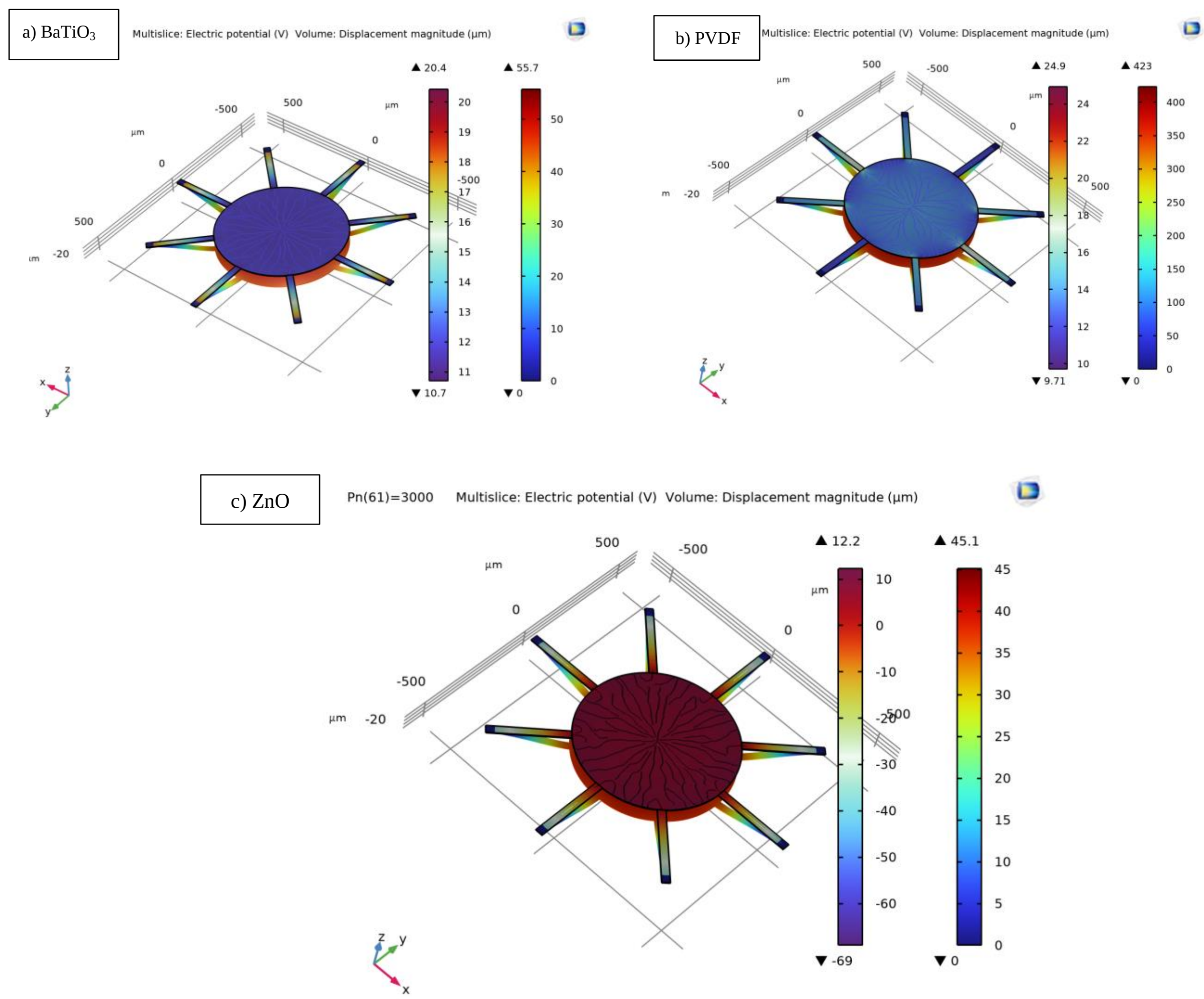

Figure 7. Volumetric Displacement Analysis of a) $BaTiO_3$, b) PVDF, and c) ZnO under 3000 Pa mechanical load.

Overall, the volumetric displacement across all loading conditions was significantly influenced by both the material's intrinsic elasticity and the applied electric potential. PVDF consistently delivered the highest displacement due to its flexible nature, making it highly suitable for applications requiring large actuation. $BaTiO_3$ offered a balanced response, showing promise for hybrid actuator-sensor devices. ZnO, while limited in displacement, remained mechanically stable and highly responsive in terms of stress-to-voltage conversion, underlining its potential in rigid, precision-controlled piezoelectric systems.

3. RESULTS

These findings indicate that the selection of piezoelectric materials should not be based solely on individual parameters such as piezoelectric coefficients or stiffness, but rather on a comprehensive evaluation of their structural responses to both electrical and mechanical stimuli. PVDF, due to its low elastic modulus, stands out as a suitable candidate for flexible systems and energy harvesting applications that require large deformations. ZnO, on the other hand, demonstrates a stable and consistent response despite its rigidity, making it particularly well-suited for microsensor applications. $BaTiO_3$ exhibits a balanced behavior in terms of both deformation amplitude and structural stability, thus presenting itself as a favorable material for micro-actuator and MEMS-based applications. In conclusion, material selection in piezoelectric device design should be approached multidimensionally, considering the intended application, target deformation range, and environmental conditions. The comparative analysis conducted in the COMSOL Multiphysics environment provides a holistic and insightful perspective for evaluating the multiphysics interactions of piezoelectric materials.

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1- Study design 2- Data collection 3- Data analysis and interpretation 4- Manuscript writing			

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