# Topics in Finite-Element Modeling of Piezoelectric MEMS

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## ABSTRACT

Techniques for modeling thin-piezoelectric MEMS devices using existing finite-element packages are examined. The emphasis is on non-resonant sensors and actuators, but most results are applicable to resonant devices and large structures as well. Characteristic features and challenges of this modeling endeavor are pointed out. Piezoelectrically actuated bending is examined, and it is shown that appropriate solid elements can work remarkably efficiently despite the sheet-like structural features. Next, a method, employing finite-element analyses, for creating an equivalent circuit representing the electrical behavior of a linear device is presented. FEM discretization errors associated with this procedure are then analyzed.

***Keywords***: MEMS, piezoelectric, FEM, error, film

## 1 INTRODUCTION

Microelectromechanical devices that employ active piezoelectric materials, typically in thin-film form, show promise for a variety of applications and are currently the subject of research in a number of laboratories. These "P-MEMS" may take the form of individual or distributed mini-actuators or sensors and may function in a resonant or non-resonant mode. As these devices become increasingly diverse and sophisticated and their commercialization is established, the need arises for increasingly accurate and efficient modeling of their behavior for design purposes. Finite-element method (FEM) analysis is a nearly indispensable tool for this, but its application in this particular area is new and much expertise remains to be developed and disseminated. A few contributions are made in this paper.

In many ways, P-MEMS are similar to other, larger, structures containing piezoelectric materials. Piezoceramic-based transducers for producing and detecting ultrasound, as well as lower-frequency speakers, microphones, and hydrophones, are well established. Piezoelectric patches bonded to large structural beams and plates for vibration control (adaptive structures) are currently of great interest for aerospace applications. In all cases, the electrically active region of the piezoelectric material performs either a sensing (strain input, electrical output) or actuating (electric-field input, displacement output) function, or both.

However, some things typically set P-MEMS apart. Foremost, the piezoelectric layer is usually a deposited film with active-area width dimensions 100 to 1000 or more times the thickness. Furthermore, other mechanically and electrically active films are present and overlap each other to form geometrically and functionally complex layered structures. Also, the smallness of the active part of the device makes its behavior more sensitive (in an adverse way) to electrical aspects of its environment; hence, good electrical modeling is needed.

The coupling of electrical and mechanical fields that is intrinsic to a piezoelectric material is not accomplished by traditional FEM elements. Driven by the non-MEMS applications, people have developed, mainly in the last decade, a variety of piezo-capable FEM elements. Many of these are tailored to particular structures, especially beams and plates, and are not more generally applicable. In the early 90's, ANSYS was perhaps the first popular general-purpose commercial FEM package to include fully coupled piezoelectric elements, and both plate and solid elements are available. It is the system (version 5.5) used in this study.

While it may seem that the sheet-like nature of structures in P-MEMS would make them good candidates for FEM using plate elements, the overlapping mentioned above often makes the physically correct interaction between different elements difficult if not impossible to set up. In addition, normal stresses and shear strains, which most plate elements do not model, may be very relevant, especially within the piezoelectric layer. Finally, a solid model imported from another CAD application is far more easily meshed into solid elements than other kinds. For these reasons, we will address issues associated with the use of solid elements only. The most obvious issue is that meshing a thin sheet into low-aspect-ratio elements requires a prohibitively large (in terms of computational resources) number of elements, while too low a mesh density might result in severe discretization and element-shape errors.

In this study, we use simple, carefully constructed FEM analyses to shed light on the fundamental ways in which mesh discretization creates error in piezoelectric actuating and sensing situations. The sensing investigation relies upon a FEM-based electrical modeling scheme that we have not seen presented elsewhere.

## 2 ELEMENT and MATERIALS

The ANSYS element used here in all analyses, for all materials, is called "PLANE 13." It is a four-node isoparametric element. Used as a piezoelectric element, the nodal degrees of freedom (DOF) are UX ($x$ displacement), UY ($y$ displacement), and VOLT (electrical potential). The same configuration works for non-piezoelectric structural materials also. For two-dimensional models, the plane strain option was used. Otherwise, the axisymmetric option was used, creating a 3-D model. With the option "extra shapes excluded," the element interprets the DOF quantities as varying linearly within the element between nodes. With "extra shapes included," the interpolation functions for both displacements contain second-order terms, but electrical potential remains linear. Both shape options were examined.

The piezoelectric film material had either material properties similar to those of ceramic PZT (with large piezoelectric and dielectric constants) or ZnO (with relatively small piezoelectric and dielectric constants). The isotropic "substrate" material had elastic and density properties similar to amorphous silicon nitride.

## 3 ACTUATION

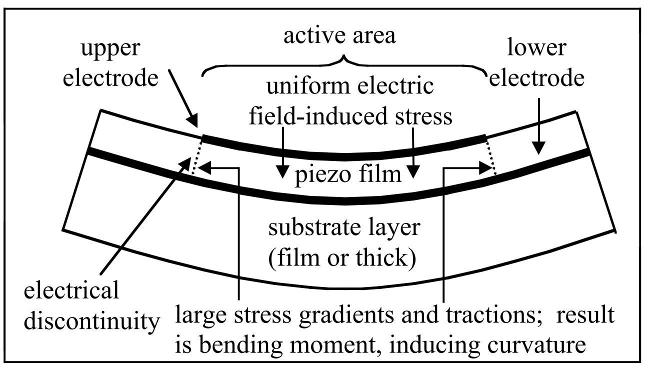


Figure 1: Features of piezoelectrically actuated bending. A voltage $V$ is applied to the top electrode relative to the bottom.

The most common way in which a thin piezoelectric layer performs an actuating function in non-ultrasonic MEMS is illustrated, in a most basic configuration, in Fig. 1. It is a *bending* effect. The piezoelectric film, partially mechanically constrained by the "substrate" to which it is bonded, develops an in-plane stress as a result of the electric field in it caused by the applied voltage. This stress causes the substrate (and therefore the film itself) to bend. A detailed analysis (not shown here), as provided by FEM with a very fine mesh in the vicinity of the electrical "discontinuity" (the term is an exaggeration, but reflects the existence of high field gradients) at the edges of the active area, reveals that the interfacial tractions exerted by the film on the substrate, which are what mechanically accomplish the bending, are large and oscillatory very near the discontinuity, but essentially die away a few film thicknesses distant.

Since meshing that produces elements far wider than the film thickness cannot possibly accurately model this realistic local stress state, nor even its St. Venant's Principle equivalent (which still must be localized), one can easily imagine that this lack of field-distribution accuracy will be the cause of significant discretization error in the macroscopic bending behavior.

To test this hypothesis and more generally investigate discretization effects on actuated bending, we analyzed the model shown in Fig. 2. For constant applied voltage, material properties, and element type, the static $y$-deflection of points **A** (below the edge of the active region) and **B** were computed as a function of mesh-division parameters $N_X$, $N_{Y1}$, and $N_{Y2}$.

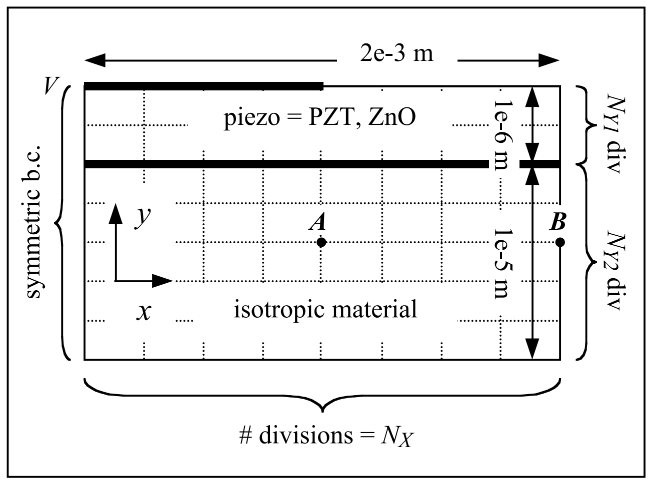


Figure 2: Model to test effects of mesh density on bending.

The results for when the elemental "extra shapes" was activated were interesting. Quite surprisingly, the computed deflection at point **A** varied by less than 0.2% for all combinations of $\{N_X, N_{Y1}, N_{Y2}\}$ from {100, 4, 10} down to {4, 1, 1}! (The deflection was also in similarly excellent agreement with analytical results.) Our hypothesis of significant discretization error was wrong, at least regarding deflections at nodes below the active area. The deflection at point **B**, however, did vary with $N_X$. We were able to make quantitative sense of the trend in the following way: Realistically, the slope of the structure past the end of the active region should be constant and equal to the slope at point **A**, which can be calculated from the deflection at **A** and the assumption of constant curvature within the active region. Comparing the final positions of **A** and **B** gives the FEM slope, which is plotted in Fig. 3 relative to the realistic slope. The error in slope is approximately proportional to element width. Analysis of the proportionality factor suggests a logical cause for the error: The slope behaves as if the column of elements just outside the active region has an average (and excess) curvature of approximately 25% of the uniform active-region curvature. This is quantitatively what would be expected from an excess $y$-direction electric field present in the piezoelectric elements neighboring the active region due to linear interpolation of electric potential. In other words, the active region is effectively enlarged due to discretization adjacent to the electrical discontinuity.

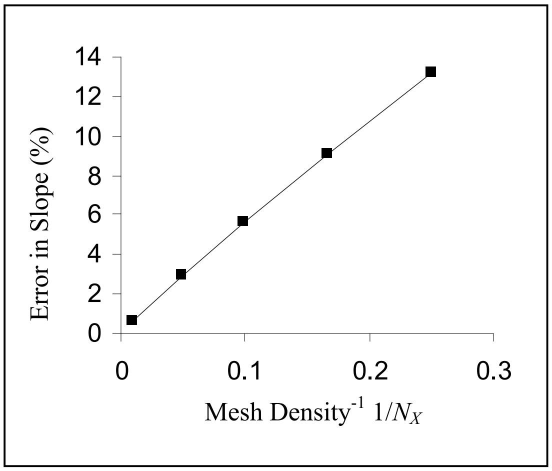


Figure 3: Excess in slope of Fig. 2 structure beyond active region, relative to theoretical.

For the same structure and element type, the resonant frequency, determined by reduced modal analysis, was very insensitive to mesh density, varying less than one percent for $N_X = 20$ to 4.

When “extra shapes” was suppressed, the results were very inaccurate. For example, with $N_X = 100$, the static deflection at **A** was only 36% of its correct value; with $N_X = 10$, only 1%. Bilinear elements are evidently unsuitable for thin-layer applications.

## 4 ELECTRICAL MODEL

Kagawa, *et al.* [1] pioneered the use of FEM to determine the electrical input admittance of radiative ultrasonic transducers with and without passive mechanical loads. The essential method was to compute the charges as well as voltages on the electrodes as a function of time or frequency while simultaneously modeling the mechanical load. However, for sensor applications, the mechanical load is *active*, which makes the admittance an unknown function of a parameter that may be an arbitrary variable. What is needed is an electrical model that takes this variable into account explicitly.

Let us consider a linear-behaving piezoelectric device that has one electrical port defining voltage $V$ and that is piezoelectrically responsive to a knowable mechanical load parameter $M$. We point out that an equivalent circuit containing two discrete circuit elements can fully model the electrical behavior of the device under quasistatic conditions or harmonic conditions, and we will explain how the values of the elements are can be determined from FEM analysis as constants (at a given harmonic frequency $\omega$) or simple functions of $M$.

Since the device is assumed to be electrically and mechanically linear,

$$Q = k_M M + k_V V \tag{1}$$

where $Q$ is the charge output from the “top” electrode, given in ANSYS as the sum of “reaction charges” on top-electrode nodes. $k_M$ and $k_V$ are constants, determined respectively by $Q_M$ … $Q/M]_{V=0}$ and $Q_V$ … $Q/V]_{M=0}$ from appropriate FEM analyses. One possible circuit equivalent to Eq. (1) in the harmonic case is: a source current $I^S = j\omega k_M M$ (upward) in parallel with a capacitance $C = -k_V$. Another circuit, applicable to quasistatic and harmonic cases, is: a voltage source $V^S = -Mk_M/k_V$ (+ toward top electrode) in series with a capacitance $C = -k_V$. These circuits electrically model the sensor attached to a passive electrical load for any known phasor $M$. They also apply to the actuator case, where the electrical load is active and the mechanical load passive, but $M$ may not be known.

## 5 SENSOR OUTPUT

As described in Section 4, a key to developing a useful electrical model of a piezoelectric sensor (those for which the magnitude of electrical-port voltage or charge, rather than resonant frequency, is the output parameter) is the determination of changes in electrode charge associated with electrical and mechanical influences. Again we sought to identify and quantify sources of error that might be associated with model discretization.

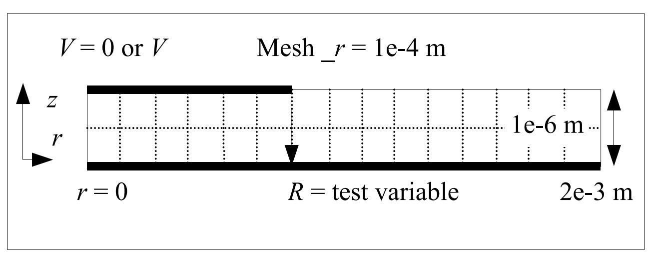


Figure 4: Model for testing reaction charge computations.

The axisymmetric model of Fig. 4, representing a piezoelectric disk uniformly meshed in the radial direction, was initially used in the investigation. In the first test, vertical displacement for all nodes was constrained to be zero while radial displacements were set to produce a uniform isotropic in-plane strain. The resulting top-electrode $Q_M$ ($M$ being the strain here) was computed for electrodes of varying radius $R$. The theoretical (analytical) value is

$$Q_M = 2\pi e_{31} M R^2 \quad (2)$$

where $e_{31}$ is a piezoelectric constant. With $R$ equaling the disk radius, the reaction charge was precisely in agreement with Eq. (2). The results for smaller $R$ are shown in Fig. 5. The relative error is quite large for the smallest electrodes. In the next test, strain was made uniformly zero, and a voltage $V$ was applied. The resulting data for relative error in computed $Q_V$ versus $R$ was almost exactly the same as for $Q_M$. Relative-error results were independent of piezoelectric material and whether or not "extra shapes" was activated.

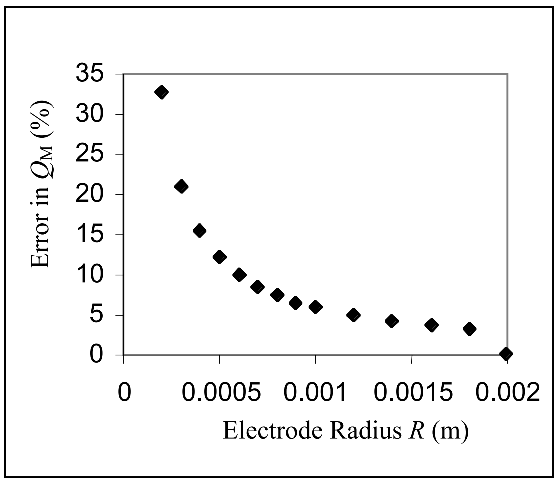


Figure 5: Excess in strain-induced charge, relative to theoretical, as a function of top-electrode radius.

Analysis of the above data and the results of other tests in which plane-strain elements were manipulated pointed to the following phenomenon as the source of the observed errors in $Q$: As a result of elemental node sharing, there is an excess computed $Q$ equal to approximately 28-29% (depending on shape) of the reaction charge that *would* appear on the set of elements adjacent to but outside of the active area *if* they were electroded and shared nodes with no additional elements and had unchanged strains. In other words, dielectric and piezoelectric charge responses from outlying elements leak unrealistically into the active area in an amount proportional to the area of these elements and (in the $Q_M$ case) the strains within them. Hence, there is a discretization error that can be reduced by meshing more finely perpendicular to and outside of the active-area edge.

## CONCLUSIONS

Due to geometrical and functional aspects of typical P-MEMS devices, employing solid rather than commonly available plate elements in the FEM modeling of them is recommended for reasons of set-up simplicity and potential accuracy.

It was found that use of a coupled-field solid element with second-order displacement interpolation yielded good results in the analysis of bend-actuated structures. Within and below the piezoelectrically active region, nodal displacement was accurate and virtually independent of mesh density. In the flexible part beyond that region, displacements exhibited error that was linked to electrical-potential discretization in elements adjacent to but not within the nominal active region. The use of a bilinear element in similar tests yielded poor results for practical mesh densities.

A method for creating an equivalent circuit that models the electrical behavior of linear piezoelectric devices subjected to mechanical influences was presented. The constant parameters in this circuit are derivable from the charge-output results of two FEM analyses of the device.

For both voltage-driven and strain-driven charge outputs, it was found that there is FEM discretization error associated, again, with elements bordering but outside of the nominal electrically active region.

While this work involved a limited number of types of elements and situations, it is anticipated that the FEM conclusions hold at least qualitatively quite generally.

## ACKNOWLEDGMENT


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## REFERENCES


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