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Shock induced phase transition in ferroelectric materials

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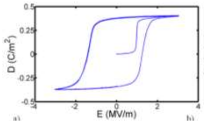
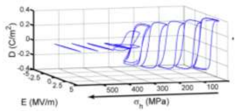
Introduction

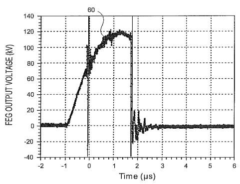
- Ferroelectric materials are special class of materials that exhibit non-zero polarization below a certain Curie temperature.
- Ferroelectric materials are used as capacitors, memory devices, actuators, sensors and tunnel junctions.
- In a ferroelectric material, the electrical, thermal and mechanical properties and responses are coupled nonlinearly.

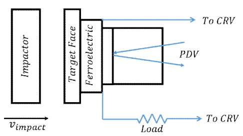


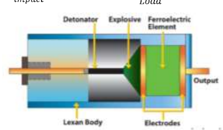
(Left) Characteristic $D-E$ curve of a ferroelectric material characterized by non zero D at $E=0$. (Right) Influence of hydrostatic loading on the $D-E$ loop of the material.



- Ferroelectric material is also used as a ferroelectric generator where the material is subjected to shock loading to generate large current or voltage output.
- Shock causes phase transition in the material – Ferroelectric to Antiferroelectric transition is typically exploited.
- PZT 95/5 is the most commonly used material for such purposes.



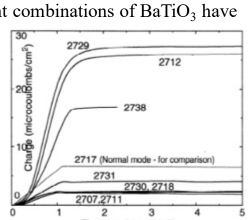


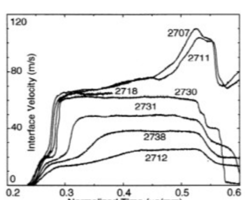


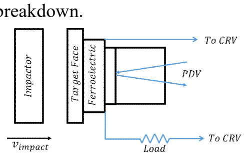
Schematic of ferroelectric generators employing impact (above right) or blast loading (right). Profile of voltage generated by a ferroelectric generator (above). The magnitude of voltage achieved is huge.

Depolarization experiments

- Over the years, many shock induced depolarization experiments have been conducted on various ferroelectric materials.
- First experiments were conducted in 1959 by Berlincourt and Krueger on PZT and $BaTiO_3$.
- Materials tested over the years include various combinations of PZT such as 95/5, 65/35 and 52/48. Different combinations of $BaTiO_3$ have also been explored.
- Axially and normally poled samples are commonly tested in open and short circuit configurations.
- We will be focusing on impact experiments on axially poled PZT 95/5 by Furnish (2000).
- Loading at 0.9 GPa results in current discharge corresponding to complete depoling.
- Higher loads result in lower current suggesting the possibility of dielectric breakdown.



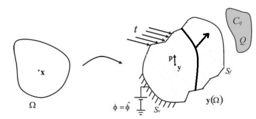




[Left] Schematic of impact experiment used by Furnish (2000). [Top Right] Charge profiles obtained for different impact speeds. [Right] Particle velocities at the far end of the target.

Governing equations

- We are studying large deformation dynamic behavior analysis for ferroelectric materials.
- We are considering impact induced ferroelectric to anti-ferroelectric phase transitions in isothermal and adiabatic environments.
- We consider a sharp phase boundary propagation in the medium.
- The possibility of dielectric breakdown is accounted for by introducing surface charges on the phase boundary S.



- Stored energy in an arbitrary volume $B \subset \Omega$

$$\mathcal{E} = \int_B W_0(p_0, F)dx + \int_{y(B)} \frac{\varepsilon_0}{2}|\nabla_y \phi|^2 dy + \int_B \frac{\rho_0}{2}|\dot{y}|^2 dx + \int_{S\cap y(B)} W_\sigma dS_y$$

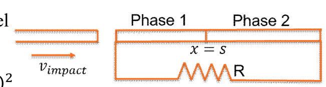
- Rate of work done

$$\mathcal{F} = \int_{\partial y(B)} \phi \frac{d}{dt}\left((-\varepsilon_0 \nabla_y \phi + \boldsymbol{p}) \cdot \hat{\boldsymbol{n}}\, dS_y\right) + \int_{y(\partial B)} t \cdot v\, dS_y$$

- $\frac{dQ}{dt} = \int_B \rho_0\, \dot{r} dx - \int_{\partial y(B)} q \cdot \hat{n}\, dS_y$
- Conservation of energy and the second law collectively yields the following expression for traction jump across the phase boundary and the driving force acting on the phase boundary.
- $\nabla_y \cdot (T + T_M) - \rho \ddot{y} = 0$ on $y(B)$
- $[\![t_0]\!] = [\![(T + T_M) J F^{-T} \hat{n}_0]\!] + (W_\sigma + \sigma\phi)\kappa J F^{-T} \hat{n}_0$ on $S_0 \cap B$
- $d = [\![H_0 + \langle \eta_0 \rangle \theta + \nabla_y \phi \cdot p_0 + J(\hat{n} \cdot T_M \hat{n}) - F\hat{n}_0 \cdot \langle (\hat{n} \cdot T_M \hat{n} + T) J F^{-T} \hat{n}_0]\!] + \langle J \rangle (W_\sigma + \sigma\phi)\kappa$
- Driving forces and the traction jumps depend on the curvature of the phase boundary due to he presence of surface charges.

Numerical Forumulation

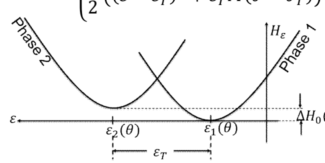
- One dimensional material model

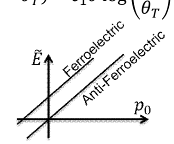


$$W_0 = W_p(p) + W_\varepsilon(\varepsilon, \theta)$$

$$W_p = \frac{\alpha_p}{2}(p_0 - p_1)^2, \frac{\alpha_p}{2}(p_0 - p_2)^2$$

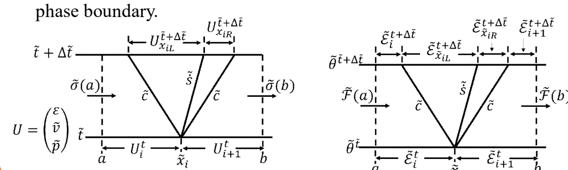
$$W_\varepsilon = \begin{cases} \frac{E}{2}\varepsilon^2 - \alpha E \varepsilon(\theta - \theta_T) - c_1 \theta \log\left(\frac{\theta}{\theta_T}\right) \\ \frac{E}{2}\left((\varepsilon - \varepsilon_T)^2 + \varepsilon_T M(\theta - \theta_T)\right) - \alpha E \varepsilon(\theta - \theta_T) - c_1 \theta \log\left(\frac{\theta}{\theta_T}\right) \end{cases}$$





[Left] Piecewise quadratic profile of energy depending on strain and temperature. The energy wells move depending on the temperature. [Right] Piecewise linear profile of electric field with respect to polarization.

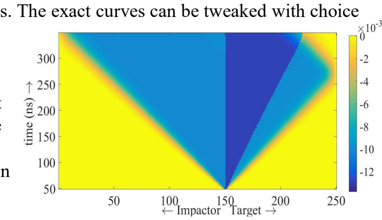
- Linear thermoelastic impactor and no dielectric breakdown.
- Electro-thermo-mechanical coupling makes the problem nonlinear.
- We solve Riemann problems at each time and track the location of the phase boundary.

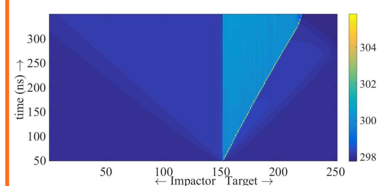


[Left] Riemann problem solved at the node corresponding to the phase boundary. This problem is solved isothermally. Temperature is updated based on conservation of energy [Right].

Results

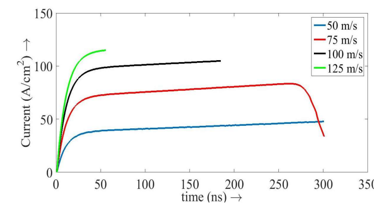
- We track current flowing through the R under linear and stick-slip linear kinetics.
- We observe that as the impact speeds increase, the current output increased. The temperature variation was very small $\sim 5-10K$ due to low impact speeds.
- Current output and charge profiles show similar magnitude when compared to experiments. The exact curves can be tweaked with choice of parameters.
- Linear and stick-slip linear kinetics yield similar results in current profiles and temperature variations.
- Wave reflections result in changes in current.

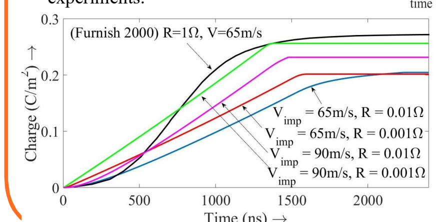




[Above] Strain map in $X-t$ diagram. An elastic wave travels ahead of the phase boundary, reflects off the free edge and interacts with the phase boundary. Temperature map depicted in the $X-t$ diagram [Left] shows 5K rise in temperatures at 75m/s speeds. The current drops as soon as the elastic wave reflected off the free edge interacts with the phase boundary. [Below]

- Current shows an exponential profile and achieves a steady value.
- Magnitude increases with impact speeds.
- Magnitude similar to experiments.





Comparison of charge profiles obtained in the simulations with experiments. The qualitative behavior and the order of magnitudes are much more important than exact values. This is due to the fact that parameters chosen are matched up to the order of magnitude.

References

- Agrawal V. and Bhattacharya K., Impact induced depolarization in ferroelectric ceramics (to be submitted).
- Valadez J., Pisani D. and Lynch C.S., Proc. SPIE 8689, 2013.
- Abeyaratne R. and Knowles J., Arch. Rat. Mat. Anal., 126 (3), 1994.
- James R.D., Cont. Mech. and Therm., 2002
- Xiao and Bhattacharya, Arch. Rat. Mech. Anal., 2008
- Furnish M.D. et al., AIP Conference Proceedings, 505, 975(2000)

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