Modelling of 3-3 piezocomposites

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Abstract

Three-dimensional modelling of a 3-3 piezoelectric structure was carried out using ANSYS finite element modelling software. Hydrophone figures of merit were calculated for structures with increasing amounts of interconnecting porosity present. In addition to air being the second phase, polymer fillers were added to the three dimensional model in order to observe the effect of polymer Young's modulus on the piezoelectric properties of the bulk material. Results show that increasing the porosity has the effect of improving the hydrostatic piezoelectric properties for applications such as low frequency hydrophones.

1 Theoretical background

Traditionally research into piezoelectric devices has concentrated on producing materials with high density. However, for certain applications it can be shown that ceramic piezoelectrics with low density, i.e. a high amount of open porosity, can have superior hydrostatic properties. One area of particular interest is that of low frequency hydrophones [1].

At low frequencies (<100kHz) the wavelength dimensions are greater than that of the hydrophone and the stress on the device due to the acoustic wave is effectively hydrostatic. For piezoelectric devices in active (driven) applications it is advantageous for the material to have a high $d_{33}$ (strain per unit electric field in the direction of polarisation). Unfortunately dense materials usually also have a high $d_{31}$ (a contraction normal to the direction of polarisation). A figure of merit, which represents the hydrostatic strain per unit electric field, is used to assess the performance of a material in the active mode and is known as the hydrostatic strain constant, $d_h$.

$$d_h = d_{33} + 2d_{31} = \text{hydrostatic strain constant (m V}^{-1})$$

(1)
For piezoelectric devices in passive applications (listening) the figure of merit, $g_h$, is used. This is defined as the electric field generated per unit hydrostatic pressure and is known as the 'hydrostatic voltage constant'.

$$g_h = \frac{d_h}{\varepsilon_{33}^T} \text{ (Vm}^{-1}\text{ Pa}^{-1})$$

(2)

It can be seen that $d_h$ and $g_h$ are related by the permittivity at constant stress, $\varepsilon_{33}^T$.

A third figure of merit is used in the case of the materials being used in both a passive and active mode. This is simply the product of the two figures of merit $d_h$ and $g_h$, and is termed the 'hydrostatic figure of merit' ($d_h g_h$).

For dense materials the hydrostatic figure of merit, $d_h$, is low due to the fact that both $d_{33}$ and $d_{31}$ are large but of opposite sign. It is possible to increase the value of $d_h$ by reducing the absolute value of $d_{31}$. This can be achieved by manufacturing a porous piezoelectric structure [2,3] and the mechanism by which $d_{31}$ is reduced is explained in subsequent sections of this paper.

The research reported in this paper is concerned with 3-3 piezocomposites. This is a matrix of two materials (one is piezoelectric as an active phase, the other is polymer as a passive phase), that are completely interpenetrating, so that each phase forms a three-dimensional network around the other phase as shown in Figure 1.

In addition to increasing $d_h$ the inclusion of a second phase (air or polymer) reduces the overall permittivity ($\varepsilon_{33}^T$) of the device which increases the value of the piezoelectric voltage constant, $g_h$. Further gains in performance can be achieved by considering the density of the composite. A decrease in density of the device will result in a lower acoustic impedance, leading to improved impedance matching between the acoustic medium (water or air) and the piezocomposite. Processing costs for open porosity piezocomposites can be considerably lower than those for dense materials. In addition, near net shape forming is possible and any post sintering machining costs will be small.

Figure 1: An example of a 3-3 composite.
A number of manufacturing methods can be used to produce a variety of porous structures at relatively low cost [4]. However, little work has optimised the performance of 3-3 piezocomposites with respect to pore content, pore morphology and properties of the passive phase. While models, including finite element models, have been developed to optimise other piezocomposites (such as 1-3 structures), no such model exists for 3-3 type piezocomposites. Therefore, the current research is aimed to optimise the properties of 3-3 piezocomposites by using finite element modelling.

2 Modelling of 3-3 piezocomposites

There are numerous physical properties that will have an effect on the final performance of a hydrophone device. The properties that have been examined are the volume fraction of porosity/polymer and the Young’s modulus of the passive phase (polymer). The effect of changing these variables on the figures of merit $d_{33}$, $g_{33}$, and $d_{33}g_{33}$ will be discussed.

In order to model a porous structure, a unit cell was chosen to represent part of the structure which would be characteristic of the whole system. One such unit cell is shown in Figure 2. In order to vary the porosity the model was changed by increasing and decreasing the effective wall thickness of the unit cell. This enabled the model to be recalculated for any porosity from 0 to 100%, however, for practical reasons only porosities from 10 to 90% were calculated.

The model material chosen was PZT-5H, a commercially available soft PZT and all piezoelectric data [5] relevant to this material was entered into a commercial finite element analysis (FEA) package and the unit cell was constructed as shown in Figure 2. Electrodes were applied to the top and bottom of the unit cell and symmetry was applied to 3 of the 6 faces. This symmetry allowed the results from the unit cell to be calculated as if the cell was part of a larger array.

![Figure 2: Sample unit cell used for FE modelling.](image-url)
To calculate \( d_h \) a potential difference was applied to the electrodes on the unit cell. The subsequent displacement and strain per unit field in the z direction (\( d_{33} \)) and the strain in the x or y (\( d_{31} \)) direction was measured, as shown in Figure 3. These two values were used to calculate \( d_h \) (\( d_h = d_{31} + 2d_{33} \)).

In order to calculate \( g_h \), one electrode was set to 0V, while the other electrode was free to attain an equilibrium potential (Figure 4). A hydrostatic pressure was applied, acting to compress the structure, on the three surfaces of the unit cell. After the finite element model solution was calculated the voltage generated in the free electrode was measured allowing the calculation of \( g_h \), the electric field generated per unit hydrostatic pressure.

The product of the values \( d_h \) and \( g_h \) was used to calculate the hydrostatic figure of merit \( d_h g_h \).

3 Results

3.1 Effect of Young's modulus and polymer volume fraction on \( d_h \)

The following set of calculations was completed to assess the effect of volume fraction of polymer filled porosity on \( d_h \). In addition, the Young's modulus of the polymeric second phase was varied from 2GPa to 10GPa which represent typical values of silicone polymers to hard set epoxies.

The results from this set of calculations can be seen in Figure 5 which shows a maximum value of \( d_h \) at around 50% for the low modulus polymers and at around 35% for the high modulus polymers.

The behaviour in Figure 5 can be explained in terms of 'active volume' as illustrated in Figure 6. The term 'active volume' is the volume of piezoelectric ceramic responsible for the strain in a particular direction. In the case of \( d_{33} \), the 'active volume' is the pillar height of ceramic in the z direction. This volume
Figure 5: Chart showing \( d_h \) vs. polymer volume fraction at various Young’s moduli.

decreases with increasing polymer volume content causing \( d_{33} \) to decrease at higher polymer volume content (Figure 6b and c). Similar trends can be observed for \( d_{31} \) which rapidly reduces as the polymer volume fraction increases (Figure 6d-f).

However, the reduction in \( d_{31} \) with increasing polymer content is quicker than \( d_{33} \) as shown in Figure 7. The \( d_{31} \) ‘active volume’ is reduced due to the fact that only the volume of ceramic contained within the pillar in the \( z \) direction experiences a significant electric field. This is due to the low permittivity of the polymer compared to the ceramic \((\varepsilon_{\text{ceramic}}/\varepsilon_{\text{polymer}} \approx 400)\). The relatively slow reduction in \( d_{33} \) and a rapid reduction in \( d_{31} \) results in an increase in the figure of merit \( d_h \) to increase with increasing polymer volume fraction at polymer volume fractions up to 50%.

At higher polymer volume fractions there is insufficient piezoceramic for the polymer phase to strain with the ceramic, leaving a depressed region in the surface (Figure 6a). As the value of \( d_{33} \) is calculated by averaging over the whole upper surface this depression reduces the value of \( d_{33} \) and subsequently \( d_h \).

The value of \( d_h \) is also a function of the Young’s modulus of the polymer phase and increases with decreasing Young’s modulus. This is simply because a stiffer polymer will inhibit the movement of the active volume. It can be postulated that to maximise the performance of an active transducer a polymer volume fraction of around 50% with a low stiffness polymer should be used.
Figure 6: Schematic of how $d_{33}$ and $d_{31}$ vary with polymer volume fraction.

Figure 7: Effect of polymer content on the $d_{33}$ and $d_{31}$ values.
3.2 Effect of changing polymer volume fraction on $g_h$

A striking trend can be seen from Figure 8 where $g_h$ is seen to increase with increasing polymer volume fraction and reduction in polymer stiffness. The diagram shown in Figure 9 helps to explain this behaviour. The high stiffness of the ceramic relative to the polymer results in the majority of the applied stress in any direction being transferred into the ceramic. If a constant strain model is assumed, then the high Young's modulus of the ceramic will cause more stress transfer into the ceramic than into the polymer. Thus, load per unit PZT area will increase with increasing polymer fraction. This results in high values of $g_h$ (electric field per unit hydrostatic stress). As the polymer volume fraction increases this value will rise. However, there is a limit where the ceramic part of the composite will fail or there will be critical stress where domain switching occurs. Therefore, increase to infinity in Figure 8 is actually prevented by realistic considerations.

The results for $g_h$ show that in order to maximise the properties of a passive hydrophone device it is advantageous to have a high polymer volume content with a low stiffness polymer as a second phase. At the time of preparation of this manuscript, a set of porous ceramics with different pore content and pore size are prepared and filled with passive polymer to be tested experimentally in order to validate the findings of FE analysis on 3-3 piezocomposites in this work.

3.3 Effect of changing polymer volume fraction on $d_{31}$ & $g_h$

The previous charts Figure 5 and Figure 8 have shown the effect of polymer volume fraction and Young's modulus on $d_h$ and on $g_h$ respectively. If a material is to be used in both passive and active mode, both of the figures of merit are of

![Figure 8: Effect of polymer volume fraction and Young's modulus on $g_h$.](image)
Figure 9: Schematic of how $g_h$ varies with polymer volume fraction.

Figure 10: Effect of polymer volume fraction and polymer Young's modulus on $d_hg_h$.

importance. These can be combined to give the hydrostatic figure of merit, $d_hg_h$. This resulting curve is simply a combination of these two curves.

Figure 10 shows that for a passive/active device the optimum volume fraction porosity is around 82% for a low Young’s modulus polymer filler and slightly lower at 75% for a high Young’s modulus polymer filler. Optimum volume fraction is therefore a function of polymer stiffness.
4 Conclusions

There are a number of trends and conclusions that can be drawn from the finite element modelling results reported in this work.

- The figures of merit $d_h$, $g_h$ and $d_h g_h$ are enhanced as the Young's modulus of the second phase decreases for a fixed polymer volume fraction.

- The hydrostatic strain constant, $d_h$, reaches a maximum around 50% polymer volume fraction.

- The hydrostatic voltage constant, $g_h$, increases with decreasing ceramic volume fraction.

- The hydrostatic figure of merit $(d_h g_h)$ which describes an active/passive transducer, reaches a maximum at ~80% polymer volume fraction. Practical experiments are underway in order to quantify the accuracy of this model although the results are in good agreement with results reported in the literature [6].

References


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