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Modelling Porous Ferroelectrics to Assess Piezoelectric Energy Harvesting Capabilities

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Aim: To evaluate the effect of porosity and porous structure on the energy harvesting capabilities of ferroelectric ceramics using a Finite Element Modelling approach.

Context
Porous piezoelectric ceramics are of interest for energy harvesting applications due to porosity causing significant reductions in permittivity, $\varepsilon_{33}$, compared with relatively small reductions in longitudinal strain coefficient, $d_{33}$, leading to increases in energy harvesting figures of merit, where $\text{FOM}_{33} = d_{33}^2/\varepsilon_{33}$ [1]. The development of an FE Model will allow different porous structures to be evaluated for their energy harvesting capabilities.

Pre- and Post-Poling Porous BaTiO$_3$ network

(a) 30$^3$ cells randomly designated material properties of either unpoled BaTiO$_3$ (blue) or air (empty), depending of density defined for run and (b) post-poling procedure with poled (red) and unpoled BaTiO$_3$ (blue) and air (empty). BaTiO$_3$ elements are poled when local E-field exceeds coercive field.

FE Modelling Process

1. Generate network model geometry
2. Determine random two phase distribution (unpoled BaTiO$_3$ and air) for given volume fraction of porosity
3. Apply poling voltage to ‘electroded’ surfaces
4. Establish distribution of polarised material
5. Characterise porous piezoceramic performance in terms of $d_{33}$, $\varepsilon_{33}$, and energy harvesting FOM
6. Record results
7. Clear model

Fig. 2: Flow diagram of modelling process used to generate randomly distributed porosity with piezoelectric ceramic (adapted from [2]).

Initial Results

(a) $d_{33}$ (\text{pC/N}) vs. Relative density (%)
(b) Relative permittivity vs. Relative density (%)
(c) FOM$_{33}$ (\text{kJ/m$^2$/N}) vs. Relative density (%)

Fig. 3: FE model data (blue) compared to experimental data BaTiO$_3$ (red) for (a) $d_{33}$, (b) relative permittivity and (c) FOM$_{33}$, all plotted as a function of relative density. Experimental data measured from BaTiO$_3$ ceramics with range of porosities obtained using the burnt out polymer spheres (BURPS) process.

Discussion & Outlook
- Want to bring model and experimental data closer together
  - More accurate input data required
- Use model to investigate EH capabilities of different structures/ connectivity
  - Currently, only randomly distributed porosity (3-0/3-3) generated
  - Structure has effect on key properties, i.e. $d_{33}$, $\varepsilon_{33}$ and $S_{33}$ (elastic compliance)

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