

Estimation of the Effective d_{31} Coefficients of the Piezoelectric Layer in Rainbow Actuators

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We have analyzed the performance of Rainbow (reduced and internally biased oxide wafer) actuators by assuming that the key difference between these devices and unimorph actuators is the presence of internal stress that alters the extrinsic (domain switching) contribution to electromechanical response, and thus, the effective d_{31} coefficient of the piezoelectric layer. Based on this assumption, we calculated the d_{31} coefficient as a function of device geometry and electric field and found that the coefficients ranged from approximately -300 to -600 pm/V. The highest d_{31} value was obtained for a Rainbow actuator that was fabricated by reducing 1/3 of the piezoelectric layer; other studies indicated that this device possessed the highest tensile stress in the surface region of the piezoelectric. We observed that geometric effects on calculated d_{31} coefficients were as significant as voltage effects. The analytical approach utilized also permitted estimation of the relative contributions of mechanical and stress effects to the performance of these devices, which were determined to be dependent on field and geometry. Although the estimated d_{31} coefficient for certain geometries is twice the typical low field value, it must be remembered that this value represents an “average” value for the entire piezoelectric layer, which is under a stress gradient; i.e., the lower region of the piezoelectric is in lateral compression, while the upper region is in lateral tension. This suggests that the true electromechanical coefficients of the lead zirconate titanate composition utilized in these devices would display an even broader range of d_{31} values, if d_{31} was characterized as a function of uniform lateral stress.

I. Introduction

RAINBOW (reduced and internally biased oxide wafer) and RThunder® (thin unimorph driver) actuators form a unique family of stress-biased piezoelectric devices that display displacement and load-bearing responses that are substantially enhanced compared with more traditional electromechanical devices.^{1–5} As a result, the devices are of immense interest in applications where high strain is required and device space is restricted.⁶ The

performance characteristics of Rainbow actuators have been summarized by Haertling,¹ and a comparison of the performance characteristics of the two stress-based devices has been given by Wise.⁵ Despite the great interest in these devices, further work is required to better understand the various factors that contribute to their performance. In this paper, we employ unimorph theory to examine the effects of actuator geometry on the effective d_{31} coefficient of the piezoelectric layer within the devices. We also show that this method can be used to determine the relative importance of mechanical and geometric (stress) contributions to the strain response of these actuators under different operational conditions.

Rainbow ceramics are fabricated by an elevated-temperature process in which the lower region of a lead-based piezoelectric polycrystalline ceramic, such as lead zirconate titanate (PZT), lead magnesium niobate, or other electrostrictive composition is chemically reduced through intimate contact with a carbon block at temperatures ranging from 600° to 1200°C .^{1–3} The kinetics of this reduction process, which involves the formation of metallic lead species and produces a “cermet layer,” have been reviewed by Wang and Cross.⁷ During cooling from the reduction temperature, the thermal expansion mismatch between the two layers of the structure results in a domed actuator with a stress profile across the device that is strongly dependent on device geometry.^{8–10} Thunder devices are produced by a different process,⁴ but the resulting device is similar, consisting of a domed structure with a piezoelectric element bonded to a metal layer. Therefore, both devices resemble unimorph actuators, with the most significant differences being that the devices are domed and possess an internal stress profile.

To prepare Rainbows that generate the maximum displacement response, it has been noted that there are significant effects of actuator geometry on performance: devices with cermet layers of 35%⁵ to 50%¹¹ of the total device thickness demonstrate the greatest displacement. There have been numerous studies that have focused on the underlying reasons why device geometry affects strain.^{9,11–14} Suggested contributing factors include the following: (i) simple mechanical effects, as might be expected based on the resemblance of the devices to unimorph actuators;^{9,11} (ii) enhanced extrinsic electromechanical response due to stress and field effects on domain configuration and switching;^{9,11,14,15} and (iii) mass-loading effects.^{9,16} In this paper, we discuss the performance of these devices from the perspectives of mechanical effects, i.e., unimorph response,^{17,18} and stress enhancements to the piezoelectric response due to altered domain configuration and switching characteristics.¹⁵

It has been suggested that Rainbow ceramics may be viewed as unimorph actuators in which the piezoelectric layer is under a stress state that alters the effective electromechanical coupling coefficients of the piezoelectric material.¹¹ In analyzing the performance of Rainbow ceramics with unimorph theory, it was observed that the general response characteristics of the devices were accurately described, as shown in Fig. 1,¹¹ but the magnitude

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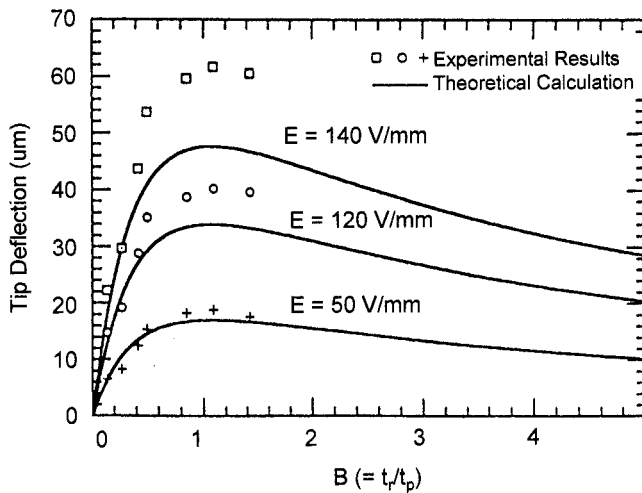


Fig. 1. Tip deflection plotted as a function of thickness ratio for cantilever Rainbow actuators under different electric fields ($f = 5$ Hz, $L = 38$ mm, $t = 1.02$ mm, and $d_{31} = 320$ pm/V).¹¹

of the response was not effectively predicted. In the analysis presented in this earlier work, a d_{31} coefficient of -320 pm/V (the value reported by the manufacturer of the piezoelectric plates) was used in the unimorph approach to model device response as a function of actuator geometry and applied electric field.

In this paper, we follow an approach different from that reported previously to understand the performance of Rainbow ceramics. Because of the effects of field and stress on d coefficients,^{19,20} it is known that the d coefficient of the piezoelectric layer in the Rainbow will vary significantly from the value of a standard poled polycrystalline ceramic.¹⁵ In fact, this is pointed out by Wang and Cross.¹¹ Hence, rather than using unimorph theory with the standard value of d_{31} to analyze displacement response, we assume (as previously suggested) that Rainbows are unimorph devices, but because the piezoelectric layer is under stress, it will show different electromechanical behavior. We then rearrange the unimorph equations and use measured cantilever displacements to estimate “effective” d_{31} coefficients of the piezoelectric layer in Rainbow ceramics that are operated under different electric fields. We also evaluate the performance of actuators fabricated with different piezoelectric/reduced layer thickness ratios, and thus, which possess different internal stress, to illustrate the importance of stress on d_{31} of the piezoelectric layer. The approach that we follow allows for a decoupling of field and stress (geometric) effects from simple mechanical effects. We show that devices fabricated with high tensile stress in the surface region of the piezoelectric have the highest electromechanical coefficients. We also demonstrate that the effective d_{31} coefficient of the piezoelectric layer and, more importantly, the balance between mechanical and geometric contributions to electromechanical response of the devices are dependent on both device geometry and operational conditions. In this paper, we use the word “effective” to describe the average electromechanical response of the piezoelectric layer. We emphasize that by reporting a single d_{31} value for the piezoelectric layer in these devices, this value must be considered as an average value for the layer. In actuality, the stress gradient across the piezoelectric results in different d_{31} values at different locations within the layer.

II. Analytical Approach

The general method used to analyze the performance of the lead zirconate titanate, PZT 5H-based Rainbow ceramics is derived from the constituent equations for unimorphs of Smits,¹⁷ which were subsequently modified by Wang *et al.*¹⁸ The following equations from Wang *et al.* were utilized previously to describe

cantilever tip deflection in terms of applied force and applied voltage:¹⁸

$$\delta = aF + bV \quad (1)$$

$$a = \frac{4s_{11}^p L^3}{wt_p^3} \frac{AB + 1}{1 + 4AB + 6AB^2 + 4AB^3 + A^2B^4} \quad (2)$$

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

$$A = \frac{E_m}{E_p} \quad (4)$$

$$B = \frac{t_r}{t_p} \quad (5)$$

In the above expressions, δ is the tip deflection of the cantilever, the term a relates the tip deflection to an applied force, F , at the cantilever tip, and the term b describes the tip deflection, δ , per applied volt, V . w is the width of the cantilever, L is the length of the cantilever, t_p is the thickness of the piezoelectric layer, and t_r is the thickness of the reduced layer. s_{11}^p is the elastic compliance of the piezoelectric layer and d_{31} is the piezoelectric coefficient. The term A shows the effects of the ratio of Young’s moduli 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 reduced layer to the piezoelectric thickness (t_r/t_p) on the tip deflection. Thus, the tip deflection of the cantilever for a given applied voltage can be described in terms of the ratio of Young’s moduli of the two layers, the piezoelectric coefficient, and the dimensions of the device, including the relative thickness of the two layers. In this paper, we are mostly interested in the displacement response due to an applied voltage. The typical response predicted for these devices, together with the experimentally observed response, is shown in Fig. 1. Significant differences between observed and predicted responses that are both geometry and field dependent may be seen. Experimental details of fabrication and displacement characterization may be found in Ref. 11.

Unimorph analysis of these devices may be taken a step further by assuming the devices are accurately modeled by unimorph theory, and that the observed differences in performance compared with the predictions of unimorph theory are due to stress (geometric) and voltage effects on the effective d_{31} coefficient of the piezoelectric layer. Using this assumption, for the case where $F = 0$, we may rearrange Eq. (1) to solve for b in terms of the measured tip deflection and the applied voltage:

$$b = \delta/V \quad (6)$$

We may then rearrange Eq. (3) to solve for the effective d_{31} coefficients of actuators fabricated with different dimensions and operated under different applied voltages when there is no applied force:

$$d_{31} = \frac{bt_p^2}{3L^2} \frac{1 + 4AB + 6AB^2 + 4AB^3 + A^2B^4}{AB(B + 1)} \quad (7)$$

In addition to modeling Rainbow response, Wang and Cross¹¹ also reported tip deflections for actuators with different dimensions operated at different fields. These results, which are reproduced in Figs. 2(a) and (b), are utilized in the estimation of effective d_{31} coefficients in this paper by using the reported actuator dimensions and Eqs. (6) and (7).

III. Results and Discussion

First, we consider the effects of actuator geometry on the low-field performance of Rainbow devices using the results shown in Fig. 2(a). As noted previously,¹¹ under low applied electric fields, a linear displacement behavior is predicted due to the

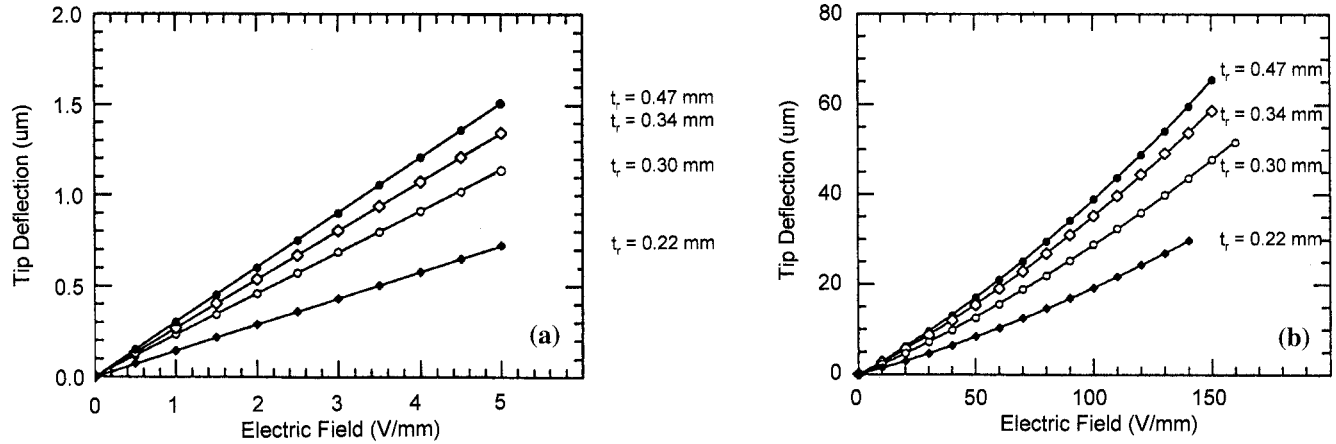


Fig. 2. Tip deflection as a function of electric field for Rainbow actuators fabricated with different reduced layer thicknesses under quasi-static conditions ($f = 5$ Hz, $L = 38$ mm, $t = 1.02$ mm, and $d_{31} = -320$ pm/V):¹¹ (a) low field; (b) high field.

absence of field enhancement effects to electromechanical response. This linear behavior is, in fact, observed, although even at low electric fields, effects of actuator geometry may be noted. Differences in tip deflection (for a given applied electric field) due to different t_r/t_p ratios are expected due to the mechanical enhancement of actuator response associated with the unimorph nature of these devices. Because of the low applied electric fields, we would expect the intrinsic piezoelectric response mechanism to dominate, and initially, we might believe that we could account for these geometric effects (shown in Fig. 2(a)) on tip deflection using only Eqs. (1) to (5), and the reported d_{31} value for the polydomain polycrystalline material (-320 pm/V). The results of these calculations, which were conducted at an applied electric field of 5 V/mm, are shown in Table I, together with the measured tip deflections. As may be seen, even at low electric fields, unimorph theory cannot fully account for the observed tip deflections of devices fabricated with different t_r/t_p ratios. At low t_r values, unimorph theory predicts a slightly greater response than observed, while at higher t_r values, unimorph theory predicts a smaller tip deflection than observed. The greatest discrepancy between the predicted and observed responses (22.9%) occurs for a t_r value of 0.34 (i.e., when the piezoelectric layer has been reduced 33.3%). Below, we further consider the implications of these discrepancies.

Using Eqs. (6) and (7), we have also used the results of Fig. 2(a) to calculate the effective d_{31} coefficients of these Rainbow ceramics at low electric field (5 V/mm). The results of these calculations are also presented in Table I. For the smallest t_r value, the calculated d_{31} coefficient, -297 pm/V, is slightly less than the d_{31} coefficient of -320 pm/V reported by the manufacturer. However, for higher values for t_r , there is an apparent enhancement of the effective d_{31} value, with the maximum value observed for $t_r = 0.34$ (33.3% reduced). It is expected that this device would have the highest tensile stress in the surface region of the piezoelectric.²¹ For this device, an effective d_{31} of -407 pm/V is determined, corresponding to an increase in the effective d_{31} coefficient of 27% compared with the reported value, and 37% compared with

the estimated d_{31} value for the actuator with $t_r = 0.22$. This suggests that, even for low applied electric fields, geometric effects beyond those accounted for by unimorph theory are present. As discussed further below, we believe that these observations are due to variations in the extrinsic piezoelectric response that are related to the different stress profiles that exist across the piezoelectric layer of actuators fabricated with different t_r/t_p ratios. This result is, perhaps, not fully unexpected, given the fact that even at low electric fields in piezoelectric plates, differences have been observed between the electromechanical response of single-domain single crystal (i.e., purely intrinsic) and polydomain polycrystalline (i.e., poled ferroelectric ceramic; intrinsic and extrinsic response) materials.²² The present analysis not only confirms this, but begins to provide a measure of the importance of stress effects on the magnitude of the effective d_{31} coefficient of the piezoelectric layer in these devices.

We have also analyzed the high electric field results of Fig. 2(b) using Eqs. (1) to (7) to compare the predictions of unimorph theory with the observed responses, and to determine the effects of actuator geometry and electric field on the effective d_{31} coefficients in Rainbow actuators. The first part of this analysis is similar to that used to generate Fig. 1, while the second part of the analysis is similar to that used above to calculate d_{31} . In this paper, we focus more on the effects of electric field on tip displacement at different actuator geometries (Fig. 3) compared with the previous analysis that concentrated more on the effects of actuator geometry on tip displacement (Fig. 1 above, and Ref. 11, Fig. 7). Again, our purpose for pursuing this approach is to separate simple mechanical effects (i.e., performance enhancements due to the unimorph structure of these devices) from true differences in the electromechanical response of the piezoelectric layer in these devices that are associated with variations in actuator geometry (t_r/t_p ratio).

The results of these analyses are shown in Figs. 3 through 5 and Table II. In Figs. 3(a) and (b), tip deflection is plotted as a function of electric field for devices with two reduced layer thicknesses. From unimorph theory, we predict that tip deflection will be a function of actuator geometry and will vary linearly with the electric field (see Eqs. (1) and (5)). The linear response that is predicted arises from the fact that d_{31} is assumed to be invariant with geometry (stress profile) and electric field. In terms of geometric effects (t_r/t_p ; the parameter B), a response similar to that seen at low electric fields (Table I) is predicted: actuators fabricated with higher t_r values exhibit greater tip deflections for a given applied voltage. This unimorph enhancement may be considered by looking at the predicted displacement responses for actuators fabricated with $t_r = 0.22$ mm and $t_r = 0.34$ mm, shown in Figs. 3(a) and (b), respectively. For an equivalent electric field (for example, 100 V/mm), the actuator with $t_r = 0.34$ is predicted to have a tip deflection that is 35.6% greater than the actuator fabricated with $t_r = 0.22$. This predicted enhancement in response,

Table I. Effect of Actuator Geometry on Tip Deflection at Low Electric Fields[†]

Reduced layer thickness (mm)	t_r/t_p ratio	Piezoelectric reduced (%)	Tip deflection (μm)		Difference (%)	Calculated effective d_{31} coefficient (pm/V)
			Predicted [‡]	Measured		
0.22	0.275	21.6	0.76	0.72	-5.7	-297
0.30	0.417	29.4	0.96	1.15	15.7	-376
0.34	0.500	33.3	1.03	1.34	22.9	-407
0.47	0.854	46.1	1.18	1.51	21.4	-399

[†]Total actuator thickness: 1.02 mm. [‡]Unimorph theory.

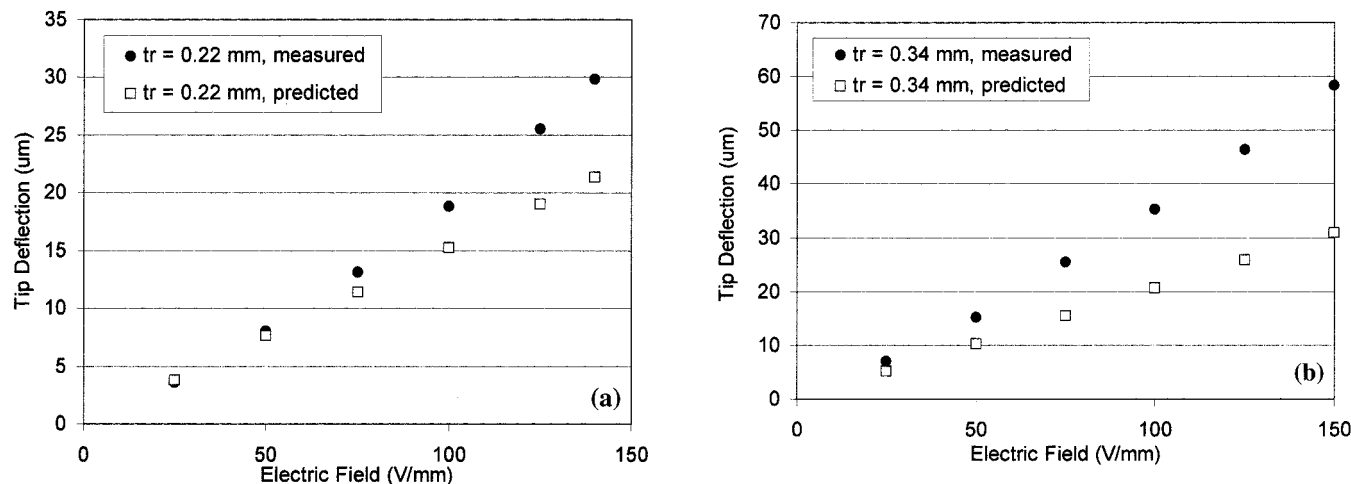


Fig. 3. Predicted and measured tip deflection responses of Rainbow actuators as a function of applied electric field. Data taken from Ref. 11: (a) $t_r = 0.22$ mm and (b) $t_r = 0.34$ mm.

which is qualitatively similar to that observed for the actual devices, is simply due to changing the thickness of the reduced layer within the device; no mass loading effects or variation in extrinsic contribution to electromechanical response are considered. It is evident in these figures, however, that unimorph theory alone cannot describe the observed device response.

In addition to the predicted responses, there are two other interesting aspects of Figs. 3(a) and (b); these may also be seen in Table II. First, it may be seen that the differences between the predicted and observed tip deflections increase as electric field increases. This is an anticipated result based on the enhanced extrinsic contribution to electromechanical response anticipated at higher applied electric fields. The nonlinear nature of this behavior is also evident in both figures. Second, a perhaps more surprising, but equally interesting result, is that the discrepancy between the predicted and measured tip deflections is geometry-dependent: actuators prepared with higher t_r values show a greater discrepancy

between the predicted and measured responses than do actuators fabricated with low t_r values. As shown in Table II, these differences are greatest for Rainbows fabricated with $t_r = 0.34$ mm. Thus, there are field-dependent differences in electromechanical response that are also dependent on actuator geometry, as observed at low electric fields. We believe that these results strongly indicate that the contributions of extrinsic effects (domain configuration/domain wall motion) to electromechanical response are greater for actuators fabricated with $t_r = 0.34$ mm (i.e., $t_r/t_p = 0.5$; $t_r/t_t = 0.33$, where t_t is the total thickness of the Rainbow actuator). Thus, Rainbow actuators that are reduced 33% during fabrication display the greatest extrinsic response contributions to device performance, as evidenced by the greatest difference between the predicted and the observed responses. However, these actuators may not display the greatest overall response because of the presence of other mechanical effects (i.e., standard unimorph enhancements). This is evidenced by the overall greater response of the $t_r = 0.47$ mm actuators, as shown in Fig. 2.

Thus, both mechanical effects and enhanced extrinsic piezoelectric behavior, each of which is geometry dependent, contribute to the observed performance of Rainbow actuators. We suggest that a rough estimate of the relative contribution of each of these effects to the observed performance of the devices may be gained by a review of figures such as those presented here, and a comparison of the predicted and observed responses. We present an example to demonstrate this. At high fields (Fig. 3(a), $E = 140$ V/mm), for the device fabricated with $t_r = 0.22$ mm, $\sim 2/3$ of the observed performance is derived from unimorph-dictated mechanical effects; the other $1/3$ is due to enhanced extrinsic contributions to electromechanical response. In contrast, for the device prepared with $t_r = 0.34$ mm, the relative contributions to the observed performance are different. At $E = 150$ V/mm, only about one-half of the response is due to the mechanical aspects of the device (unimorph enhancement) while the other half is due to greater extrinsic piezoelectric contributions. Obviously, the relative magnitudes of these two contributing factors will also be dependent on electric field, and it is important to note that frequently, these devices are operated at still larger electric fields. Because of the nonlinear nature of the observed δ - V response, we predict that under these conditions, the relative importance of extrinsic domain wall motion effects would be even greater; i.e., more than half of the observed response would be due to the higher effective d coefficients of the piezoelectric layer, rather than simple mechanical effects. Hence, at higher fields, we would expect still greater performance from these actuators compared with analogous unimorph devices.

To further quantify field and geometric effects on electromechanical response, we have utilized Eqs. (6) and (7) to calculate the

Table II. Predicted and Measured Tip Deflections, and Differences between Measured and Predicted Tip Deflections for Actuators Fabricated with Different Reduced Layer Thicknesses (t_r) for Various Electric Fields

t_r (mm)	Electric field (V/mm)	Tip deflection (μm)		Difference (%)
		Measured	Predicted	
0.22	25	3.6	3.8	-6.3
0.22	50	8.0	7.61	5.2
0.22	75	13.2	11.42	13.1
0.22	100	18.8	15.23	19.2
0.22	125	25.5	19.03	25.3
0.22	140	29.8	21.32	28.4
0.30	25	5.7	4.78	16.1
0.30	50	12.3	9.56	22.5
0.30	75	20.4	14.34	29.9
0.30	100	28.6	19.11	33.0
0.30	125	37.3	23.89	35.9
0.30	150	47.6	28.67	39.7
0.34	25	7.0	5.16	26.3
0.34	50	15.2	10.33	32.0
0.34	75	25.4	15.49	39.0
0.34	100	35.3	20.65	41.4
0.34	125	46.4	25.81	44.3
0.34	150	58.4	30.98	46.9
0.47	25	7.6	5.91	22.1
0.47	50	16.7	11.83	29.2
0.47	75	27.0	17.74	34.3
0.47	100	38.7	23.66	38.8
0.47	125	51.1	29.57	42.1
0.47	150	65.2	35.49	45.5

effective d_{31} coefficients of the piezoelectric layers in these actuators. Use of these coefficients in future work may allow for more accurate predictions of the displacement response of these devices under different drive conditions. The results of these calculations are shown in Figs. 4 and 5. In Fig. 4, we have plotted the effective d_{31} coefficient of the piezoelectric layer of actuators fabricated with different geometries as a function of applied electric field. As expected from the above results, the effective d_{31} coefficients are a function of both geometry and electric field. With increasing electric field, d_{31} increases by $\sim 50\%$, independent of geometry, at least for the geometries studied. For the device with $t_r = 0.22$ mm (26.1% reduction), the d_{31} coefficients vary from approximately -300 pm/V ($E = 25$ V/mm) to approximately -450 pm/V ($E = 140$ V/mm). Analogous variations in d_{31} are noted for other actuator geometries, but for reasons discussed below, we suggest further studies of geometric effects on $\Delta d_{31}/\Delta E$, i.e., the field-induced nonlinearity in d , before concluding that it is truly "independent" of Rainbow geometry. It is also interesting to note that while nonlinearity is readily apparent in the tip deflection response (Fig. 3), nonlinearity in $\Delta d_{31}/\Delta E$ is not especially obvious. A linear regression analysis performed on the d_{31} versus E behavior shown in Fig. 4 suggests that $\Delta d_{31}/\Delta E$ is of the order of -1.27 (pm/V)/(V/mm).

In addition to field effects on the effective d_{31} value, Fig. 5 also shows that the geometry of the Rainbow actuator is at least as important as the electric field in defining the effective d_{31} of the piezoelectric layer. For example, in considering the effective d_{31} coefficient at 25 V/mm, the lowest coefficient is observed for actuators with $t_r = 0.22$ mm and with increasing t_r , in general, d_{31} increases. The highest value of d_{31} is noted for devices with $t_r = 0.34$, or when the piezoelectric has been reduced during fabrication by 33.3% (out of the four examined values of 21.6%, 29.4%, 33.3%, and 46.1%). As discussed below, by reducing the piezoelectric layer by this amount, a device with maximum lateral tensile stress in the surface region is formed. This generates a domain configuration with the highest percentage of a -domains, and hence, a device with a maximized extrinsic (domain switching) contribution to the electromechanical response. While there is evidence of some domain pinning in Rainbow actuators with high lateral tensile stresses, the altered initial domain configuration and greater a - to c -domain switching overcome this effect, yielding high displacement devices.¹⁵

The effects of actuator geometry on d_{31} are further examined in Fig. 5. For all samples, the highest electric fields always generated the highest tip displacements. However, in this figure, it may be seen that the effects of geometry are equal in importance to electric field with regard to enhancement of the effective d_{31} coefficient.

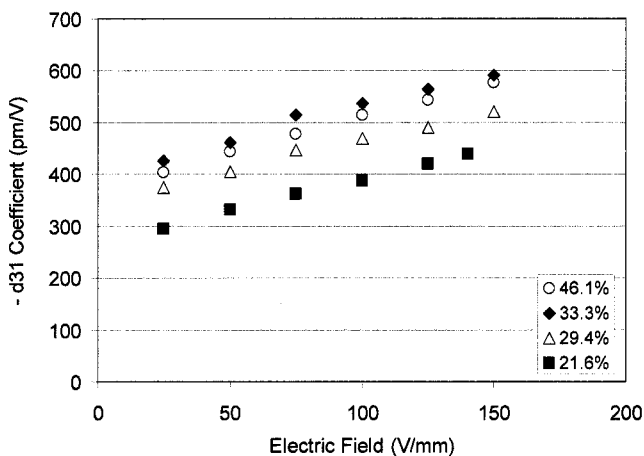


Fig. 4. Calculated effective d_{31} coefficient as a function of electric field for Rainbow actuators with different reduced layer thicknesses as a function of applied electric field: 21.6% reduced, $t_r = 0.22$ mm; 29.4% reduced, $t_r = 0.30$ mm; 33.3% reduced, $t_r = 0.34$ mm; and 46.1% reduced, $t_r = 0.47$ mm.

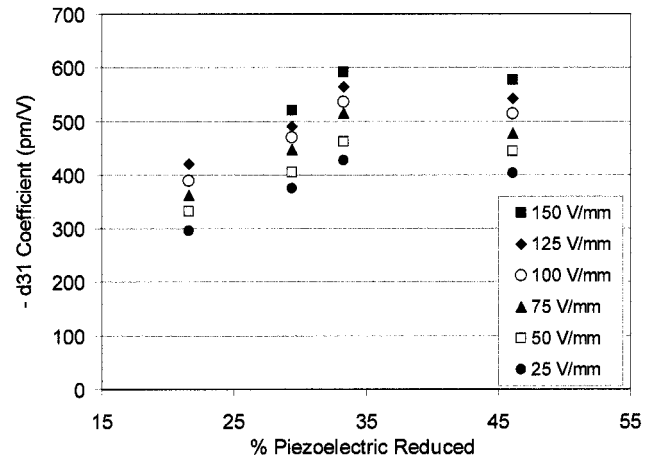


Fig. 5. Calculated effective d_{31} coefficient of Rainbow actuators as a function of relative percent piezoelectric reduced: 21.6% reduced, $t_r = 0.22$ mm; 29.4% reduced, $t_r = 0.30$ mm; 33.3% reduced, $t_r = 0.34$ mm; and 46.1% reduced, $t_r = 0.47$ mm.

Comparing the effects of field and geometry, 100% enhancements in the value of the effective d_{31} of the piezoelectric layer are possible by using high electric fields and fabricating devices that are reduced by $\sim 33\%$. We note that these enhancements are for the particular field and geometric conditions studied; still further enhancements in actuator performance are likely attainable through optimization of geometric factors such as the length/width ratio⁹ and the t_r/t_p ratio.¹² For example, 35% reduction versus the evaluated 33.3% ($t_r = 0.34$ mm) may give a greater response, but this has not been tested. Although further optimization of actuator displacement response should thus be possible, Figs. 3 through 5 clearly show the importance of actuator geometry effects on electromechanical response that go well beyond simple unimorph enhancements.

As suggested by Haertling,¹⁴ we believe the enhanced electro-mechanical response of Rainbow devices is at least partially attributable to the altered domain configuration that is present (a higher population of a -domains near the surface) due to the tensile stress in this region of Rainbow actuators fabricated with commonly used reduction ratios. The important factor here is that the presence of lateral tensile stress generates a domain configuration similar to that used by Wang and Cross²³ in their polydomain single-crystal BaTiO₃ actuator, and those actuators that have the highest a -domain percentages would display the highest piezoelectric coefficients. Because lateral tensile stress is expected to promote the formation of a -domains, we would predict that under fabrication conditions where the tensile stress is maximized, the highest d_{31} coefficient should be observed, assuming that the tensile stress is not sufficiently high to induce clamping of domain wall motion under the applied electric fields that are utilized.^{19,20}

To determine the validity of this concept, we have used finite element (FEA) modeling to study the effects of percent reduction on stress within the piezoelectric layer for devices that have similar geometries (5 mm width, 30 mm length, and 0.5 mm thickness).^{9,24,25} The results of this analysis are summarized in Table III, and a full discussion of the modeling approach may be found in Ref. 24. Also shown in this table are the results of a heterogeneous thin plate analysis^{26,27} of the stress magnitude at the surface of circular Rainbows prepared with various degrees of reduction.²¹ While the stress values obtained by these methods differ substantially (for reasons discussed below), it may be seen that, irrespective of the modeling method, or circular versus rectangular parts, the highest tensile stresses (for the four t_r/t_p ratios studied) are in fact noted for Rainbows that have a reduced layer thickness of 35% of the total actuator thickness. Nearly identical fabrication conditions (33.3% reduction) result in devices with the highest d_{31} coefficients as seen in Fig. 5. Thus, devices with the highest tensile

Table III. Compressive and Tensile Stresses at the Reduced Layer/Piezoelectric Interface and the Surface of Rainbow Actuators Prepared with Different Extents of Reduction Calculated by Finite Element Analysis,^{24,25} and a Heterogeneous Thin Plate Approach²¹

% reduced	Stress (MPa)		
	Finite element analysis [†]		Heterogeneous thin plate analysis at the piezoelectric surface [‡]
	Piezoelectric surface	Interface with the reduced layer	
20	225	−380	27
30	260	−460	35
35	285	—	39
50	230	−410	32

[†]Actuator geometry: 30 mm long × 5 mm wide × 0.5 mm thick rectangular parts.
[‡]Actuator geometry: 25.4 mm diameter, 0.5 mm thick circular parts. Stress magnitudes reported are for actuators with a grain size of 5.5 μm.²¹

stresses in the surface region of the piezoelectric layer possess the highest effective d_{31} coefficients.

The magnitude of the stresses derived from finite element modeling^{9,24} is quite high, ranging from 225 MPa tensile stress at the surface to 460 MPa compressive stress at the lower interface. While these values are in agreement with previously published results for similar analyses,¹² an important aspect of the piezoelectric layer has been neglected in these simple finite element approaches, causing an overestimation of the magnitude of the stresses in these devices. In these previous FEA approaches,^{9,12,24} the investigators did not account for the ferroelastic nature of the material. This behavior not only contributes to the high a -domain population in the surface region of the devices that is observed, but also contributes to the mechanical softening of the piezoelectric layer during processing. This results in actual stress levels that are significantly lower than those calculated. By comparing the stress levels estimated by FEA with actual measurements of device deformation after processing,²¹ it has been estimated that the maximum tensile stress levels in the surface region of the device are of the order of 40 to 50 MPa, rather than 225 MPa. This explains why clamping of domain wall motion, as would be expected for such high stress levels,^{19,20} does not occur. Also, the 40–50 MPa values estimated from the thermoelastic theory approach and the measured dome heights result in values that are close to the reported tensile strengths (38 to 51 MPa) for PZT materials.²⁸ Although the results of the FEA simulations are not quantitatively correct, the relationship between the relative stress magnitude and device geometry is still accurate. We thus use these values in our analysis of device geometry and stress effects, and we note that the use of the lower stress values obtained by the heterogeneous thin plate approach applied to circular actuators yields a similar result. Studies of domain configuration and switching as a function of device geometry support this interpretation.¹⁵

We want to consider the magnitude of the observed variation in the effective d_{31} of the piezoelectric layer as a function of stress. Since device geometry defines the stress profile that exists across the Rainbow, as well as the magnitude of the stress, the observed effects of geometry on displacement response (Fig. 3) that are not due to unimorph mechanics effects are due to stress (and field) effects on d_{31} of the piezoelectric layer. Stated otherwise, the results of Fig. 5 show more inherently the effects of stress on d_{31} , rather than the effects of sample geometry on d_{31} . It may be concluded that the effects of lateral stress on the effective d coefficients of these materials are pronounced. Devices that show relatively minor stress variations (225 MPa for 20% reduction vs 285 MPa for 35% reduction) demonstrate large differences in the effective d_{31} coefficient. Rainbow or other actuator devices that are fabricated with stresses that are either smaller or still greater would be expected to show effective d coefficients that are even more different from standard poled polycrystalline materials. Further, it is also important to recall that the effective d_{31} coefficients determined in this paper as a function of Rainbow

geometry represent only an “average” value for the entire piezoelectric layer, which is subject to a stress profile that ranges from compressive at the interface with the reduced layer to tensile at the surface. We, therefore, expect the d_{31} value in the surface region of the material to be even higher than our estimated value, due to a domain configuration that has a higher a -domain population compared with the piezoelectric layer as a whole. In the lower region of the piezoelectric, which is under compressive stress, and which we would expect to have a lower a -domain population than a standard poled polycrystalline ceramic,¹² we expect the d_{31} value to be lower than the average value reported. In the limit, the d_{31} value of this region of the piezoelectric might approach the value of solely the intrinsic response. The variation in the piezoelectric coefficient as a function of position within the layer has previously been suggested by Li, Furman, and Haertling,¹² and a recent study of the effects of stress on d_{31} lends credence to this hypothesis.¹⁵ We note, however, that our estimated d_{31} values are higher than those suggested by Li, Furman, and Haertling¹² in their analysis of Rainbow actuators. A contributing factor to this difference may be the rectangular versus circular geometry of the two sets of devices studied. To fully understand the response of Rainbow devices, studies of the specific effects of lateral tensile and compressive stresses on domain configuration and domain wall motion in less complex systems where the stress state and magnitude are uniform are required.

IV. Summary

By assuming that Rainbow ceramics are unimorph devices that possess a superimposed stress field, we have estimated the effective d_{31} coefficients of the piezoelectric layer in these devices as a function of electric field and actuator geometry. We found that both field and geometry have significant effects on d_{31} . The d_{31} coefficient varies from approximately −300 pm/V for devices fabricated with small reduction ratios that are operated at low fields, to more than −600 pm/V for devices with a reduction ratio of 33.3% operated at high electric field. The calculated d coefficients allow for predictions of device performance as a function of actuator geometry. More significantly, the approach utilized allows for estimation of the relative importance of the two contributing mechanisms, mechanical effects due to unimorph enhancements and increased piezoelectric response, that serve to define the high strain capabilities of these devices. We also observed that the balance between these two performance-enhancing mechanisms was dependent on both applied field and device geometry. When the devices studied were operated under comparatively low electric fields (5 V/mm), the majority of the device response can be accounted for by unimorph theory; extrinsic contributions to performance are minimal. However, under higher electric fields, and especially for devices prepared with reduction ratios of ~33%, the balance between these two mechanisms was shifted, and increased effective d_{31} coefficients were responsible for at least 50% of the observed displacement response of the devices. Taken together with the results of other studies, these results confirm that the enhanced response of these devices is due, in part, to the effective enhancement in the piezoelectric coefficients that arises from the internal stress field within the device, likely, the tensile stress in the surface region. Since the estimated d_{31} coefficients represent an “average” value for the piezoelectric layer, still more widely varied coefficients are expected for the surface and interface regions of the device, where higher than average tensile and compressive stresses exist, respectively. Further studies of the effects of lateral stress on the nonlinear response of the d coefficients are required. It is also interesting to consider the use of unimorph theory to study force effects on these devices (i.e., the first term in Eq. (1) above). However, we anticipate that the nonplanar geometry of these devices would complicate the analysis of device response to applied force to a much greater extent than the free displacement analysis presented here.

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