MODELING AND CHARACTERIZATION OF GEOMETRIC EFFECTS ON THE PERFORMANCE OF RAINBOW AND THUNDER ACTUATORS

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I. Summary

Dome formation in Rainbow and Thunder actuators occurs to relieve thermal expansion mismatch stress between the metallic and piezoelectric layers during cooling from device fabrication temperatures. Accompanying this process is the generation of an internal stress profile within the devices and the development of significant tensile stresses within the surface region of the piezoelectric. These tensile stresses affect the domain configuration (ratio of c-to-a domains), and improve the 90° domain wall movement response of the device in this region of the piezoelectric. This results in improved electromechanical performance compared to standard direct extensional and flextensional devices, presumably because of the contributions of stress to the non-linearity of the piezoelectric d-coefficients.[1] Interestingly, this improvement in response seems counterintuitive; a stress perpendicular to the direction of the applied electric field should impede, not contribute to 90° domain switching. Further consideration of the lower region of the piezoelectric that is under compressive stress thus appears warranted.

The specified objectives of the research were to:

1. Conduct finite element and equivalent circuit simulation-based investigations to understand the effects of actuator geometry on internal stress distribution and actuator performance (displacement and load-bearing capabilities).
2. Use the results of the modeling studies to predict the processing conditions (geometry and thickness ratio) required for the fabrication of Rainbow ceramics with optimized performance.

Goal 1 outlined above was met during the time period of the contract. A number of finite element simulations of actuators fabricated with different geometries were carried out and the impact of geometry and shape on stress level was successfully modeled.

Goal 2, verification of modeling results was not completed due to the extent of activities aimed at meeting Goal 1 and other proposed activities in equivalent circuit modeling of device performance. These additional studies also yielded interesting results that are summarized below and which suggest that in addition to stress effects, mass loading and more straightforward mechanics effects (i.e., modulus and geometry effects on performance that are independent of stress) also contribute to the enhanced performance of these devices.

The results of both the finite element and equivalent circuit modeling that have been obtained to date were initially summarized in an interim report[2] to Dr. Wallace Vaughn (Advanced Materials and Processing Branch). Results in both of these areas obtained since the submission of the interim report this past March are summarized below.

In previous research carried out on this contract, we used 3-dimensional finite element modeling to demonstrate that the tensile stress levels in the surface of Rainbow actuators were dependent on the geometry of the device and were significantly greater than the stresses present in analogous Thunder devices.[2] Further, the predicted stress levels in the devices are in agreement with the observed displacement performance of the two families of actuator devices.[3]

Higher stress levels were predicted by finite element modeling for the Rainbow devices compared to Thunder devices. Testing of both of these devices[3] indeed shows that the Rainbow devices generate greater displacements, again emphasizing the importance in understanding the effects of internal stress on the d-coefficients of these materials.

The influence of a variety of specimen geometry effects (reduced layer ratio, circular, and rectangular geometry, and device thickness) on the internal stress profile and dome formation within the material have also been modeled.[2] Maximum stresses are predicted for reduced layer thicknesses of approximately 35%, in agreement with results of previous 2D finite element studies.[4] Initial results indicate that reduced layer/piezoelectric layer ratio and device thickness are key parameters in defining stress level. More recent results obtained by non-linear finite element analysis also indicate that actuator geometry (circle vs. rectangle and rectangle aspect ratio) has a significant effect on stress profile, which suggests that the devices will display significant performance differences. The properties of rectangular actuators prepared with different aspect ratios are under investigation to verify these predictions. Modeling results are presented below.

In addition to the finite element studies, equivalent circuit modeling of Rainbow devices has also been carried out to predict the resonance and strain behavior of these actuators. In this approach, the devices were modeled as a black box equivalent circuit.[5] Results of these studies displayed good agreement with published results[6] for resonance frequencies, but the strains predicted significantly exceed the reported values. Recent studies aimed at further characterization of cantilever geometry effects indicate excellent agreement between predicted and measured resonance frequencies for actuators with both different length and thickness ratios. In these studies, the highest predicted strains were observed at ~ 26% reduced thickness/total thickness ratio, close to the experimentally observed value of 30–35%,[4] suggesting that not in addition to stress, mass loading and other mechanics effects must also be considered.

II. Discussion of Results

A. Background

The intrinsic strain that can typically be obtained from a piezoelectric material is about a few tenths of 1%. Unimorph and bimorph technologies were developed to amplify this strain, although this performance improvement was accompanied by a decrease in the load-bearing capabilities of the device. A thorough review of applications of unimorph and bimorph benders is given by Smits et al.[7] For applications requiring still larger displacements, two recent actuator technologies have been devised to amplify the strain. These actuators include THUNDER[8] (THin layer UNimorph DrivER) and RAINBOW[9] (Reduced And INternally Biased Oxide Wafer) ceramics. In particular, Rainbows are not only able to generate very high displacements (100-300% strain), but they do so with reasonable load bearing capabilities. It has been demonstrated that Rainbow actuators can sustain point loads of about 10 kg.[10] Haertling has previously reviewed the performance characteristics of Rainbow devices.[1]

The Rainbow device is obtained by the controlled partial reduction of $Pb(Zr,Ti)O_3$ (PZT), $(Pb,La)(Zr,Ti)O_3$ (PLZT) or other high-Pb containing, piezoelectric oxide materials.[11] The typical manufacturing process involves the following steps. A ceramic disc is placed onto a carbon block in a furnace at temperatures between 600 and 1200°C; typically, a temperature of 975°C is employed. Oxygen from the air reacts with the carbon to produce CO, which in turn reacts with the ceramic that is in contact with the block. The ceramic in this region is chemically reduced, forming metallic Pb distributed in a multiphase ceramic matrix. Following the reduction step, the carbon block and composite are removed from the furnace and cooled. During cooling, thermal expansion mismatch between the two layers causes the formation of a domed, or saddle-like, geometry depending upon the lateral/thickness dimension ratio. The thermal expansion mismatch between the two layers is most pronounced below the Curie transition of the piezoelectric layer; most of the doming and stress development in the structure thus occurs in this temperature range. Investigators have prepared circular, square, and rectangular Rainbows with a variety of sizes and thickness ratios.[12]

Rainbow and Thunder actuators are referred to as "stress-biased" actuators due to the presence of an internal stress profile. This internal stress contributes to the enhanced performance of these devices that is observed compared to more traditional direct extensional and standard unimorph and bimorph flextensional devices. The fabrication process for both of these devices involves an elevated temperature processing step, and the stress profile that is generated is primarily the result of the thermal expansion mismatch between the piezoelectric and the underlying reduced (Rainbow) or metallic (Thunder) layers. Details of the fabrication process and the performance characteristics of the devices may be found in References 1 and 11.

In order to model the performance of Rainbow actuators, several groups have studied the mechanical properties of the reduced layer and have reported on the modulus and thermal expansion behavior.[13,14] It is interesting to note that depending on the reduction conditions, detailed studies of the thermal expansion behavior[15] of this phase suggest that it retains some ferroelectric character. A distinct change in the thermal expansion behavior is observed at a temperature of ~ 330°C, indicative of a phase transformation (i.e., the Curie transition).[15] The presence of this ferroelectric phase in studies of device performance has not been accounted for,[16] and it is also neglected in the analysis below.

In the development of these devices, some attention has been given previously to the nature of the stress profile by Li, Furman, and Haertling.[4] Interest in the stress profile of these devices arises because of its effects on domain configuration and domain wall movement phenomena, which concurrently impacts the electromechanical response of the devices. Alternatively, we may state that the d-coefficients of the device are dependent on stress, and as the stress state of the device is altered, as might occur through changes in the fabrication process for example, differences in device performance are anticipated.

Using this approach, the effects of stress on the non-linearity in the electromechanical response are considered. It has been suggested that it is this significant stress-induced non-linearity that results in the enhanced performance of the Rainbow and Thunder devices compared to more traditional devices. This explains our interest in understanding the nature of the internal stress profile within these devices. By defining which process techniques and device geometry aspects may be manipulated to optimize this stress profile, we may develop devices with still greater performance compared to current Thunder and Rainbow devices. These issues have been discussed in greater detail previously.[2]

The Thunder actuator is fabricated by bonding a thin metal layer to a piezoelectric ceramic using a curable polyimide polymer.[8] This three layer structure is then heated to elevated temperatures, typically around 350°C, which results in curing of the polymeric layer. During subsequent cooling, in an analogous manner to the Rainbow ceramic, the thermal expansion mismatch between the metallic and ceramic layers results in a domed or saddle-like configuration for the actuator. The strain characteristics of the Thunder devices are, in general, similar to those of the Rainbow[3] but the load-bearing capabilities of the Thunder devices appear to have not been investigated as thoroughly. Also, the attainable displacements of the Thunder devices appear to be somewhat less than those of Rainbow ceramics.[3]

Thus, the general configurations of Rainbow and Thunder ceramics are similar to standard unimorph devices, only they are domed and can possess a significant stress profile across both the reduced and the unreduced piezoelectric layer. Li, Furman and Haertling have modeled the performance of Rainbow actuators by assuming that the d_{31} coefficient in the surface region of Rainbow ceramics, which is under tension, is as high as –508 pC/N compared to a value of –271 pC/N for a standard ceramic. Studies of the (200) and (002) x-ray diffraction peak intensities tend to support these conclusions.[4]

Since the d-coefficients may be significantly impacted by the magnitude of the stress, a quantitative understanding of the stress profiles in these devices may potentially lead to a better understanding of the performance of these devices and strategies to further improve actuator performance. In this report, we summarize our studies of the effects of actuator geometry on planar stresses in these devices through finite element simulation. A variety of circular and rectangular devices were modeled and the stress levels present in the piezoelectric layer were correlated with device geometry using both linear and non-linear analysis approaches.

Before considering these results, it is appropriate to make a few other comments regarding the performance characteristics of Rainbow and Thunder devices and which additional aspects of these devices may contribute to the enhanced response that is observed. For stress-biased, as well as standard unimorph actuators, the observed displacement response will be dictated by the effective d_{31} coefficient of the piezoelectric layer. This coefficient is well defined for single crystal materials such as $BaTiO_3$, and is, of course, also known for polycrystalline ceramics, including lead zirconate titanate materials of a variety of compositions. While in single crystal materials, the observed d_{31} response is truly an "intrinsic" effect, in polycrystalline ceramics, even in materials that are poled, the observed response has contributions from both intrinsic and extrinsic effects, i.e., domain wall motion effects. In addition, the domain configuration may also affect what is typically referred to as the "intrinsic" response since the a- and c-crystallographic directions in these materials have different inherent polarizabilities. The extrinsic response is affected by material properties such as grain size and stress state, and for at least the past 10 years, investigators have attempted to take advantage of an increased extrinsic response to improve the performance of piezoelectric actuators.[17] Zhang and Cross[17] prepared single crystal based bimorphs, which due to the presence of an internal stress, demonstrated a mixed c- and a-domain configuration. Upon application of the field, a greater strain response was obtained due to domain switching with the metallic layer providing a restoring elastic force to regenerate the original domain pattern after the removal of the electric field. Analysis of the results of these investigators indicates that a performance enhancement of a factor of 30 compared to a typical single crystal device is possible.[18] For a more direct comparison, the response of poled polycrystalline actuators was considered, and again, improved performance for the bimorph device was noted.

Other approaches to predict the performance of Rainbow and Thunder devices have also been pursued. For example, Wang and Cross have modified the standard constituent equations for unimorph actuators to describe the performance of Rainbow ceramics and have acknowledged that stress effects may impact the effective d_{31} coefficient.[16] However, while variations in d_{31} with stress are, in fact, pointed out in this paper, no attempt was made to incorporate influences of this type into the model that was used to describe performance. The presence of the internal stress profile was, however, highlighted as the major difference between Rainbow and standard unimorph-type actuators.[16]

While there are a few reports in the literature on the effects of stress on the ferroelastic properties of ceramics such as PZT[19,20] and $BaTiO_3$, there are few, if any, reports on the effects of both electric and mechanical stresses on the electromechanical response of these materials. Therefore, in the single crystal domain actuator,[16] and in stress-biased devices such as Rainbow and Thunder actuators, it becomes quite difficult to predict the performance of the devices due to the unknown magnitude of the extrinsic contributions to the response, the presence of a radically different domain configuration compared to a standard poled piezoelectric unimorph, and the presence of a restoring stress field that tends to bias the structure toward an a-domain configuration while the electric field tends to enforce the formation of a c-domain configuration. Due to the ferroelastic nature of the material, the presence of both mechanical and electrical fields can also be expected to promote substantially more complex aging and fatigue behavior that can impact the utilization of the devices in a variety of applications.

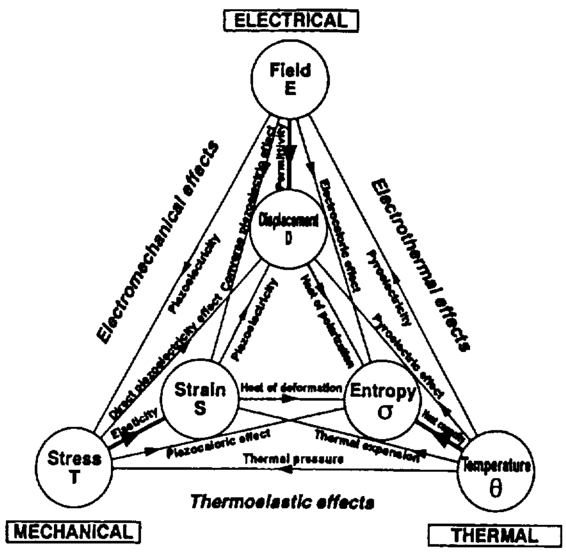
During the course of this program, due to the complexity of these devices, we initiated efforts to understand a variety of effects that we felt could contribute to the performance of these actuators. Specifically, we have begun to look at mass loading effects on the generated strain (displacement) of these devices using an equivalent circuit approach. This method allows for prediction of the macroscopic behavior of the piezoelectric device without requiring an in-depth knowledge of the microscopic characteristics.[21] The equivalent circuit model views the piezoelectric device as a "black box" having some combination of resistance, capacitance, inductance, etc.[22] Based upon these bulk properties and material properties such as Young's modulus, a macroscopic model is developed to predict the response of the device to an input electrical signal.[5,23] The effects of mass loading appear to have been neglected in previous analyses of both Rainbow and Thunder devices, as well as in the study of unimorph and bimorph devices. The possible importance of this device "geometry" parameter is further discussed below.

In the presentation of program results that follows, the enhanced performance of stress-biased piezoelectric actuators such as Rainbow and Thunder devices is further discussed. While a quantitative model that predicts device performance was not developed, nor was this a goal of this program, a number of aspects of the devices that may contribute to their response are investigated. First, results that were obtained using the standard constituent equations for unimorphs will be discussed to suggest that at least part of the observed response of these devices is due to simple mechanical effects. Second, results of equivalent circuit modeling studies will be presented that imply that mass loading effects in these devices also play a role in their performance. Third, we examine the results of a study of the effect of stress on dielectric constant. And finally, we present the outcome for finite element analyses of the stress profile and surface stresses in these devices. These results will illustrate that the geometry of the device has a significant effect on the mechanical stress field, which may impact the extrinsic piezoelectric contribution to the performance of these devices.

B. Application of unimorph theory to Rainbow and Thunder actuators

Prior to discussing the extension of unimorph theory to predict the performance of stress-biased actuators, some background on the derivation of standard unimorph theory for predicting tip displacement and charge generation is discussed. Briefly, the standard unimorph equations are derived from the general constitutive equations that describe electromechanical response shown in Figure 1. These modified equations, shown below, indicate the dependence of unimorph performance on material properties such as s and d, and geometrical parameters such as w, l, and thickness ratio. These equations have since been further modified by Wang and Cross[16] to more directly relate actuator performance to device parameters such as the ratio of the piezoelectric layer to the metallic layer compliance and the ratio of the metal layer to the piezoelectric layer thicknesses.

Other approaches, based on the use of unimorph theory and standard beam theory, have also been used recently to predict the performance of Rainbow and Thunder stress-biased actuators.[16,24] These methods have focused on the prediction of the tip displacement of the actuators when fabricated in rectangular cantilever geometries. The need to include non-linear contributions to piezoelectric response of the devices has also cited,[16] although no modeling has been carried out with the inclusion of these effects.



CONSTITUTIVE EQUATIONS

$T = c^E S - e' E$ $\quad$ $D = e S + \varepsilon^S E$

$T = c^D S - h' D$ $\quad$ $E = -h S + \beta^S D$

$S = s^E T + d' E$ $\quad$ $D = d T + \varepsilon^T E$

$S = s^D T + g' D$ $\quad$ $E = -g T + \beta^T D$

Figure 1. Heckmann diagram and constitutive equations to describe the electromechanical response of piezoelectric ceramics.

Cantilever tip deflection was predicted using the constituent equations for unimorphs of Smits[7] and Wang et al.[25] For study of device performance in applications such as positioning, we are primarily interested in the displacement performance of the devices under an applied electric field, and the following equations from Wang et al. were utilized:[25]

$$\delta = aF + bV \tag{1}$$

$$b = \frac{3d_{31}L^2}{t_p{}^2}\,\frac{AB(B+1)}{1+4AB+6AB^2+4AB^3+A^2B^4} \tag{2}$$

$$A = \frac{E_m}{E_p} \tag{3}$$

$$B = \frac{t_m}{t_p} \tag{4}$$

where the term b describes the tip deflection, δ, per applied volt V, d_{31} is the piezoelectric coefficient, L is the length of the cantilever, t_p is the thickness of the piezoelectric layer, and t_m is the thickness of the metallic, or for the case of Rainbows, the reduced layer. The term A shows the effects of the ratio of the Young's modulus of the metallic (E_m) to the piezoelectric layer (E_p) on tip deflection, and the term B describes the effects of the ratio of the piezoelectric to metal thickness (t_m/t_p) on the tip deflection of the cantilever. For Rainbow actuators, the modulus values used are presented below in Table I; for the Thunder actuator that was modeled, a modulus of 6.9×10^{10} N/m^2 was used for the underlying aluminum layer.

TABLE I.

Material properties utilized in equivalent circuit and unimorph modeling of Rainbow ceramics.

	Equivalent Circuit Model	Unimorph Model
Motional time constant	1×10^{-12} sec	
Permittivity	1.53×10^{-8} F/m	
Conductivity	0	
Coupling Coefficient	0.60	
Rel. Permittivity (Piezo. Constant)	1730	
Density – Piezoelectric layer	7.95 g/cm^3	
Density – Reduced layer	6.90 g/cm^3	
Elastic Constant – Piezo layer	1.11×10^{11} N/m^2	7.42×10^{10} N/m^2
Elastic Constant – Reduced layer		6.26×10^{10} N/m^2

Using Eqn. 1-4, the relative displacement of unimorph actuators fabricated with the materials employed in Rainbow and Thunder devices (PZT 5A and reduced PZT 5A for the Rainbow simulation; and PZT 5A and aluminum for the Thunder simulation) were predicted. The results of these analyses are shown below in Figure 2. Interesting, these predictions indicate that both devices should display similar effects of the t_m/t_p (metal/piezoelectric thickness) ratio, despite the slight differences in the moduli of the reduced layer (in the Rainbow) and the metal (aluminum) often used in the fabrication of Thunder devices. The use of stainless steel as the metal layer shifts the curve to the left. We note that, in this figure, the maximum device displacements are predicted for a metal (or reduced) layer thickness of approximately 30 – 35 % of the total device thickness. Interestingly, this value is close to that observed experimentally for the Rainbow devices that the generate maximum displacement (see Figure 3a). This suggests that while surface tensile stresses may be maximized for this device geometry (see discussion both above and below), other simpler geometrical or mechanical factors also play a role in the maximized performance of these devices. Stated otherwise, the maximization of the tensile stresses for this geometry may simply serve to further enhance the performance of "unimorph" devices prepared with this configuration.

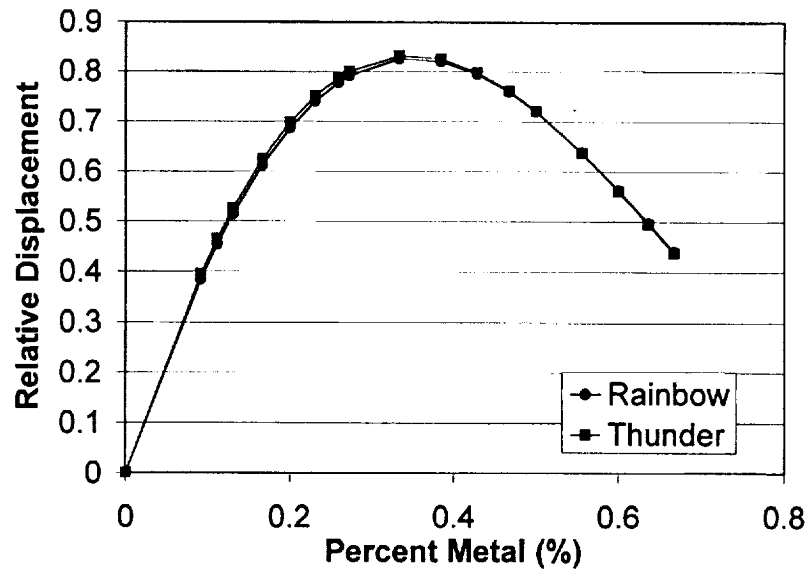


Figure 2. Unimorph predictions of Rainbow and Thunder geometry effects on relative displacement of the cantilever tip.

These predictions are somewhat different from those of Wang and Cross who reported that maximum tip displacements are obtained for a t_m/t_p ratio of 1, i.e., a metal thickness that is 50% of the total device thickness. However, as mentioned above, the value of 30 – 35 % is close to that observed experimentally for Rainbow devices that generate maximum displacement response. For example, Haertling and coworkers have reported that maximum displacements (at least for circular domed devices) are obtained for a thickness ratio of approximately 2:1 Piezo thickness:reduced layer thickness.[4] Similar observations have been noted for the performance of Thunder devices, with devices that are constructed with a metal layer that is 50% of the thickness of the piezoelectric layer displaying the greatest displacement response.[26] The difference between these results and those of Wang and Cross[16] may be related to device geometry effects (rectangle vs. circle), or tip deflection vs. mid-point deflection measurement, but further investigation is required.

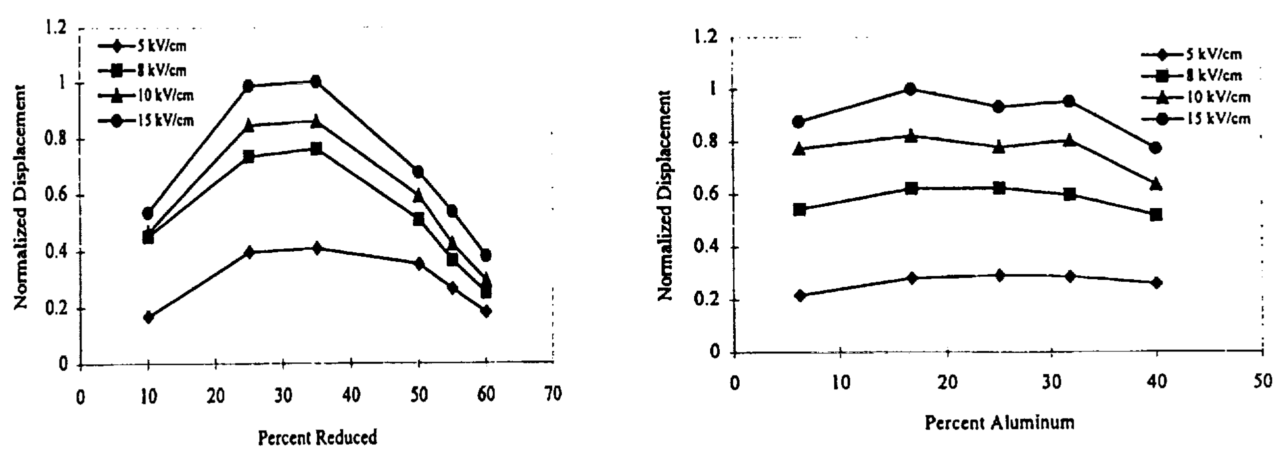


Figure 3. Measured displacement performance of (a) Rainbow and (b) Thunder actuators.[3]

The application of unimorph theory to these devices therefore appears attractive in modeling some of the general aspects of device performance, although similar predictions of response vs. actuator geometry are really not observed for the Thunder data of Wise.[3] This is perhaps related to the polymeric layer that is present in the devices, or the fact that the stress-biased devices are driven at higher fields.

While unimorph theory qualitatively predicts the effects of device geometry on displacement performance, this "mechanical" aspect alone does not explain the enhanced response of Rainbow and Thunder actuators. An additional contribution to the performance of these actuators is still believed to originate from the stress profile that exists in these devices.[14,17,27] To illustrate this point, Wise has already discussed the performance of Rainbow and Thunder devices and has reported that Rainbows demonstrate a greater displacement response.[3] The modeling results presented below suggest that, in fact, as has been speculated, internal stress is important in the performance of these devices. Finite element modeling has shown that the Rainbow devices possess significantly higher maximum stress (400 MPa) than Thunder devices (60 MPa). X-ray diffraction studies by Moon (summarized below) of actuators fabricated with different stress levels support the argument that enhanced domain wall motion occurs at higher stress.[28] Again, this result is contrary to expectations for the ferroelastic response of PZT materials, but the studies by Moon[28] and other investigators[4] support this conclusion. Further studies of actual devices, as well as analysis of published results of device performance are required to determine the possibility of extending "standard" unimorph theory to "quantitatively" predict the performance of Rainbow and Thunder ceramics.

C. Equivalent Circuit Modeling

Another approach used to approximate the performance of Rainbow ceramics was an equivalent circuit approach. In this phase of the program, a simple, one-dimensional plate resonator model was used to predict the changes in resonance frequency and strain response for different device configurations.[5,21] The focus of the investigation was to study the effects of reduced layer thickness on device performance. In order to simulate different reduced layer thicknesses, the mass of the top electrode was varied in the equivalent circuit model. Thus, while unimorph modeling accounts principally for geometrical effects, and the finite element approach utilized below permits the investigation of stress effects, this method allows for the study of simple mass loading effects on the displacement performance of the device. Recent investigations have addressed the development of more accurate equivalent circuit models for the analysis of multilayer structures,[29] but as a first step, in this study, the simplest one-dimensional plate resonator model was utilized. PZT 5A ceramic was used as the basis of the model with zero acoustic wave transmission from the piezoelectric layer to the electrode. A variety of simulations were carried out by running the equivalent circuit model using MATHCAD and the material parameters are shown above in Table I.

In the initial simulations, a device geometry (actuator thickness, width, length, and reduced layer/total thickness ratio) identical to that reported by Elissalde[6] was utilized, so that results of the simulations could be compared to experimentally reported results. The initial output of the model indicated that the resonance frequencies predicted were a function of several competing variables. It was interesting to note, however, that as shown in Figure 4, the predictions of the equivalent circuit model were in good agreement with the published resonance frequency results of Elissalde.[6] The primary variables that defined the resonance frequency were the dimensions of the device, but additional variables, such as load (in this instance, electrode mass) and the ratio of reduced thickness to the unreduced thickness, also impacted the resonance behavior of the actuator. In comparing the results of the equivalent circuit model with those in the literature, it is interesting to note that even for the simple one dimensional model that was developed, the predictions of the model correlated fairly closely with the observed experimental results.

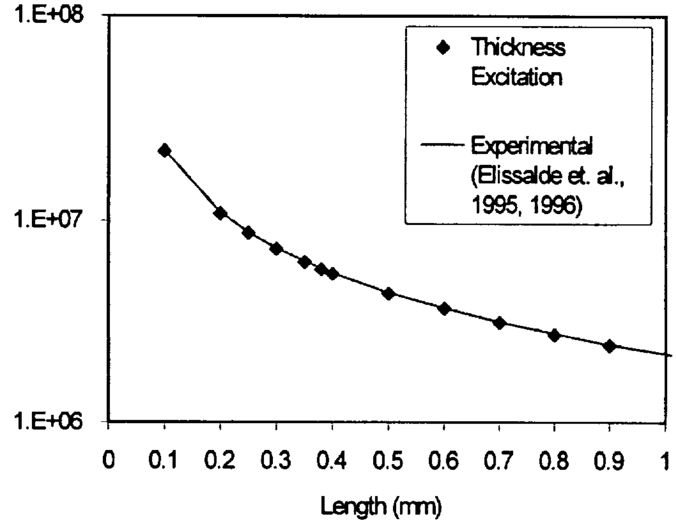


Figure 4. Comparison of equivalent circuit modeling results of Rainbow resonance frequencies vs. actuator length with experimentally measured values of Elissalde.[6]

Additional simulations have also been carried out accounting for the effects of reduced layer thickness. In this first scenario, the simple approach of approximating this layer as a massy electrode is utilized. Specifically, the primary device parameters that were examined included the ratio of oxide thickness to reduced layer thickness, i.e., electrode mass at constant wafer thickness, and off resonance performance for different t_p/t_m thicknesses (different electrode masses). The general trends observed in the literature for these effects were duplicated by our simulation efforts, with one striking difference. The maximum strain at resonance was strongly dependent on mass loading. Therefore, a "resonance" behavior for strain was observed as shown in Figure 5. Keeping in mind that the reduced layer was being treated simply as a mass on one surface of the piezoelectric wafer, it was possible to simply adjust this mass, or thickness of the wafer, to change the amount of loading on the surface. It is important to note that this loading level (which corresponds to a reduced layer/total thickness ratio of 26.2%) again correlates surprisingly well with the value of 30 – 35 % reported by Haertling for actuator fabrication parameters that gave optimized strain responses.[1,4] As internal stress is not a component within the model, it leads one to believe that additional reasons, beyond the maximization of surface tensile stress for this reduction ratio, exist for the enhanced performance of the devices that have been reduced 30 – 35%. The equivalent circuit modeling results suggest that even simple mass effects contribute to the enhanced performance of devices with this geometry. It should also be noted that because of the nature of the assumptions invoked in the derivation of the model, the magnitude of the strain cannot be taken at its absolute value, but rather must be examined qualitatively relative to other predicted displacement values. However, it is still interesting to note that maximum displacements are again predicted for the Rainbow geometries (~30 – 35%) that display the highest strains. Recent experimental studies[30] of the effects of mass loading on strain confirm these predications, although the enhancement in response is not three orders of magnitude as suggested by Fig. 5.

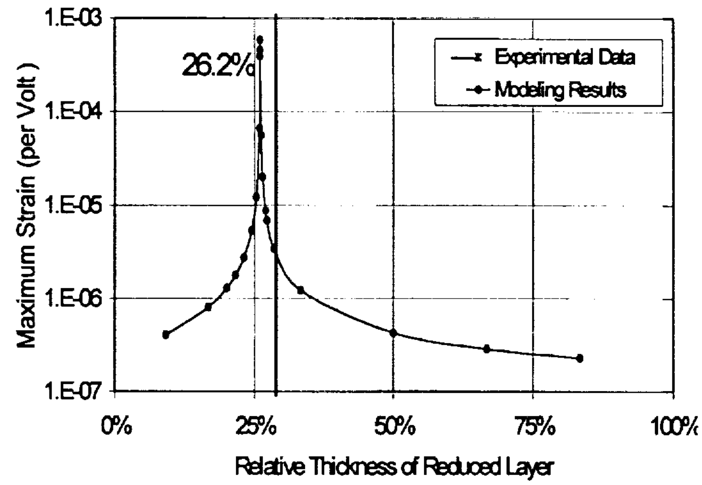


Figure 5. Effect of mass loading (relative thickness of the reduced layer) on the displacement performance of Rainbow actuators. The experimental data is indicated as the line in the figure.

D. Finite Element Modeling

Approach

This section describes the key results obtained to date from the finite element modeling simulations. A few of these results presented below were documented previously in the Interim Report.[2] Together with these results, significant new results are also discussed.

In the Interim Report, surface stresses, stress profiles and device deformations (as a result of the thermal expansion coefficient mismatch) were studied for circular, square, and a variety of rectangular Rainbow geometries. Compared to previous studies by other investigators,[4,14] we used a 3-dimensional approach to model deformation and internal stress. We also used a different thermal coefficient of expansion (TCE) for the piezoelectric layer compared to that used previously by other investigators.[2] Here, we used two TCEs for the thermal response of the material above and below the Curie point. We anticipate that this should improve the accuracy of the analysis.

Briefly, the model that was developed for simulation of the Rainbow's dome shape was constructed as a two-layer plate, with each layer having the same lateral dimensions but a different thermal coefficient of expansion. Further, the basis of the model, i.e., that dome formation and internal stress result during cool down from the reduction temperature, is in agreement with experimental results that indicate that most of the dome formation, and therefore, most of the stress development, occurs during cooling below the Curie transition.[28]

The thermal expansion values were assigned based on a review of the literature[31] and previous experimental characterization of expansion behavior carried out at Clemson University.[28] The temperature of the two plate structure was then set to the reduction temperature, 1250 K, followed by cooling of the structure to room temperature, 300 K. During the cooling process, a dimensional mismatch between the two layers occurs for the reasons identified above, leading to doming of the Rainbow device and the development of an accompanying internal stress distribution.

The finite element model was constructed and analyzed using ANSYS (version 5.4), a commercially available software package. The models were constructed using three dimensional, 8-node brick elements.[14] Because the structures that were modeled were symmetric about the x and y axes, it was only necessary to model one quarter of the structure. Another aspect of the model is that symmetry conditions require that displacements of nodal points lying on a symmetry plane be constrained to be zero normal to that plane. The central axis of the structure was allowed to move vertically, except for the point at the lower edge, where it was completely fixed. To simulate the dome formation that occurred during cooling to 300 K, temperature-independent isotropic material properties were used for both the reduced and oxide layer elements. The values for these properties are reported in Table II.

Table II.

Material properties of the reduced layer and oxide layer required for finite element modeling.

	Young's Modulus (N/m^2)	Poisson's Ratio	Density (kg/m^3)	Thermal Expansion Coefficient
Reduced Layer	6.26×10^{10}	0.342	6900	1×10^{-5}
Oxide Layer	7.42×10^{10}	0.390	7700	0.25×10^{-5} (300-643 K) 0.67×10^{-5} (643-1250 K)

Linear 3-D models

In our studies of circular geometries, which can also be studied by 2-dimensional finite element methods,[4] using a linear analysis, we obtained similar results to those previously reported for the stress profile, as shown in Figure 6a.[2] This figure shows the internal stress as a function of position (thickness) for different directions in a 30 mm diameter, 0.5 mm thick circular Rainbow. The results presented are for the center of the circular sample, and the thickness ratio (reduced layer/total sample thickness) for this particular sample was 0.3. The region of tensile stress on the left of the figure is associated with the reduced region while that on the right is associated with the surface of the piezoelectric oxide region. The x and y components of internal stress, normally called the planar stresses, are identical and vary through the thickness of sample. It is evident that the entire reduced layer is subjected to a tensile stress while the lower part of the oxide layer is under compression and the surface region is in tension. There is an abrupt change in the planar stress at the reduced layer/oxide layer interface. The intersection between the stress lines and x-axis signifies the location of the neutral plane within the Rainbow oxide layer. In general, the z-component of the internal stress is negligible.

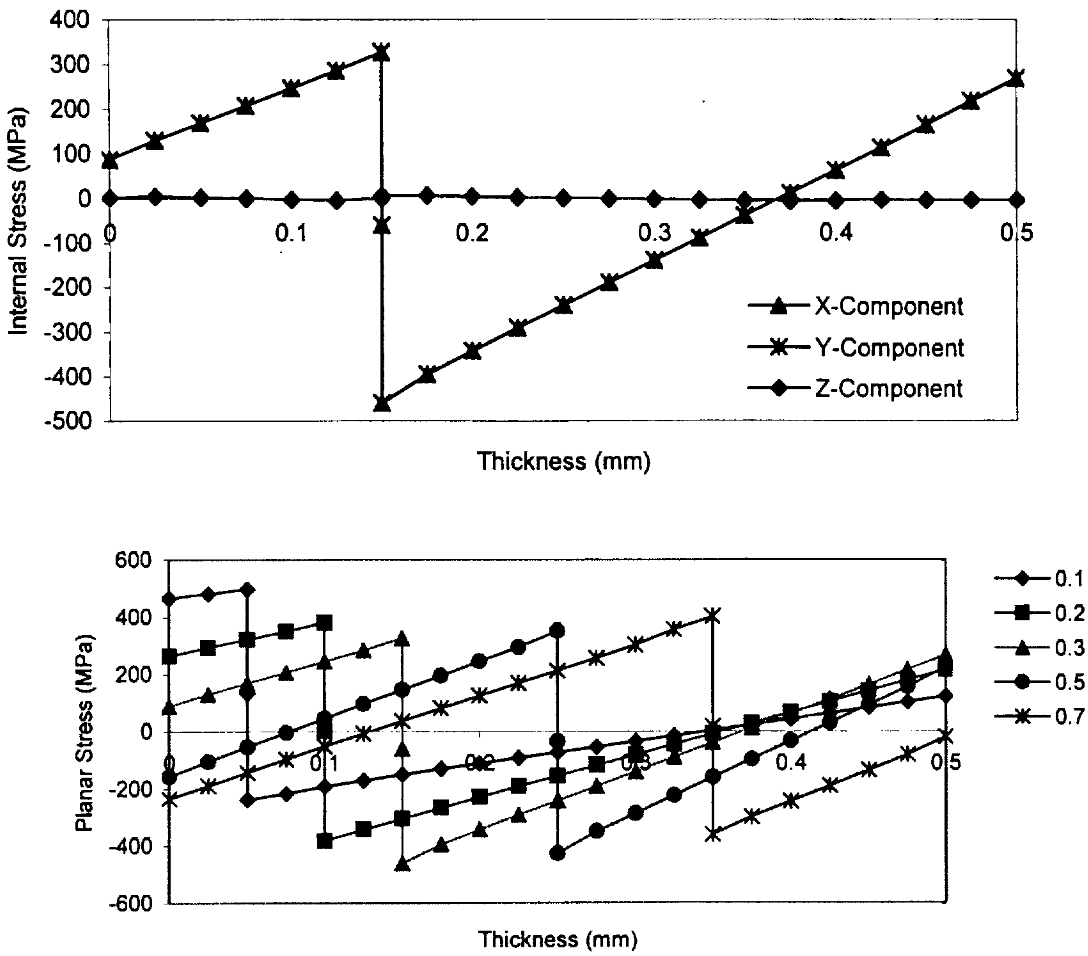


Figure 6. (a; top) The distribution of internal stress when a circular Rainbow is cooled down from reduction temperature to room temperature. Positive values on the vertical scale represent tension. Results presented are for the center of the circular specimen; and (b; bottom) the distribution of planar stress through the thickness of a circular Rainbow with different thickness ratios. Results are for the center of the circular specimens.

These results are qualitatively similar to those of Li and coworkers[4,14] who carried out two dimensional finite element analyses of circular Rainbow ceramics. The tensile stress within the surface region of the ceramic, which approaches 300 MPa for this sample geometry, results in a different domain configuration (higher a-domain percentage) compared to typical monolithic PZT piezoelectrics and a higher effective d_{31} piezoelectric coefficient in the surface region.[4]

To further study the effects of actuator geometry on stress, the stress profiles for actuators with different reduced layer-to-piezoelectric layer thicknesses were also studied. The results of these simulations are shown in Figure 6b. Maximum tensile stresses in the surface region of the actuators are obtained when approximately 30 – 35 % of the piezoelectric is reduced during the fabrication process. These results are further illustrated in Figure 7 which plots the stress at the surface of the center of a circular Rainbow as a function of reduced layer ratio. Given the effects of tensile stress on enhancement of the d-coefficients, thickness ratios of approximately 30 – 35% appear optimal for maximizing Rainbow electromechanical response. It may also be noted in this figure that other actuator geometries can result in compressive stresses throughout the piezoelectric layer, which would suppress the electromechanical response of the device, even compared to standard unimorph actuators.

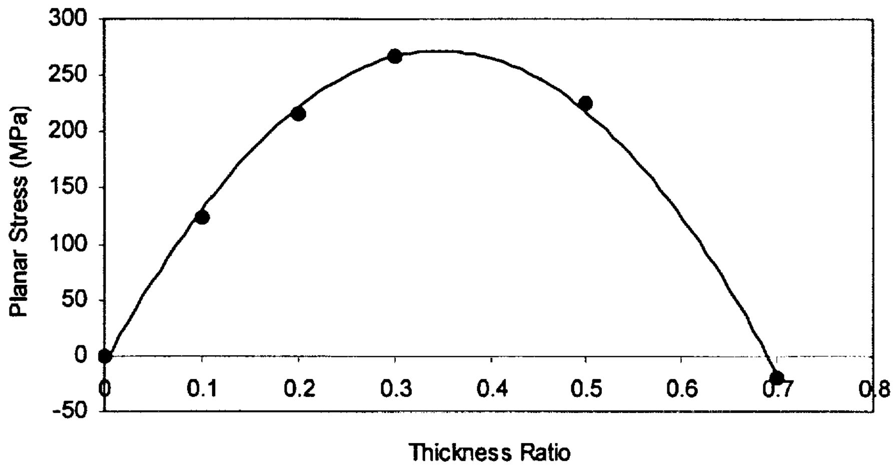


Figure 7. The planar stress at the surface of the oxide layer in the center of the sample as a function of reduced layer/total thickness ratio.

Linear 3D modeling – Comparison of Thunder and Rainbow devices

A similar modeling approach was carried out on Thunder actuators using a 0.3 thickness ratio of stainless steel to total device thickness. Tensile stress levels in the surface of the device were predicted to be approximately 60 MPa, compared to ~ 350 MPa for the Rainbow device.[2] While this effect might be expected based on the lower processing temperature of Thunder devices, the relative magnitudes of predicted stresses are in agreement with the observed displacement performance of the two families of actuator devices.[3] Because higher stress levels would be expected to result in a higher effective piezoelectric coefficient, higher displacements are predicted for Rainbow compared to Thunder actuators, in agreement with experimental studies of the two families of devices.[3]

Non-linear analyses

While linear analyses such as those above are useful in understanding general characteristics of the dome formation and internal stress profile, the bending deformation that occurs during Rainbow processing is generally so large that nonlinear analysis is required. Modeling approaches currently under investigation utilize a non-linear method, and the stress profile does indeed display a dependence on radial position as expected (i.e., the stress at the center vs. the edge of the device varies). For circular Rainbows, higher stresses are noted near the outer 1/3 of the devices, in agreement with observed x-ray diffraction results for (200) and (002) peak intensities compared to the central region of the Rainbow.[4] These results are shown in Figure 8. Also in this figure, it is interesting to note that both hoop and radial stresses may be predicted. Hoop stresses represent the x-component of stress in the y-direction (and y-stress in x-direction), while the radial stresses are the x-stress in the x-direction and the y-stress in the y-direction. Both show a trend of increasing stress with distance from the center of the surface of

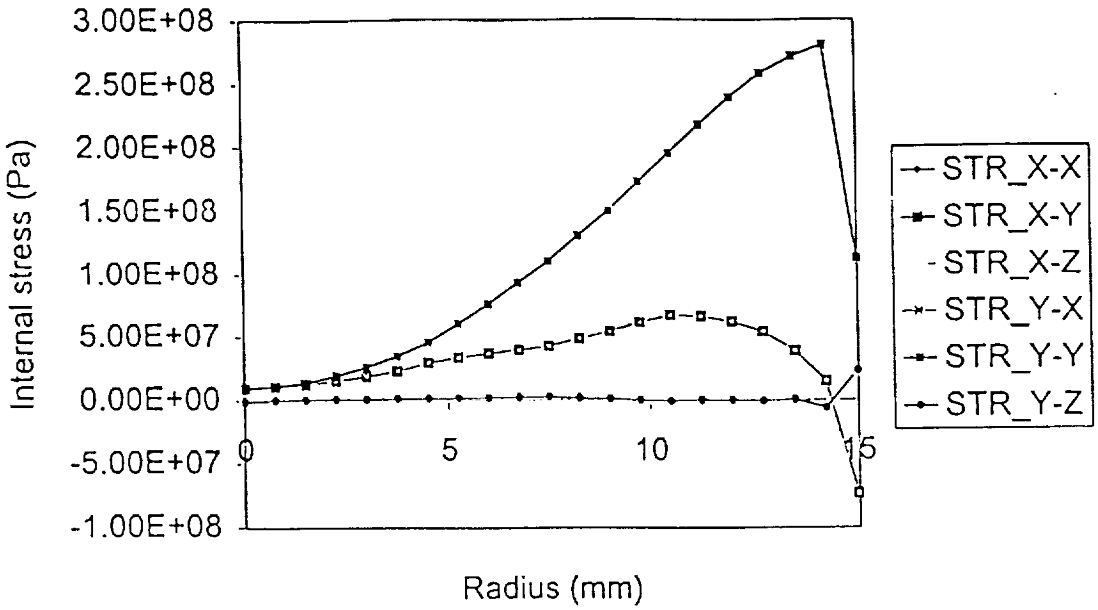


Figure 8. Stress across the surface of a circular Rainbow ceramic with a 0.3 thickness ratio, 15 mm radius and 0.5 mm thickness; center (0 mm) and outer edge (15 mm). Definition of nomenclature: 1st coefficient: direction; 2nd coefficient: stress direction.

the piezoelectric, although the variation in radial stress is greater, and the magnitude of the radial stress is higher toward the edge of the actuator. It is important to note that both stresses are expected to contribute to the non-linear piezoelectric coefficient, which will be defined by the planar stress. Considering the variation in surface stress from the center to the edge of the device, this figure also demonstrates the need to model stress profiles in these devices using non-linear modeling approaches. Previous linear analysis studies[2] of the stress across the surface indicated that the stress was relatively uniform.

Results for thickness ratio effects on surface stress determined by non-linear analysis methods are shown in Figure 9. The results are similar to those of the linear approximation in that the highest tensile stresses are again predicted for a reduced layer thickness ratio of 30 %, in agreement with experimental observations of actuator displacement performance. As with the linear analysis of the stress at the center of the actuator, compressive surface stresses are predicted for higher reduced layer thickness ratios.

Similar studies have been carried out on rectangular cantilevers of different geometry and the results are presented in Figures 10 through 12. Figure 10 illustrates the results of non-linear analyses of the stress profile at the center of the cantilever actuators. As may be seen, the aspect ratio of the actuator has a significant effect on stress profile, with higher aspect ratios generating higher tensile surface stresses at the center of the actuator. However, the results also indicate that the compressive stresses in the lower part of the piezoelectric are greater for this actuator, which may reduce the effective piezoelectric coefficient of this region of the device,[4] and hence, reduce the displacement performance of the devices. Actuators that have an aspect ratio of 3:1 (length: width) may offer the optimum combination of high tensile stresses in the upper portion of the device and lower compressive stresses in the lower portion of the device. Devices with aspect ratios of 2:1, while having lower compressive stresses in the lower part of the device also have reduced tensile stresses in the upper part of the device, and may, as a result, display reduced displacement performance.

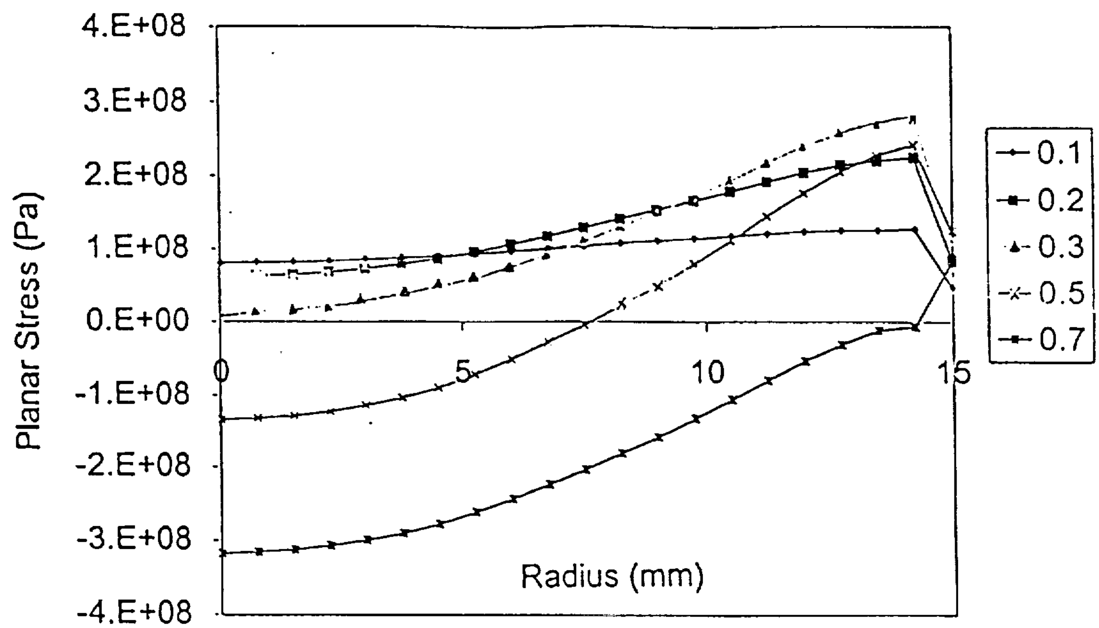


Figure 9. Effect of thickness reduction ratio on the stress at the surface of the piezoelectric layer, from the center (0 mm) to the edge (15 mm); circular Rainbow ceramics with 15 mm radius and 0.5 mm thickness.

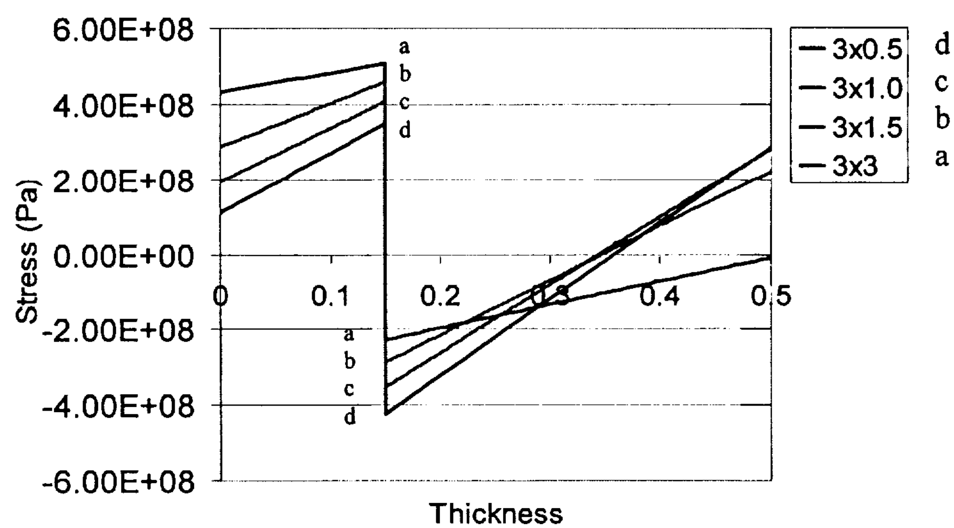


Figure 10. Effect of Rainbow actuator aspect ratio on the surface profile at the center of rectangular actuators with a 0.3 (30%) thickness ratio. Dimensions shown represent width and length in cm.

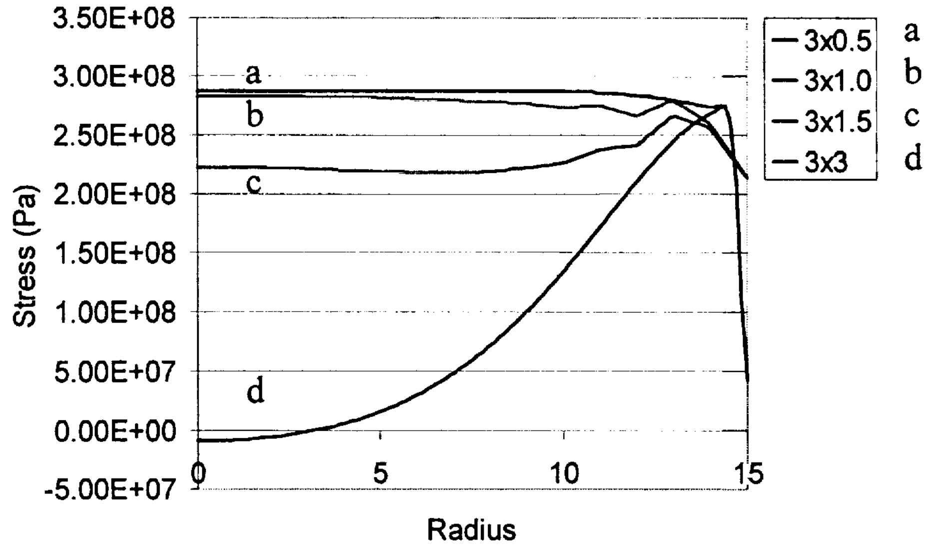


Figure 11. Planar stress along the length direction in rectangular Rainbow actuators with different aspect ratios; actuator length: 30 mm; center of rectangular actuator: 0 mm, edge of rectangular actuator: 15 mm.

Taken together, these results thus suggest that there will be aspect ratio effects on cantilever displacement performance, which is in apparent contradiction to the predictions of standard unimorph theory,[7,32] which does not include terms in the descriptive equations for the width or internal stress levels of the devices (see below). Cantilevers with an aspect ratio of 1 (square devices) have minimal stresses in the surface region of the device, similar to predictions for circular devices, and would be predicted to have generate lower displacements. However, they probably display enhanced load-bearing capabilities.

Stresses along the surface of the actuators in the length and width directions as a function of aspect ratio have also been investigated and the results are illustrated in Figures 11 and 12. Again, as with stress profile, stress along the surface of the actuators is a function of the actuator aspect ratio; higher aspect ratios produced higher tensile stresses, with the magnitude of the stress approaching 280 MPa for the 3.0 x 0.5 cm actuators in the length direction. As actuator squareness increases (decreased aspect ratio), the tensile stress toward the center of the device decreased dramatically and even becomes compressive in the center. These results for the square actuator strongly resemble those of the circular devices. Surface stress along the width direction (Figure 12) displayed similar trends.

Tests of actuators fabricated with the above geometries are in progress to verify the correlation between the magnitude of the surface stress and the displacement performance of the devices. A strong correlation is expected here because of the effects of stress on the piezoelectric d_{mik} coefficients.

Modeling deformation of Rainbow actuators

Finally, Figure 13 presents the 3-dimensional linear models of these four actuator geometries to show the induced deformation that occurs during device fabrication. The results of the simulations are in good agreement with experimental observations for rectangular actuators

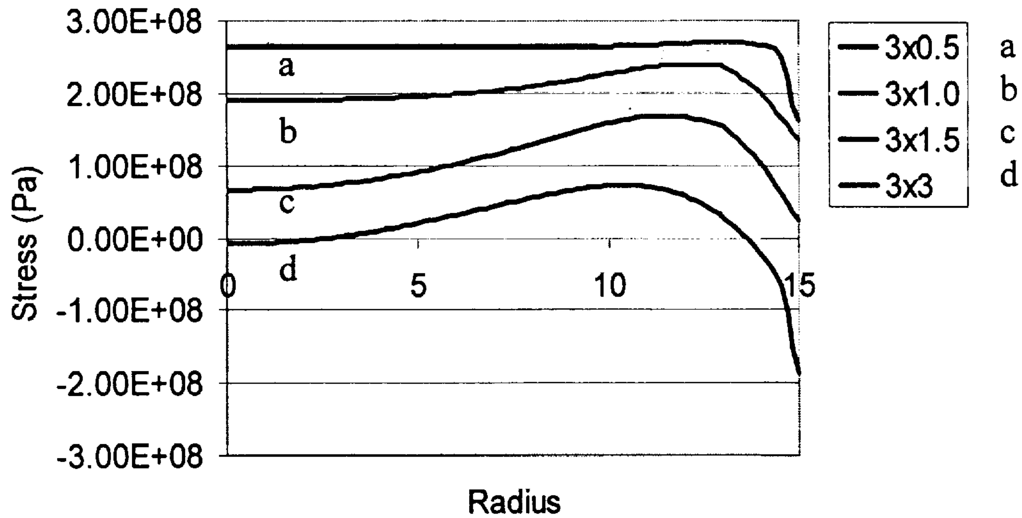


Figure 12. Planar stress along the width direction in rectangular Rainbow actuators with different aspect ratios; actuator length: 30 mm; center of rectangular actuator: 0 mm, edge of rectangular actuator: 15 mm.

fabricated at Clemson University. These 4 cm long, 1 cm wide actuators display dome heights along the x-axis of approximately 2.5 mm and 0.3 mm along the shorter y-axis. Because of the longer x-axis length compared to the model (which studied 3 cm long actuators), slightly higher curvatures are expected compared to the simulations, in agreement with observation. Deformation results for similar Thunder devices are reported below.

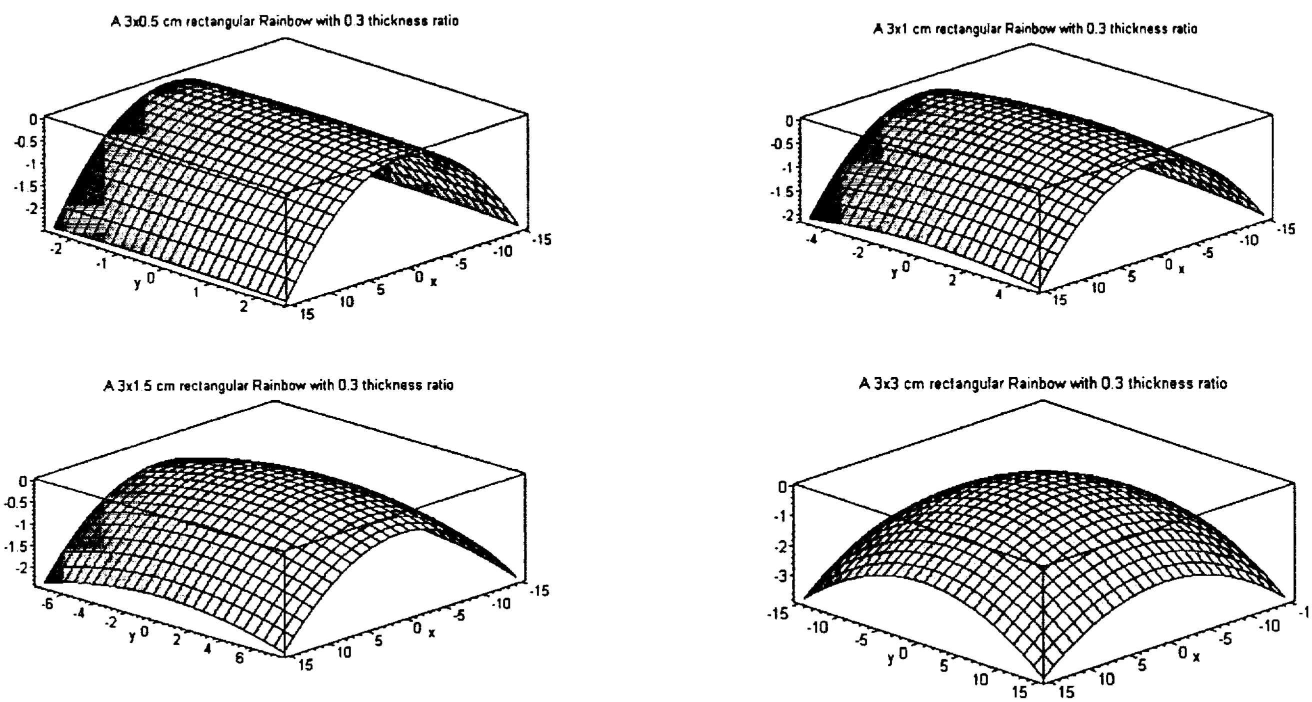


Figure 13. Equilibrium shapes of rectangular Rainbow with different dimensions. Note that the boxes have different x, y, and z scales.

Measured stress effects on domain wall movement

Recent results in other x-ray diffraction studies of (002) and (200) peak intensities at Clemson University support arguments for the stress enhancement of the electromechanical response of these devices.[28] Specifically, the presence of a tensile stress in the surface region of Rainbow ceramics appears to enhance the a-domain to c-domain switching that occurre under electric field, thus improving the strain response of the device.[12] Moon investigated this effect in greater detail by preparing Rainbows with different thickness ratios,[28] which lead to different stress levels in the surface region of the actuator. Figure 14 illustrates changes in domain wall movement for an applied electric field of 10 kV/cm for samples prepared with different reduced layer ratios. In this figure, the reported stresses are for the surface region of circular Rainbows. As may be observed, higher tensile stresses promote enhanced 90° domain wall movement and since 90° domain wall movement is associated with electromechanical response, greater electromechanical response is anticipated for the devices with higher surface stresses. This result again supports the notion that enhanced domain wall motion due to the presence of a lateral tensile stress can significantly contribute to the observed response of the devices. The domain wall motion under high stresses is, in fact, approximately three times that at lower stress. More complete data of this kind is required to begin to more accurately describe the ferroelastic response of the material, which will allow for a more accurate assessment of the intrinsic and extrinsic contributions to the performance of these stress-biased devices.

Analysis of the earlier data of Li, Furman and Haertling[4] also supports this hypothesis. In fact, a comparison of stress-enhanced domain switching with simple domain switching promoted by large electric fields in standard, poled polycrystalline ferroelectric ceramics suggests that the presence of tensile stress in the surface region of the Rainbow actuator results in a d-coefficient that is approximately 5 times larger than the high field d-coefficient of the standard poled ceramic.[18]

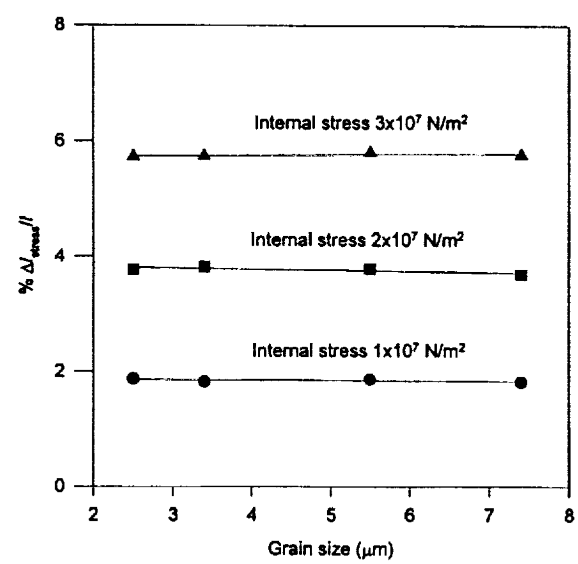


Figure 14. Variations in domain wall movement as a function of the tensile stress in the surface region of the piezoelectric. Results obtained by in-situ x-ray diffraction measurements.[28]

E. Summary of Results

Based on the results of stress effect measurements on domain wall motion, unimorph modeling, and equivalent circuit analysis, it seems reasonable to conclude that in Rainbow and Thunder devices, while the presence of the tensile stresses may significantly enhance device performance, similar mechanical issues to those which yield optimum performance unimorph devices are also critical. Considering the similar mechanical characteristics of the layers in the different devices, it should perhaps not be surprising that similar metal (reduced layer) – piezoelectric layer ratios result in the highest performance stress-biased devices. However, to accurately predict the performance of the stress-biased devices, we need to know the magnitude of the stresses present within the piezoelectric layer, and must be able to quantify the effects of stress on the non-linearity in the piezoelectric d-coefficients.

It should also be noted that in standard unimorph theory, the coefficient that relates tip displacement to applied voltage does not contain a term for the width of the device. Since we have already shown that the stress profile in these devices is dependent on the aspect ratio, some differences in the performance of devices fabricated with these geometries would be predicted. Studies of actuators with varying geometries are currently in progress and are discussed below.

III. Suggestions for Future Work

Summary

A suggested general goal of future research in this area is to further our understanding of the importance of stress, geometry, and loading effects on the displacement performance of both Rainbow and Thunder stress-biased actuators. This goal would be accomplished with further work with finite element and equivalent circuit modeling, characterization of device performance using fiber optic and LVDT sensors, and critical experiments to study domain switching under different field and stress conditions.

Research in the following areas is recommended:

(1) The use of finite element modeling in a dynamic fashion by studying the devices under load and applied electric field. This will be carried out for devices with different geometries and stress profiles to assist in quantifying effects of stress on performance.

(2) The extension of the equivalent circuit model by incorporating a recently developed five-layer model[29] that should allow for more accurate predictions of actuator performance. Both geometry and mass loading effects on actuator strain will be characterized. In addition, aging effects of the dielectric and piezoelectric constants of the devices will be studied and the results of these investigations will be incorporated into the equivalent circuit models.

(3) We will begin to quantify the effects of stress on the d-coefficients in these materials for the improved prediction of device performance by using a tensile tester to measure d_{33} under different loads. While extensive research has been carried out to determine the effects of compressive stresses on performance, relatively little work on tensile stress effects has been reported.

(4) We will use in-situ x-ray diffraction techniques to characterized the (002)/(200) peak intensity ratio of devices subjected to various electric fields. This research will be carried out at Sandia National Laboratories using a micro-spot system to focus the beam to ~ 30 μm and the devices will be characterized in a cross-sectional geometry, so that domain wall movement characteristics under different fields and different stress conditions can be determined.

(5) As studies in the finite element and equivalent circuit research areas progress, we will compare the results from the two different modeling approaches to determine which allows for the better prediction of device performance.

(6) We will explore the extension of standard unimorph theory to predict the performance of stress-biased Rainbow and Thunder actuators. Two reports of this approach have appeared in the literature[24,25] but further exploration in the use of this approach for modeling performance of stress-biased actuators is required.

(7) To use of Moire interferometry to monitor local deformation throughout the piezoelectric layer of the devices. This technique, which will involve the application of a diffraction grating to the cross-section of the device will allow for the microscopic characterization of d-coefficients throughout the piezoelectric layer, and thereby, quantification of the effects of stress on the non-linearity in the piezoelectric coefficient.

Details of Suggested Activities

1. Aging Effects

As our results on imprint testing indicate that there are significant aging and relaxation effects that would be expected to impact device performance. This work is the first to begin to quantify the temporal changes in displacement performance under dc field, dielectric constant, and stress effects on dielectric constant vs. time, despite the obvious importance of such effects on device performance, and potentially, useful lifetime. The thrust of the continued work will more fully identify the causes of aging by determining the effects of prolonged stress states on the piezoelectric, dielectric, and domain configuration of the materials used in the fabrication of Rainbow and Thunder devices. To support these studies the following experimental and modeling investigations are planned.

2. Quantification of tensile stress effects on d-coefficients

Since stress-induced enhancements to the piezoelectric d-coefficients are considered a prime driver in the large displacements of Rainbow and Thunder devices, a more quantitative assessment of d_{ij} vs. σ will be undertaken. Significant previous studies have been aimed at understanding the effects of compressive stress on dielectric and piezoelectric response, but relatively little is known about the effects of tensile stresses on these properties, even though dome and cantilever geometries exhibit both stress states. An understanding of these properties is required better predict the performance of these devices. For example, it should be possible to further develop standard unimorph theory to incorporate the stress terms in the d_{ij} coefficient (see below).

To begin to quantify the effects of tensile stress on the d-coefficients of these materials, the central region of poled rectangular ceramic plates will be electroded and the samples will be mounted in a tensile tester. A range of tensile stresses, up to mechanical failure will be applied to the piezoelectric. While holding the sample at a constant known stress state, the low field and high field dielectric constants will be measured. To characterize the non-linearity of the piezoelectric coefficient, a fiber optic displacement sensor will be used to monitor the displacement in the 3-direction under various tensile stresses applied in the 1-direction. This test situation closely resembles the field-stress conditions for both Rainbow and Thunder ceramics, and as such, should provide quantification of the non-linear piezoelectric higher order terms needed for the development of more detailed models. This will lead to better prediction of the performance of these stress-biased devices. The key experiments carried out in this task will employ PZT with the material composition and grain sizes typically used in Rainbow and Thunder fabrication. Investigations into the time-dependence of these relationships will also be carried out.

3. In-situ x-ray diffraction characterization of stress and field effects

The optimal method to fully characterize the interrelationships between electric field, applied stress, and the domain wall movement that leads to piezoelectric response is to carry out a Moire interferometry experiment (see below) to characterize the local displacement at different points within the internally stressed piezoelectric layer. The basis of this experiment is outlined below as an optional research task. However, the scope of this experiment would require a significant funding increase of the current level of support for the student working on this program.

An alternative, reasonably effective, but less expensive method to obtain similar information, is to use of micro-spot x-ray diffraction to characterize the relative intensities of the (200) and (002) peaks as a function of position within the piezoelectric layer under different electric fields. We also propose to study the peak intensity ratio of these peaks as a function of applied electric field. Because of the relationship between the a- and c-domain population and the (200) and (002) peak intensities, it will be possible to characterize the effects of internal stress profile on domain population, as well as the interaction of stress and electric field on domain wall movement. Further, since domain wall movement is strongly correlated to piezoelectric response, it will be possible by using this technique, to obtain important information to quantify the effects of stress on the piezoelectric coefficients of these materials.

This research will be carried out at Sandia National Laboratories using a micro-spot x-ray diffraction system that can focus the x-ray source to ~ 30 μm. Rainbow and Thunder actuators with approximately 500 μm thick piezoelectric layers, which will allow for determination of the peak intensity ratio at approximately 15 different locations across the depth of the layer.

4. Inclusion of property aging effects into equivalent circuit models

The experimentally determined phenomenological dependencies of stress and time on capacitance and piezoelectric coefficients will be added parametrically to the equivalent circuit models. As we have seen from Figure 10, the model is very accurate in determining the resonance behavior of Rainbow structures (despite being only exact for 1 D plates and stacks). By making the model time-dependent with actual material values for the various relaxation mechanisms, the equivalent circuit approach will become an even more powerful predictive tool to model device performance.

5. Finite element modeling of devices under load and field

In this task, we will use finite element modeling in a "dynamic" fashion by studying the devices under different load and applied electric field conditions. Again, the goal of these studies is to be able to better predict device performance under different operational conditions for different device geometries. A variety of loads will be applied as point sources to the center of circular and square actuators, and also to the tips of cantilever actuators. Initially, we will characterize the resulting deformations/displacements of the actuators under these different loads to assess the impact of variations in device stiffness and load-bearing.

Subsequently, different magnitude electric fields will be applied to the actuators without load to monitor displacement performance under different field conditions. Resonance frequencies will be identified for these conditions and the results will be compared to equivalent circuit predictions. In addition, modified unimorph theory will be used to predict displacement performance for the actuators and the results of these calculations will be compared to results obtained by finite element modeling.

Electric fields will be applied in the finite element approach to devices subjected to different loads and load/actuator displacement will be characterized for a range of applied electric fields. Again, these results of these simulations will be verified by experimentation. As with the characterization of stress profiles, these modeling efforts will be carried out for devices with different geometries and stress profiles to assist in quantifying effects of stress and geometry on actuator performance.

With regard to the performance of Rainbow devices, it is also unclear if the characteristics of the reduced layer/piezoelectric interface play a critical role in the stress profile and device performance. Therefore, the influence of a non-planar interface on actuator properties will also be modeled with regard to both stress profile and displacement performance. For Thunder devices, FEM will be used to study stress profiles for devices that include the polymeric "Robon" layer; previous models have not included this layer.

As studies in the finite element and equivalent circuit research areas progress, we plan to compare the results from the two different modeling approaches. Both methods allow for predictions of strain and frequency response as a function of actuator geometry and while the equivalent circuit method is substantially simpler, the predictions of this method appear relatively accurate with respect to resonance frequency predictions. This is because the form of the equations required to predict the response of bimorph devices closely follows that associated with more typical piezoelectric resonators, such as AT- or SC-cut quartz plate resonators, for which the equivalent circuit model originally was developed.

By extending the equivalent circuit model to look at gradient structures, even more accurate predictions of resonance and strain response should be obtained. The results of these analyses will also be compared to finite element modeling. The comparison of these results will allow for further insight into mechanics and stress effects on device performance.

We will model functionally graded structures by extending the equivalent circuit model using our recently developed five-layer model.[29] In this model, the material gradation is approximated by a number (5, or fewer, in the present case) of small uniform steps. The new model takes into account the effects of impedance mismatches between the respective layers that lead to acoustic reflections. The output remains resonance frequency, maximum displacement, and surface acceleration on the structure. This new model also will be useful in more accurately characterizing the influences of the reduced layer in the case of the Rainbow devices. Previously, this had been simply modeled as a thicker (and heavier) electrode. In theory, this approximation is fine for relatively thin electrodes, but as the reduced layer becomes a more significant fraction of the Rainbow thickness (such as the ~ 30 % reduced layer thickness that maximizes displacement) the transmission and interaction of acoustic waves through these layers must be more exactly modeled. The five-layer model is an extension of our previous single layer plate model (with mass loading of electrodes) that accounts fully for these effects. The model also simplifies to mimic the response of a cantilever structure when again the only driving force is electrical. This thrust will compare the five-layer model to the one layer model as well as the experimental results to realize better simulations to actual device performance. The effects of aging also will be included in this newest modeling effort.

6. Develop extension of standard unimorph theory for stress-biased actuators

Standard unimorph theory does not account for either internal stress or cantilever width effects in the prediction of device displacement performance. In the previous extensions of unimorph theory to predict Rainbow performance, the principal modification to the theory was the inclusion of a term for 0-field tip deflection, based on the TCE mismatch that occurs during processing which results in a domed structure.[16] The authors of this approach correctly suggest in their paper that non-linear stress effects will play a role in determining device performance and they begin to address this effect for strain and dielectric displacement, however, the magnitude of these effects is not considered. Further, based on the results of some of our previous finite element modeling studies described above, statements in the paper such as "the mechanical stress acts only along the length of the device" seem to demand further consideration. We suggest this because our finite element simulations suggest that fabrication-induced y-direction stresses in these devices are of approximately the same magnitude as x-direction (length) stresses. Further, while blocking force at the tip of the cantilever is predicted to depend on device width, tip deflection is not. Again, this analysis seems to not consider the effects of width direction stresses on the piezoelectric coefficients. As we model the performance of wider and thicker devices, the approximations made under Euler-Bernoulli beam theory are not necessarily valid, and device width may become an issue.

In this task, we will further develop standard unimorph theory by modifying the boundary conditions used to describe cantilever performance and by incorporating non-linear piezoelectric terms into the equations as possible. When coupled with the experimental results from the above studies, improved predictions of device performance for actuators fabricated with a variety of geometries, should be possible.

7. Moire Interferometric study of domain wall motion vs. piezoelectric profile

The accurate characterization of stress effects on piezoelectric coefficients is non-trivial. However, one effective experimental method is to utilize a Moire interferometry technique. In this method, the device cross-section would be polished to a reasonable smoothness. Then, a fine line diffraction grating would be applied to the device in a domed configuration. Since there is not change in the stress state of the device, there is no initial deformation of the diffraction grating and the interferogram across the thickness of the device is uniform. However, as an electric field is applied to the Rainbow (or Thunder) actuator, deformation throughout the thickness of the piezoelectric will occur. Because of the fineness of the diffraction grating, the local deformation, with micron scale resolution, can be determined. Since the sign and magnitude of the stress varies across the piezoelectric, the local deformation (strain = d-coefficient x field) will vary. Characterization of the local deformation will therefore allow for an in-situ quantitative determination of the effects of stress on the piezoelectric coefficient.

IV. List of Publications and Presentations

<u>*Publications*</u>

1. J. Ballato, R. Schwartz, and A. Ballato, "Network Formalism for Modeling Functionally Gradient Piezoelectric Plates and Stacks and Simulations of Rainbow Ceramic Actuators," *IEEE UFFC*, (1999) *Submitted.*
2. R. W. Schwartz, P. Laoratanakul, W. D. Nothwang, J. Ballato, Y. Moon, and A. Jackson, "Understanding Mechanics and Stress Effects in Rainbow and Thunder Actuators," Proceedings, SPIE, Smart Materials and Structures (2000) *Submitted.*
3. W. D. Nothwang, R. W. Schwartz, and J. Ballato, "Experimental Validation of Equivalent Circuit Modeling for Rainbow Ceramics," (2000) to be submitted to *IEEE UFFC.*

<u>*Presentations*</u>

1. R. W. Schwartz, M. L. Richard, P. Laoratanakul, P. L. Robertson, and K. Gass, "Development of Actuators for VCSEL Positioning and the Role of Stress in Stress-Biased Actuators," American Ceramic Society Southeast Sectional Meeting, Nashville, TN (November 17-18, 1998).
2. R. W. Schwartz, "Understanding Stress Effects on the Performance of Stress-Biased Piezoelectric Actuators," 3M Company, Minneapolis, MN (March 18, 1999). ***Invited.***
3. W. D. Nothwang, R. W. Schwartz, and J. Ballato, "Equivalent Circuit Modeling of Piezoelectric Rainbow Actuators," American Ceramic Society Annual Meeting, Indianapolis, IN (April, 1999).
4. P. Laoratanakul and R. W. Schwartz, "Modeling and Characterization of Stress and Geometric Effects on the Performance of Rainbow Ceramics," American Ceramic Society Annual Meeting, Indianapolis, IN (April, 1999).
5. R. W. Schwartz, "Electronic Materials and Piezoelectric Ceramics Research at Clemson University," Sandia National Laboratories, Albuquerque, NM (June 21, 1999). ***Invited.***
6. R. W. Schwartz, P. Laoratanakul, W. D. Nothwang, J. Ballato, Y. Moon, and A. Jackson, "Understanding Mechanics and Stress Effects in Rainbow and Thunder Actuators," SPIE, Smart Materials and Structures Meeting, Newport Beach (March 6 – 9, 2000).
7. Nothwang, W. D., Schwartz, R. W., and Ballato, J., "Simple Plate Resonator Modeling and Characterization of the Effects of Mass Loading on the Strain Response of Piezoelectric Actuators," American Ceramic Society Annual Meeting, St. Louis, MO, April 30 – May 3, 2000. *Scheduled.*
8. Nothwang, W. D., Schwartz, R. W., and Ballato, J., "The Use of an Equivalent Circuit Model to Describe Aging and Fatigue Effects in Piezoelectric Ceramics," American Ceramic Society Annual Meeting, St. Louis, MO, April 30 – May 3, 2000. *Scheduled.*

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