Finite Element Modelling
of Electroceramics

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January 1999

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Executive Summary

This report has been written by Fiona Lowrie of The Structural Materials Centre, DERA, Farnborough, acting as a subcontractor for NPL on the DTI-funded project 6CAM7.

The aim of this study was to investigate whether finite element analysis (FEA) could be used to accurately predict the behaviour of two piezoelectric devices. The choice of two devices, an interdigitated electrode device and a bimorph transducer, is discussed and the construction of a piezoelectric FE model explained. Models of the two devices were produced, and the strain response due to applied electric field predicted. Results were then compared to those experimentally measured, where good agreement was found between the predicted and measured strain of the interdigitated electrode. For the bimorph transducer, the non-linear behaviour of the piezoelectric parameters, due to the high applied fields, caused the modelled response to deviate from that expected. Once the non-linear behaviour was accounted for through modification of the FEA input variables, the model also agreed with the measured data.

ISSN 1361-4061

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Approved on behalf of Managing Director, NPL, by Dr C Lea,
Head, Centre for Materials Measurement and Technology

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1. INTRODUCTION

In the field of electroceramics there is a vast range of devices already in use, and new materials and devices are rapidly becoming available. It is essential that manufacturers are able to optimise device performance, and so the effect of conditions which will be encountered during operation, such as stress, field (especially high drive levels) and temperature, must be known. It is also increasingly important that a realistic assessment of the lifetime response under operating conditions can be made, i.e. the fatigue characteristics need to be better understood.

Analytical solutions of piezoelectric device performance generally examine simple shapes (e.g. discs) under static load or at resonance conditions. Analytical solutions of complex geometries (as in geometries of actual devices) often involve assumptions which simplify the stress state and electric field distribution within the device. Invariably, this leads to inaccurate predictions of the observed response.

The advantage of finite element analysis (FE) over analytical solutions is that stress and electrical field measurements of complex geometries, and their variations throughout the device, are more readily calculated. FE allows calculation of the stress and electric field distributions under static loads and under any applied electrical frequency, and so the effect of device geometry can be assessed and optimised without the need to manufacture and test numerous devices. In addition, it should be possible to give a prediction of lifetime without the need to perform numerous time-consuming tests if the relevant fatigue parameters are obtained.

The aim of this study was to investigate the capability of FE to accurately model the behaviour of two piezoelectric devices. In a second report the ability of FE to predict degradation over time will be discussed using the devices explained in the present study. In this report the details of how an FE model for piezoelectric material is constructed are explained. Models of two devices, an interdigitated electrode (IDE) and a bimorph transducer, were produced. In order to validate the models, the strain response of these devices was experimentally measured and compared to that predicted by FE.

In addition, the use of FE to predict non-linear piezoelectric behaviour is reported, using simple models of the response of a disc geometry. This is dealt with in annex A.

This work was carried out as part of the CAM7 programme, sub-contracted by NPL, and funded by DTI.

2. BACKGROUND THEORY

2.1 INTRODUCTION TO FINITE ELEMENT MODELLING

The fundamental assumption of finite element analysis is that any continuous function, such as stress, strain or electric field, can be approximated by discretisation. The original volume is divided into elements, and within each element the function is constant or a simple function of position, either linear or quadratic. At each vertex of an element is a ‘node’ and the number of variables acting at each nodal site is called the ‘degree of freedom’ (DOF) [1].

For piezoelectrics there are four DOF at each node; UX, UY and UZ (3D displacement) and voltage. To each DOF there is a reaction force FX, FY, FZ to the displacement and charge Q to the voltage. In this case it is necessary to use ‘coupled-field analysis’ to couple the interaction between applied stress and electric field. ANSYS has three specific coupled field elements for piezoelectric analysis:

SOLID5 - 3D Coupled-field solid element
SOLID13 - 2D Coupled-field solid element
SOLID98 - Tetrahedral coupled-field solid element

The choice between these three coupled field elements is dependent upon the sample geometry being modelled. For example, a tetrahedral coupled-field solid element is more suited to dividing a 3D spherical body into elements, whereas SOLID5 constructs with cuboid elements and hence is used to discretise 3D cuboid bodies.

The electromechanical constitutive equations for linear behaviour of the elements are [2]:

$\{T\} = [c]\{S\} - [e]\{E\}$ *eqn. 1*
$\{D\} = [e]\{S\} + [\varepsilon]\{E\}$ *eqn. 2*

where,
{T} = stress vector
{D} = electric flux density vector
{S} = strain vector
{E} = electric filed vector
[c] = elasticity matrix
[e] = piezoelectric matrix
[ε] = dielectric matrix

Application of the variational principle of finite element discretisation to the coupled finite element discretisation yields the following equation.[3]

$$[M_{uu}].\ddot{u} + [C_{uu}].\dot{u} + \begin{bmatrix} K_{uu} & K_{uf} \\ K_{uf} & K_{ff} \end{bmatrix}.u = \begin{bmatrix} F \\ Q \end{bmatrix} \qquad \textit{eqn. 3}$$

where

$[K_{uu}]$ = mechanical stiffness matrix derived from [c] matirx
$[K_{u\phi}]$ = piezoelectric stiffness matrix derived from [e] matrix

$[K_{\phi\phi}]$ = dielectric stiffness matrix derived from [ε] matrix
$[C_{uu}]$ = mechanical loss matrix
$[M_{uu}]$ = inertia matrix derived from density and volume
$\underline{u}$ = displacement vector
ϕ = voltage vector
F = mechanical force vector
Q = charge vector

Therefore to undertake finite element analysis and solve the above equations the following information is required:

(i) device geometry and loading conditions - this would define the quantities of stress, strain and electric field in equations 1 and 2

(ii) material property matrices as required in equations 1 and 2 which are shown below [3]

The dielectric matrix

$$\begin{bmatrix} e_{11} & 0 & 0 \\ 0 & e_{11} & 0 \\ 0 & 0 & e_{33} \end{bmatrix}$$

The piezoelectric matrix

$$\begin{bmatrix} 0 & 0 & d_{13} \\ 0 & 0 & d_{23} \\ 0 & 0 & d_{33} \\ 0 & d_{15} & 0 \\ d_{15} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The stiffness matrix

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix}$$

2.2 SENSITIVITY OF MATRICES

As discussed, the three constitutive matrices, comprising 12 unique coefficients, are required for a precise FE analysis of a generic piezoelectric device. In many cases, however, only a few of these parameters will critically affect the performance of the device, so initial work is required to investigate the sensitivity of device response to variations in specific matrix components such as d_{33}, ε_{11} or c_{33}.

2.3 NON-LINEAR BEHAVIOUR

Piezoelectric materials consist of regions called domains, where the polarisation vector is in the same direction. When a mechanical or electrical load is applied to the material, the size and position of the domains change, through movement of the domain walls, and this causes the observed piezoelectric response. There are two types of domain wall, termed 180° and non-180°. The 180° walls respond only to applied electric field, whereas the non-180° respond to both electric field and mechanical stress, and it is the movement of these non-180° walls which cause the non-linear piezolelectric behaviour which has been observed at high fields [4]. Once the field value up to which linear behaviour occurs has been exceeded, the strain response will also be hysteretic due to the loss associated with movement of the non-180° domain walls and prediction of the strain response will no longer be straightforward.

However, in order to produce higher strains and larger power output piezoelectric materials are being increasingly used in the non-linear regime, so this is an issue which must be addressed. Existing FE packages model linear piezoelectric behaviour, i.e. strain is proportional to applied field. In this study therefore, non-linear behaviour has been modelled by manually adjusting the relevant values in the model as the piezoelectric parameters change. Success of this modelling method relies on experimental measurements of electromechanical properties as a function of applied field to quantify the linear and non-linear regimes.

2.4 CHOICE OF DEVICES

Two devices have been modelled and fabricated under the CAM7 programme and their predicted performance compared to experimental results. The devices were selected as follows:

2.4.1 Interdigitated electrode device (IDE)

The IDE is used as a high strain actuator, in applications where the large actuation in the length direction is desired. IDE devices have thin arrays of electrodes screen printed onto piezoelectric material, as shown in figure (1). The poling direction, i.e. the direction of remnant polarisation induced by the application of a strong d.c. field, is along the length direction. Because of the electrode configuration a non-uniform electric field is produced which results in a stressed state in the device. The advantage of this device is that the electric field is in the direction of actuation i.e. actuation is in the d_{33} direction rather than d_{31}, and therefore takes advantage of the fact that the d_{33} is always considerably larger than the d_{31}.

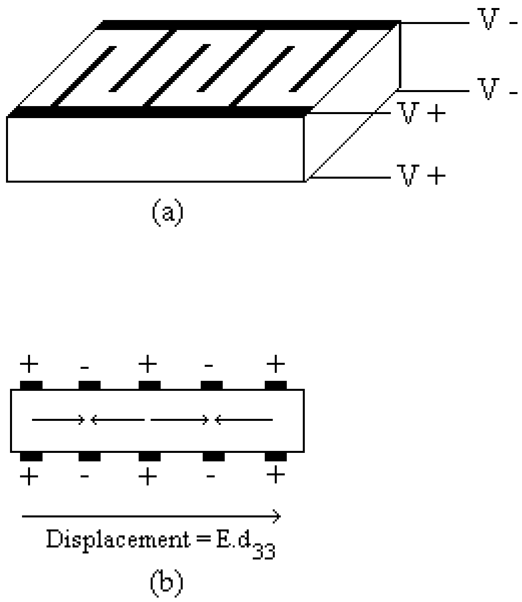

Figure 1: Diagram showing (a) the electrode configuration and (b) the field distribution and overall displacement for an IDE

This device has been chosen as its response is likely to be heavily dependent on the d_{33} value, realising simpler solutions that can be experimentally investigated and validated. In addition, the non-linear and time-dependent values of d_{33} have been measured for this study by NPL, so time-dependent behaviour of this device can also be modelled.

2.4.2 Bimorph transducer

A bimorph is used as a displacement transducer or accelerometer. The device consists of two beams of piezoelectric material joined together with an intervening electrode, as well as electrodes on the outer surfaces of the two beams. The beams are poled through the thickness direction, so when the field is applied one part of the beam will expand in the d_{31} direction, while the other contracts, resulting in a bending moment and displacement, as shown in figure (2).

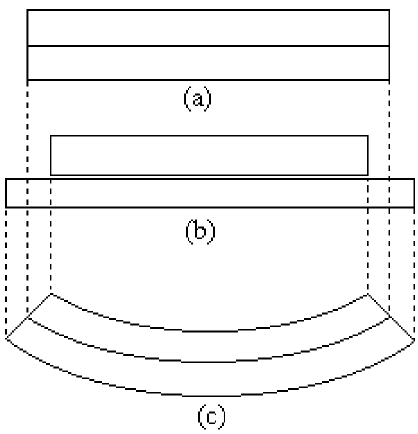

Figure 2: Diagram showing (a) undeformed bimorph, (b) separate deformation of each piezoelectric beam when electric field is applied, and (c) resultant deflection of bimorph.

This device is of interest due to the high stress induced in the material, resulting from the large deflection. Therefore, this is a good candidate for modelling electro-mechanical fatigue. It would be expected that as the device is cycled under high field, microcracking or other degradation of piezoelectric properties may occur with increasing number of cycles.

3. CONSTRUCTION OF FE MODELS

Models of both devices were constructed using ANSYS, with standard values available in literature being used for the relevant material parameters [5][6]. Plots of strain versus field and consequent internal stress distribution were predicted for each device, and the significance of each of the parameters listed in the matrices in section 2.1 investigated by individually varying each parameter, and comparing the resultant strain.

3.1 IDE DEVICE

The non-uniform behaviour of the electric field is shown by the FE model in figure (3). It is clear that directly below the electrodes is a region where the field is small and normal to the poling direction. The non-uniform field leads to internal stresses, which the model predicts as being greatest in magnitude near the electrode edges, as shown in figure (4).

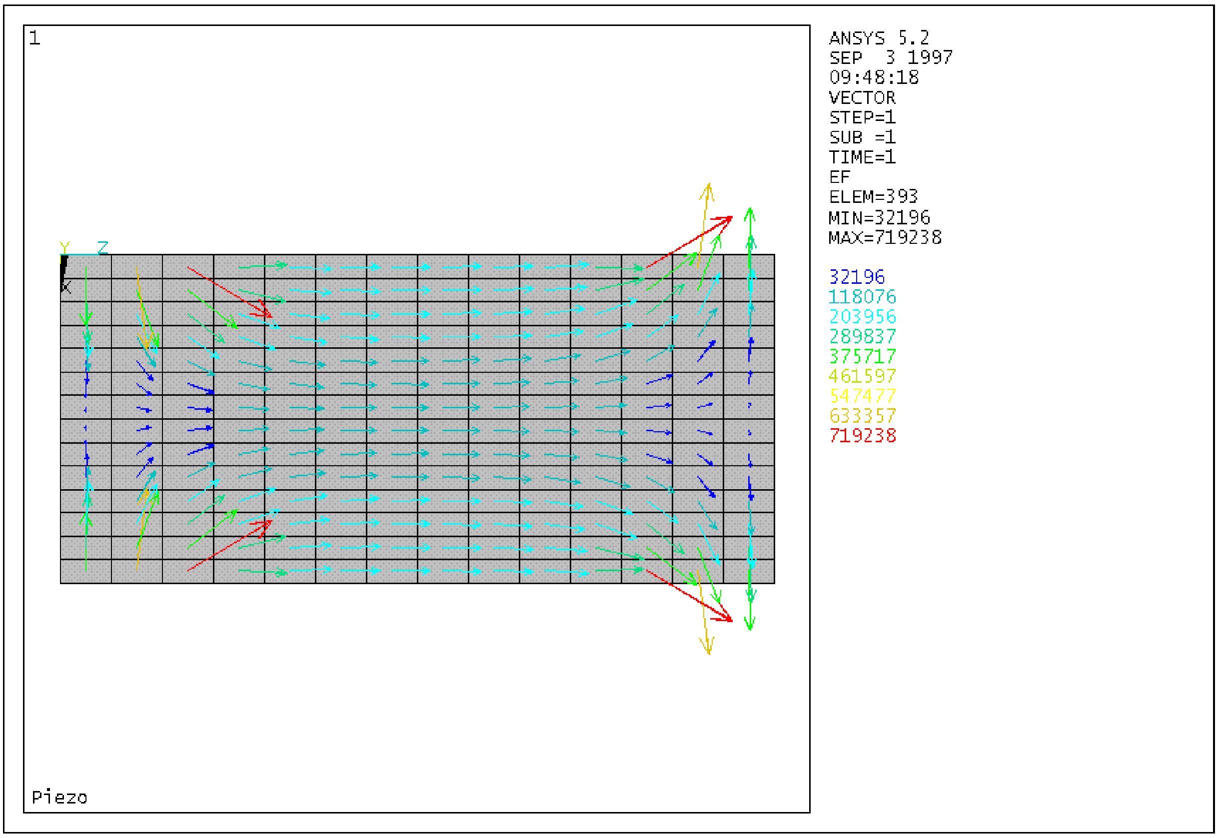

Figure 3: Predicted variation of electric field in IDE

The only parameter which was found to have a significant effect on the predicted longitudinal strain was d_{33}.

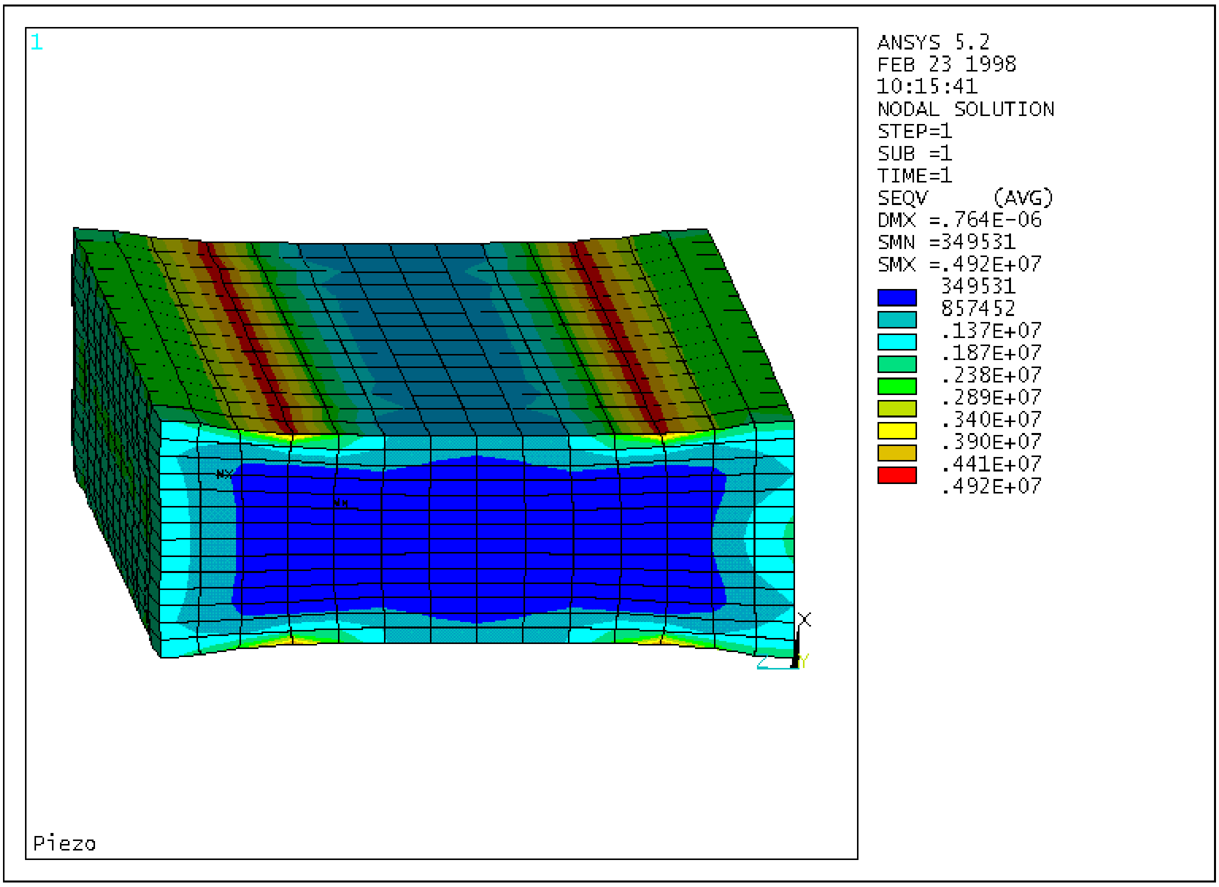

Figure 4: Predicted internal stresses produced in IDE

3.2 BIMORPH TRANSDUCER

The predicted stress distribution produced in the bimorph under an applied field of 750 V/mm is shown in figure (5a). It can be seen that the maximum stress experienced by the ceramic as it deflected was always in the ceramic region parallel to the central interface, where there was a layer of adhesive. The thickness of the adhesive layer was found to affect the predicted deflection and stress value in the ceramic; as the layer was made thinner, the deflection decreased and the stress increased. The predicted stress distribution was also affected by the clamping conditions used in the model - if deformation of the perspex clamp was not modelled the magnitude of the maximum stress was increased, and was located in the material in contact with the clamp, at the surface electrodes.

The stress experienced in the clamp is shown in figure (5b), which shows the maximum stress is located in the region where the bimorph bends against the clamp; it can also be seen that the clamp itself is deforming in this region as a result of the bimorph deflection. The maximum predicted stress in the clamp was less than that in the bimorph, being ~ 4 MPa in the clamp compared to 30 MPa in the bimorph for an applied field of 750 V/mm.

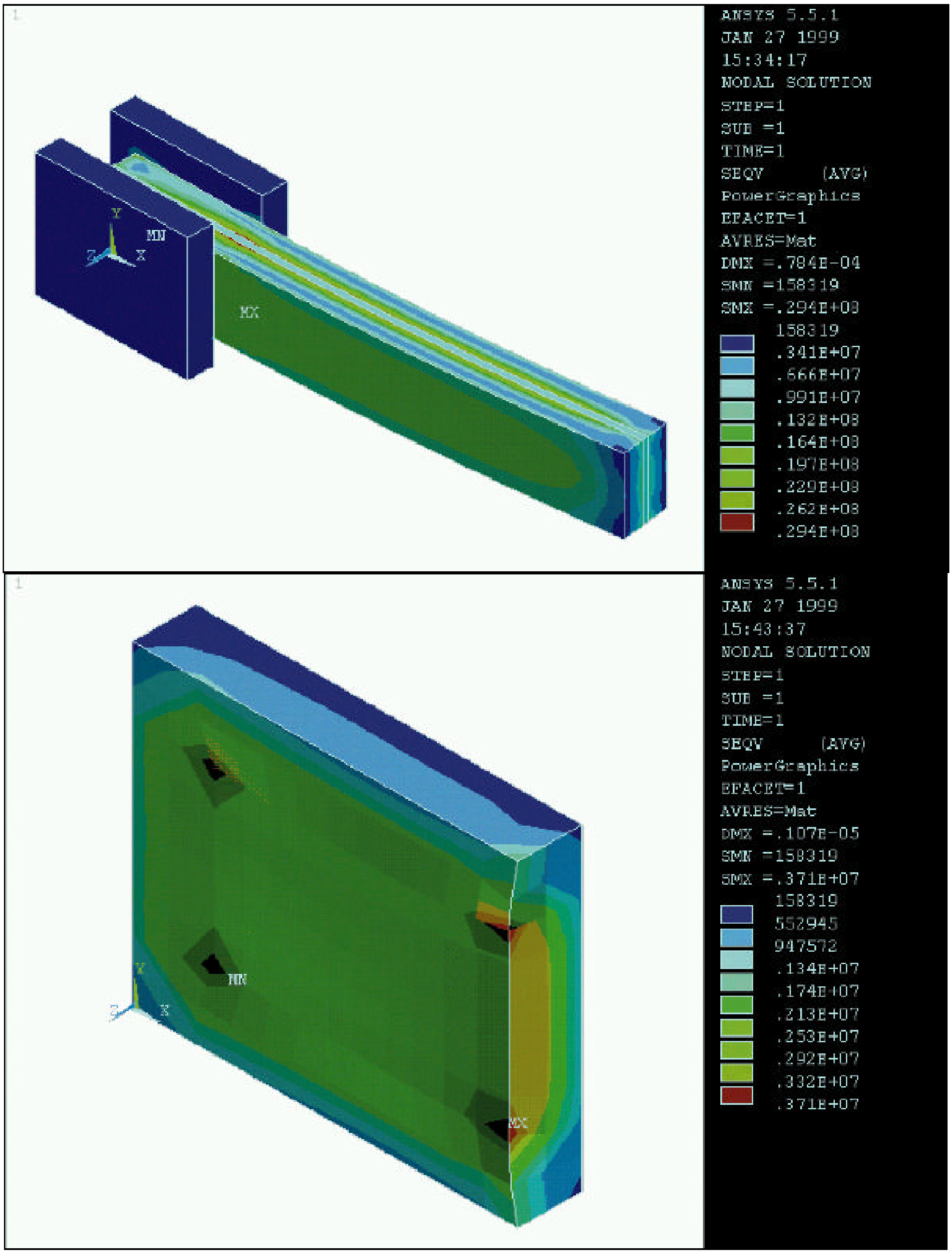

Figure 5: Stress distribution predicted by FEA in (a) bimorph and (b) clamp

Using the model which included the perspex clamp, it was found that the parameter which had a significant effect on the predicted deflection was d_{31}. The extent of this effect is shown in figure (6), where 10% and 20% changes in d_{31} caused 9% and 17% changes in respective predicted deflections.

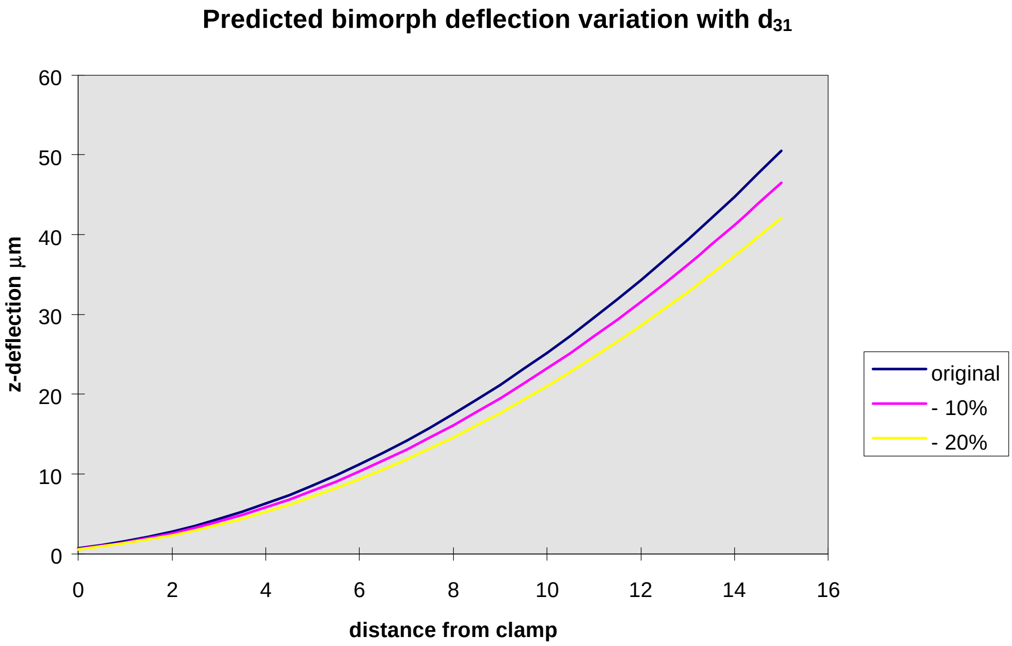

Figure 6: Graph showing the effect on bimorph deflection due to changes in d_{31}

4. VALIDATION OF FE MODELS

4.1 IDE DEVICE

IDE devices were manufactured at DERA. Substrate piezoelectric material was supplied by Ferroperm in the form of plates of PZ-26. Their dimensions were 50 mm x 25 mm x 1 mm and the i. d. electrodes were formed using a 'lift-off'[1] process. The device was then poled by the application of a static field of 3 kV/mm. Figure (7) shows the dimensions of the electrode configuration and poling direction.

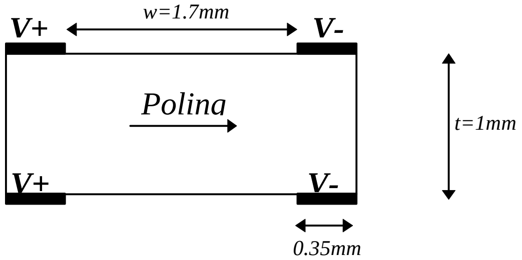

Figure 7: Dimensions of IDE used

In order to measure the strain achieved by the device, strain gauges were applied parallel and normal to the electrode lines. The potential difference across the electrodes was applied in steps of 100 V, up to a field of 700 V/mm, using a function generator and amplifier, and the corresponding strain was measured. The measured strain was then compared to that predicted by the FE [7].

4.2 BIMORPH TRANSDUCER

The material used to make the bimorph was supplied by Morgan Matroc in the form of pre-poled plates of PZT-5A, of area 20 mm^2, and 1 mm thick. These were bonded together using an epoxy resin, and cut into strips 3 mm wide, giving devices of overall thickness 2 mm. The direction of poling is shown in figure (8).

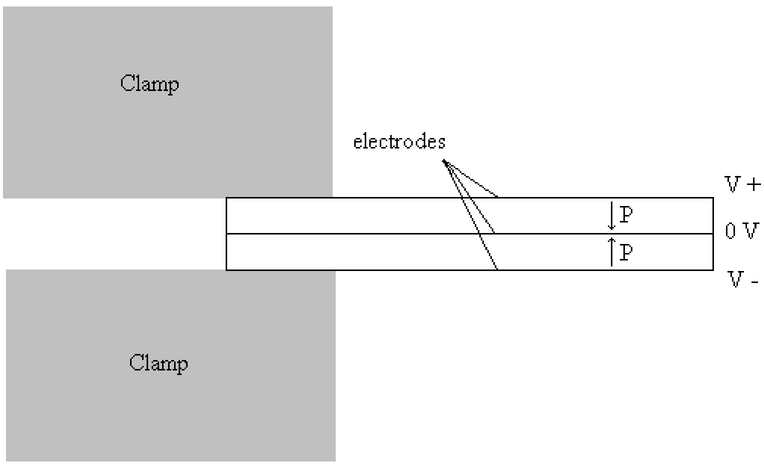

Figure 8: Poling configuration of bimorph

[1] The 'lift-off' process comprises creating a negative form of the electrode pattern on the substrate using a layer of photoresist, coating the entire surface with copper, and then removing the photoresist and overlying copper with a solvent. This leaves the copper which had been deposited directly onto the substrate in the electrode pattern.

To measure the deflection of the device, one end was held in a perspex clamp and a potential difference was applied across the top and bottom surface electrodes. The resultant deflection was measured at various positions along the length using a laser interferometer. The effect of amount of material held inside the clamp was investigated by varying the length held inside the perspex, from 5 mm to 10 mm, and measuring the deflection as before. The fields used were ± 50, 250, 500 and 750 V/mm.

5. RESULTS

5.1 IDE DEVICE

The measured strain versus field is shown in figure (9), and compared to that predicted by FE. The plots show a good correlation between the observed and modelled values, with the strain in the length direction being approximately twice that in the width direction. None of the parameters initially used to construct the model required adjusting in order that the predicted deflection should agree with that measured, so it was assumed that the piezoelectric material was maintained within its linear region over the voltage range used.

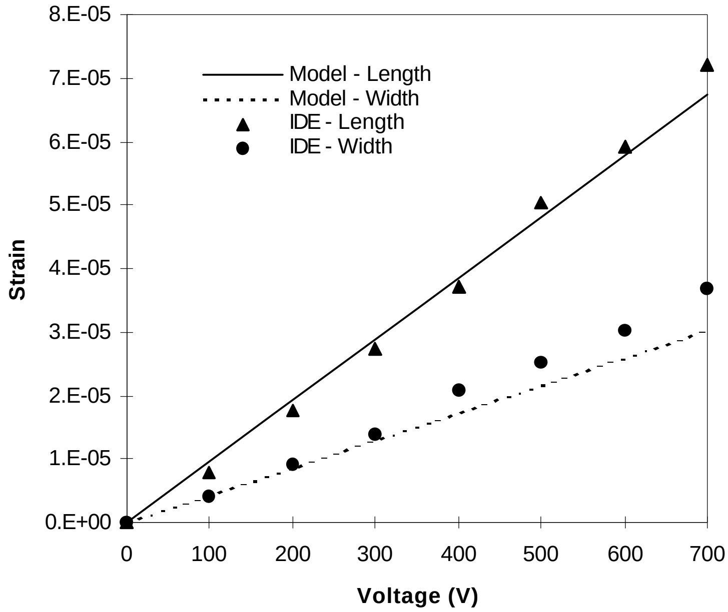

Figure 9: Comparison of modelling and experimental results for IDE

The maximum stress predicted was 5 MPa, at an applied voltage of 700 V.

5.2 BIMORPH TRANSDUCER

It was found that the deflection measured when the length of the bimorph held inside the clamp was varied from 5 mm to 10 mm was the same, within experimental error. Hence for the remaining tests the length of the bimorph held inside the clamp was always kept as 5 mm.

The plots of deflection versus position along bimorph length and deflection versus field are compared with those predicted from FE as shown in figures (10) and (11). There is good agreement between the experimental and predicted deflection at the lowest field, 50 V/mm (see figure (10)), but in order to achieve agreement at fields of 250, 500 and 750 V/mm the d_{31} value had to be increased in the model from the standard literature value initially used. Figure (11) shows a non-linear relationship between the deflection at a specific position, 10 mm along the bimorph length, and the applied field, the strain response increasing more than had been predicted assuming the initial d_{31} value. The increase in d_{31} required to give agreement between the predicted and experimentally measured deflections is given in table (1).

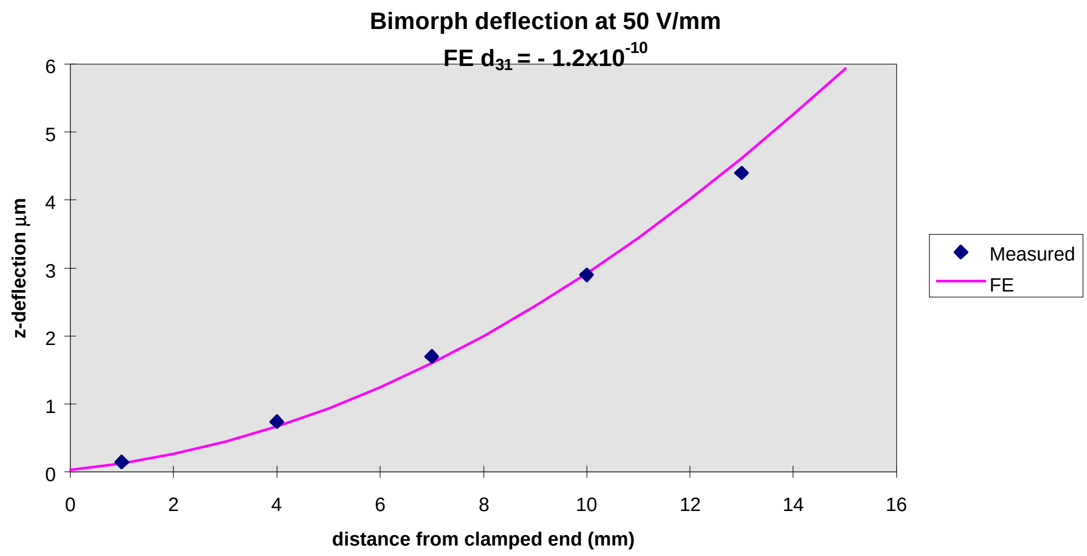

Figure (10a)

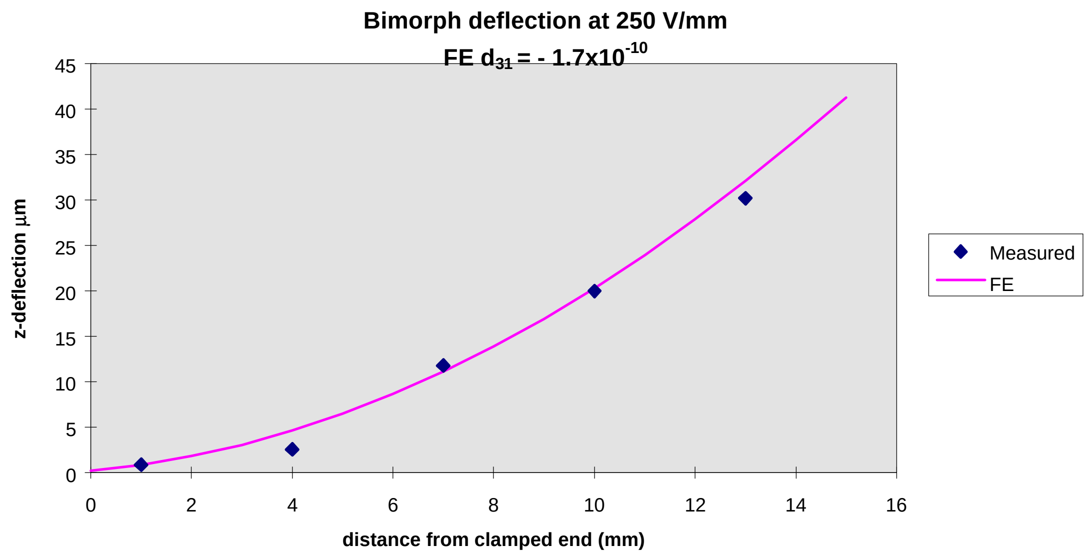

Figure (10b)

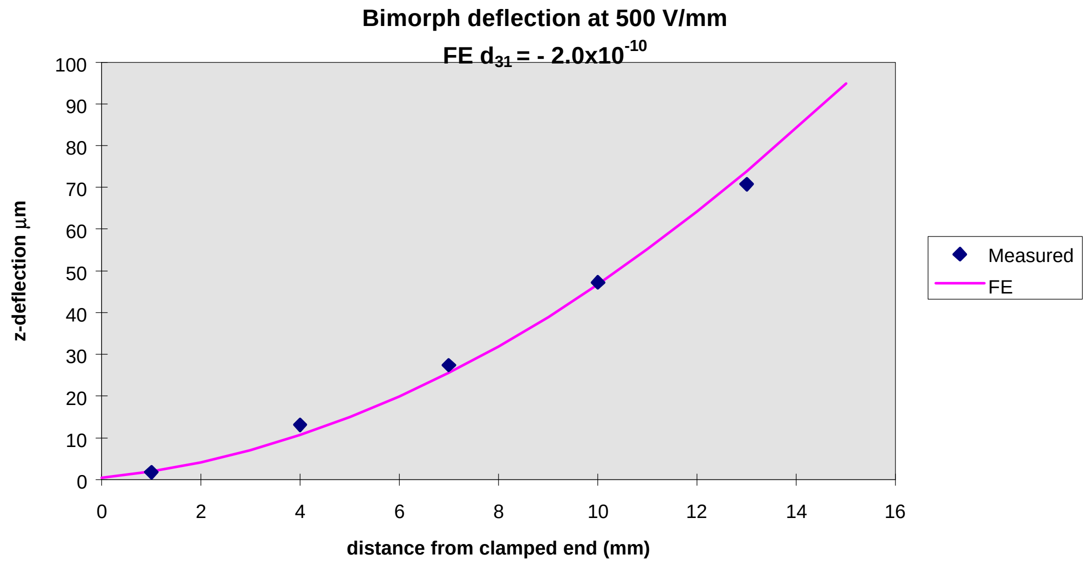

Figure (10c)

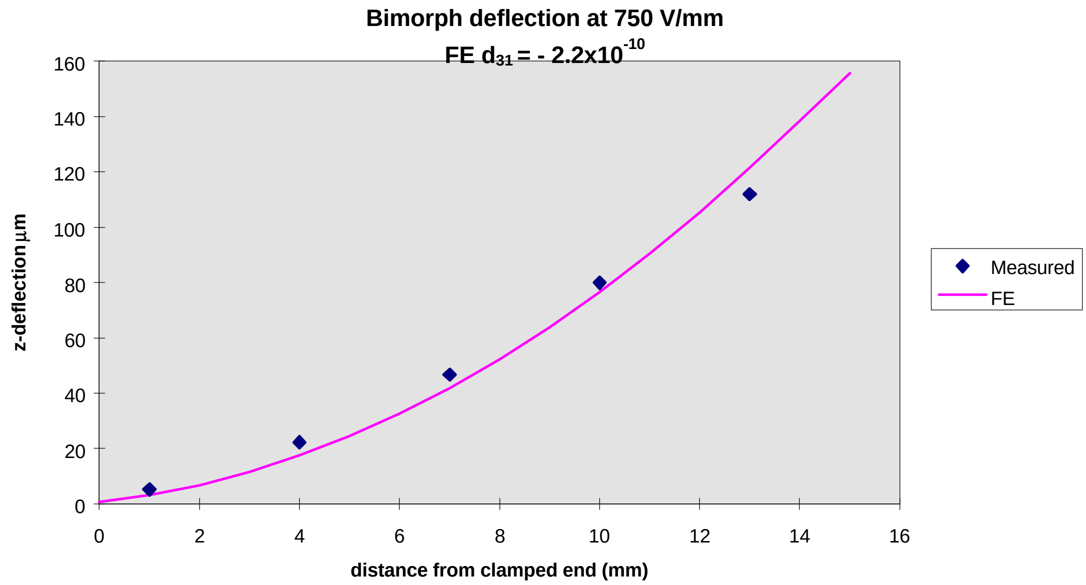

Figure (10d)

Figure 10(a - d): Comparison of predicted and measured deflection versus length of bimorph

When fields above 50 V/mm were applied, the strain response began to open out into a loop, rather than following the same path as the applied field was reversed, i.e. it had become hysteretic.

Table (1) - change in standard d_{31} required, and stress produced in bimorph

Applied field	50, V/mm	250, V/mm	500, V/mm	750, V/mm
Required d_{31}	- 120 pC/N	- 171 pC/N	- 205 pC/N	- 222 pC/N

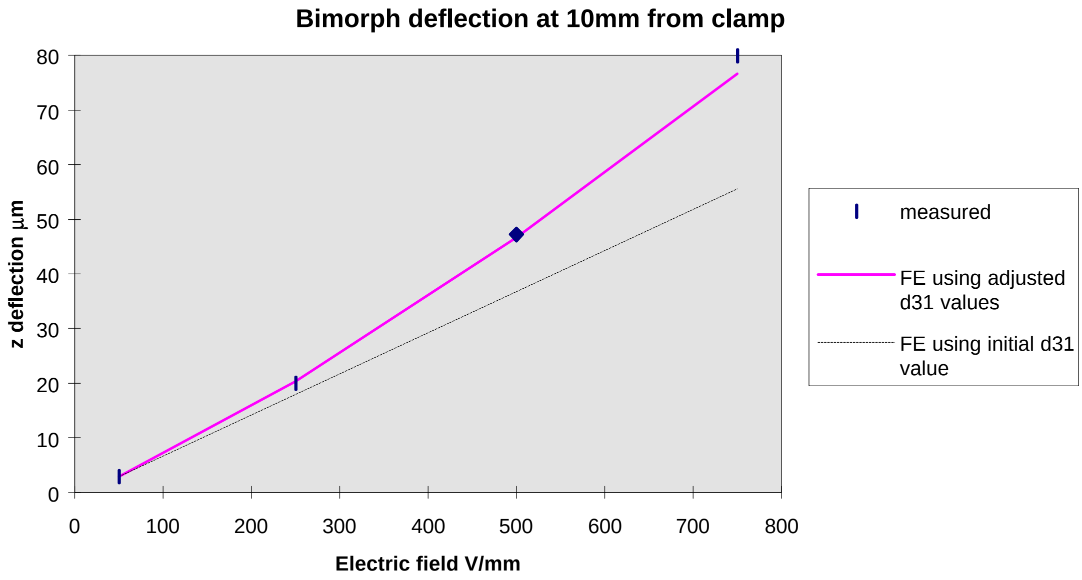

Figure 11: Comparison of predicted and measured deflection versus applied field, at 10 mm along the bimorph length

6. DISCUSSION

6.1 IDE DEVICE

Figure (3) showed that the field varied considerably through the device, with a region directly below the electrodes where, because of the field distribution, less strain would be produced than elsewhere in the device. The non-uniform strain generates stresses within the device, which were shown in figure (4) to be greatest at the electrode edges, corresponding to the greatest variation in field in this region. Although in this case the maximum stress, 5 MPa, was not at a level which is known to cause mechanical failure or to induce degradation at low numbers of cycles, if the device were to experience a large number of strain cycles, fatigue damage could become an issue. In addition, with smaller electrode spacings and a larger field, stresses large enough to cause mechanical damage could be induced.

The difference in strain (50 %) for the length and width directions was expected, since the length change is related to the d_{33} coefficient, whereas the width change was related to the d_{31}. For this material, d_{33} = 2.3 d_{31}[5], so the strain in the d_{33} direction should be at least double that in the width, as was found in this case.

The good correlation of the FE to the observed strain leads to confidence that the modelled field distribution is an accurate indication of the real field distribution. However, there are some limitations to the FE approach. The model assumes linear piezoelectric behaviour; although in this case non-linear behaviour was not observed, at higher fields this would cause a deviation from the predicted behaviour. Also, the regions of high stress at the electrode edges could affect the electromechanical properties of the piezoelectric, which again are not accounted for in this case.

6.2 BIMORPH TRANSDUCER

It had been expected that the amount of bimorph held inside the clamp would not affect the deflection, and this was found to be the case over the range of lengths tested.

Literature indicated that d_{31} would behave in a non-linear fashion at high electric fields, and this was suspected to be occurring in the bimorph material at the higher fields, since the d_{31} values had to be altered in order to maintain agreement between the experimental and predicted plots. The onset of a hysteretic strain response observed as the applied field increased indicated that the non-180° domain walls were contributing to the strain; this would explain the non-linear behaviour, since any movement of the non-180° domain walls contributes to an increased strain response. From the values which were required to fit the FE to the experimental data, a graph of d_{31} versus electric field was produced and shown in figure (12); the piezoelectric parameter had almost doubled over the range of field used. This shows the errors which can be made if assumptions are made in device response, and stresses the importance of using the correct data - had the standard value of d_{31} been used the deflection would have been underestimated by almost 50%.

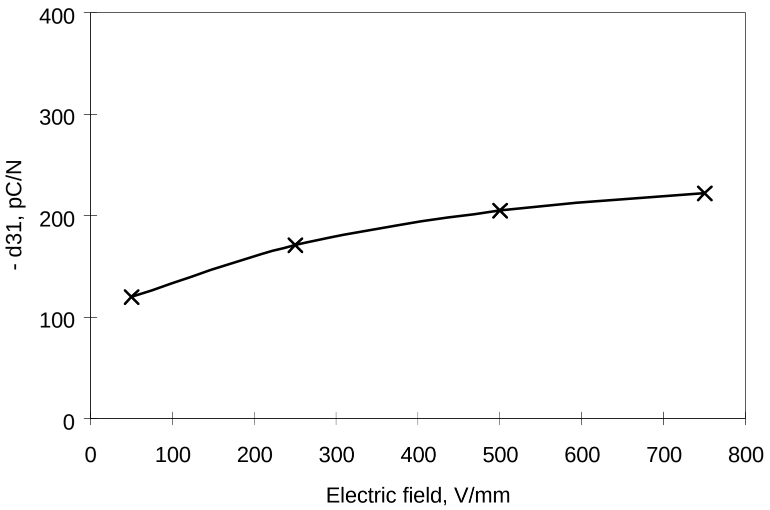

Figure 12: Graph showing the change in d_{31} with applied electric field

It must be pointed out that the variation in d_{31} shown in figure (12) is itself likely to be an underestimate. In section 3.2 it was mentioned that the thickness of the central adhesive layer would affect the deflection, with the predicted deflection decreasing as the thickness of this layer decreased. However, the minimum thickness value which could be used in the FE model was 250 µm; this was greater than the adhesive layer in the actual device, and so the model would have overestimated the deflection and hence underestimated the change in d_{31} required to correlate with the measured deflection at the higher fields.

7. CONCLUSIONS

This report has shown that FE can be used to predict the behaviour of two piezoelectric devices, an IDE device and a bimorph transducer. The strain predicted from the model agreed well with that measured for the IDE device, but for the bimorph, because the fields were larger, the piezoelectric parameters needed to be manually adjusted. By correlating the experimental and predicted values, a plot of d_{31} versus field was produced. This has illustrated the fact that FE is a useful tool for accurately predicting the behaviour of actual devices, but also highlighted the fact that an accurate model relies on the accuracy of the input data for the transducer material.

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9. ANNEX A. MODELLING OF PIEZOELECTRIC NON-LINEARITIES.

Introduction.

When quantifying the activity of a piezoelectric material, it is common place to apply a force to the sample under test and measure the resultant electrical charge flow in open circuit conditions or the potential difference developed in closed circuit conditions. Initial studies sought to investigate the effects of sample geometry on this process, making the assumption that the charge or voltage output of a piezoelectric material increased linearly with stress applied, i.e. the piezoelectric charge coefficient, *d*, and voltage coefficient, *g*, were independent of applied stress.

Modelling.

Four Finite Element (F.E.) models of piezoelectric discs were constructed for this purpose using the ANSYS F.E. package. The models could be subdivided into two groups, A and B, each containing 2 models. The first group, A, consisted of two piezoelectric discs which were subjected to a point load for charge generation, the area of contact being one tenth the sample diameter. The two models in the second group, B, were subjected to the same magnitude of stress, but in this case the stress was applied to the full surface area of the piezoelectric sample under test. One model in each of the two groups represented a thin piezoelectric disc whose thickness dimension was equal to one tenth of its radius. The other model in each group represented a thicker piezoelectric disc whose thickness dimension was equal to the radius. The radius of all the discs was 5mm. A stress of 64kPa was applied in all cases.

Methodology.

Making the assumption that the piezoelectric charge coefficient remained equal to its low stress value throughout the sample, ANSYS could calculate the charge in open circuit and voltage in closed circuit modes. Not surprisingly these values agreed very closely with analytical calculations indicating that measured piezoelectric coefficients were independent of sample geometry and method of stress application.

It was then requested that the effects of material non-linearities were examined by studying the crucial variation of piezoelectric charge coefficient, d_{33}, with applied stress using the existing F.E. models. Since ANSYS has no ability to directly assess the effect of a variation in piezoelectric coefficient a new methodology had to be devised.

In all models, the level of stress applied to generate a piezoelectric response was again set to 64kPa which allowed the utilisation of data provided by NPL, showing the variation of PZT 4's charge coefficient with stress. The aim was to examine whether any effect on the calculated piezoelectric coefficient was observed by maintaining the same stress level but varying the sample geometry and area of stress application.

Firstly, a mapping of the stress levels was generated on the four ANSYS models. The internal sample stress levels for the point contact scenarios, group A, are shown for the thin and thick samples in figures 1a) and b) respectively. It is clear that in the thicker sample the high stress levels penetrated a smaller percentage of the ceramic volume, leaving a larger proportion experiencing moderate or low stress levels when compared to the thin sample geometry. For the full surface area contact the stress distribution was highly uniform throughout the sample with only a small discontinuity at the sample edges. Utilising sample symmetry, the stress value at each node could be obtained. Examination of the NPL data showed an approximately linear increase in the charge coefficient with increasing stress. There was no indication in the data, that a 'tail-off' in the charge coefficient deviation may occur as the applied stress was decreased below 12 kPa and so a linear fit was applied to the data. From the intercept with the y axis the low stress d_{33} value of 292pC/N was obtained, which agrees well with available material data. A high stress value of 64kPa corresponded to a d_{33} coefficient of 356pC/N. By applying the relevant piezoelectric charge coefficient to the nodal stress levels, a calculation of the electrical charge developed at each individual node along the sample surface was possible. The sum of individual charges gave the total piezoelectric charge output on the conducting plates of the sample under each test condition and was a contribution from all the volumes at differing stress levels. It was then possible to back calculate a value of d_{33}, equivalent to an average of the various volumes and equal to the value that would be calculated by a test machine performing this characterisation process. This method gave a measure of sample activity which accounts for non-linear behaviour in its piezoelectric response.

Results and Discussion.

Point Load

Thin Disc

Total Charge Output = 4.21pC
Calculated piezoelectric d_{33} coefficient = 355pC/N

Thick Disc

Total Charge Output = 3.68pC
Calculated piezoelectric d_{33} coefficient = 297pC/N

Full Surface Area Load

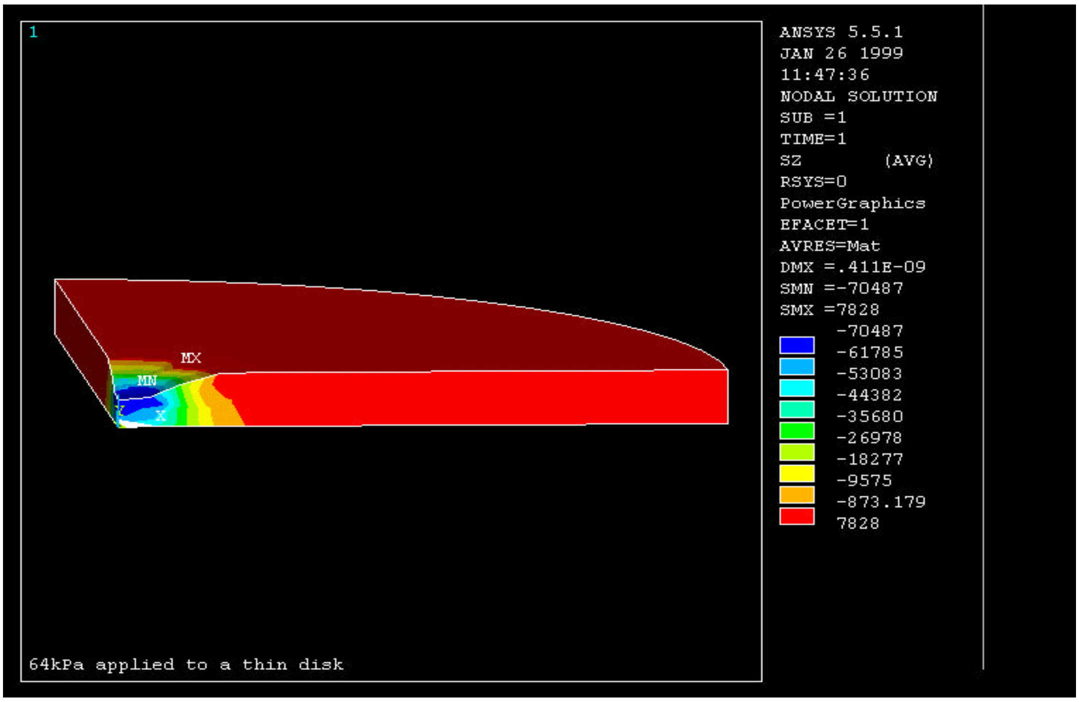
Thick and Thin Disc

Total Charge Output = 1.8nC
Calculated piezoelectric d_{33} coefficient = 356pC/N.

As would be expected a considerably larger amount of charge was generated by the full area stress application. Therefore, this method offers the possibility of good measurement resolution on a piezoelectric sample with a low activity, while maintaining no increase in applied stress levels.

If high stress levels are to be used in conjunction with point contacts then these preliminary studies indicate that the higher the thickness to width ratio, the smaller the contribution from the high stress regime of piezoelectric coefficients.

This brief study has demonstrated the feasibility of using F.E. modelling to quantify the effects of non-linearities and has shown that the extent of the effects depend upon sample geometry. In order to quantify this to a greater degree it is recommended that specialist models be developed with greater density and uniformity of finite element mesh to allow increased accuracy in the calculation of the charge developed at each individual node and the precise volume at which the stress level was present.



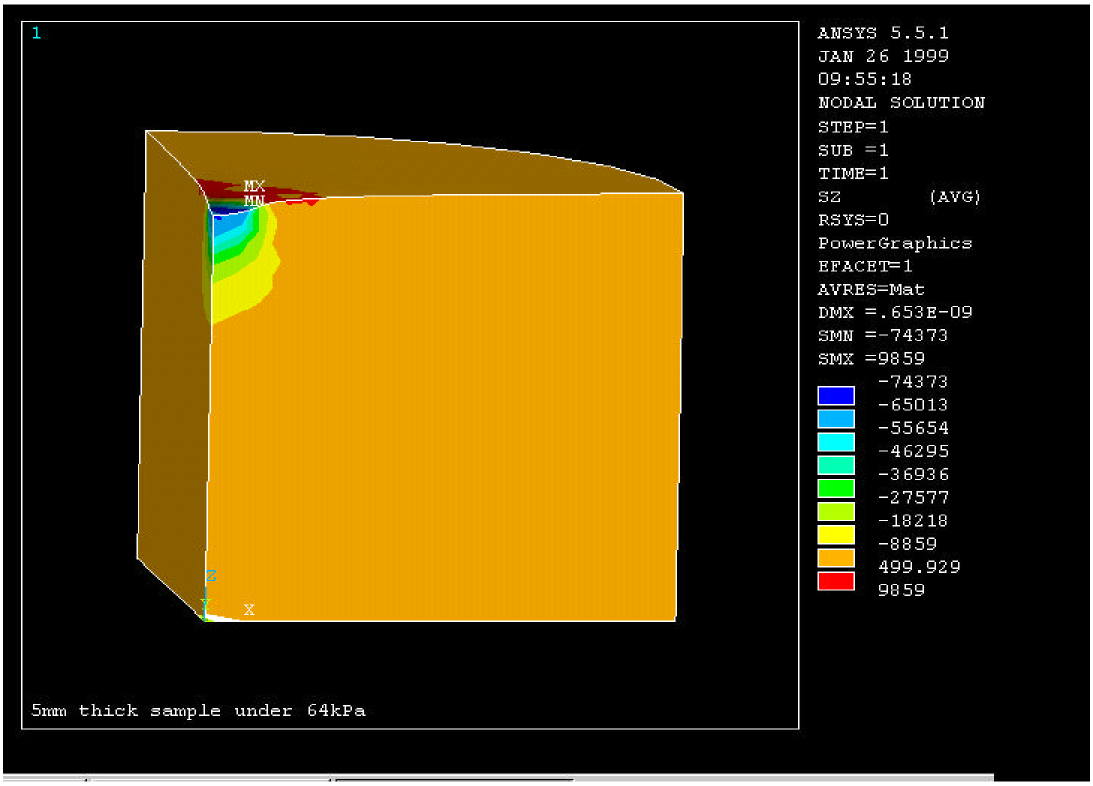


Figure 1a) and 1b). Internal stress distribution in piezoelectric samples when force is applied via point contacts.