Charge density estimation with pressure

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1 Aim of the project

To study the behaviour of piezo-electric materials in COMSOL by performing the following simulations:

1. Measure the time response of the charge density on the surface due to application of pressure/stress on the surface.
2. Measure the current flow through a known resistor by connecting a circuit to a piezo-electric capacitor due to application of pressure/stress on the surface.

2 Piezo-electric materials

These materials can generate an electric charge in response to applied mechanical stress. For weak electric fields, this effect can be approximated to be linear and the quantities are governed by the following constitutive equations:

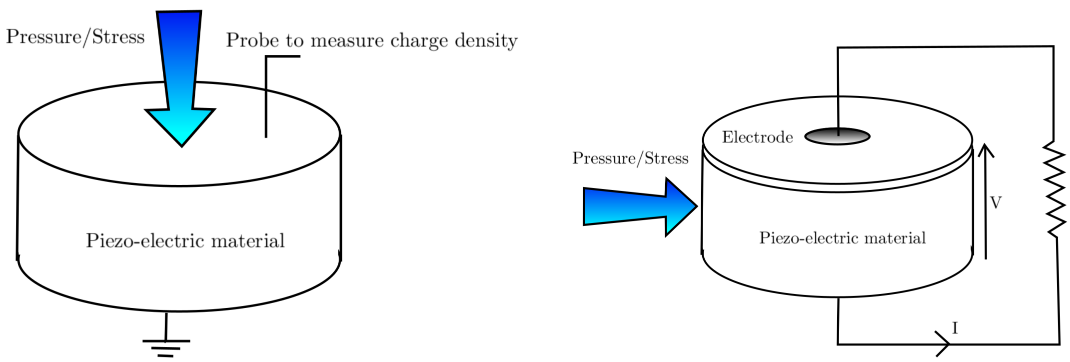
$$S = s_E \cdot T + d^t \cdot E$$
$$D = d \cdot T + \epsilon_T \cdot E$$

- **S** = Strain; **T** = Stress;
- **D** = charge-density displacement; **E** = Electric field;
- **d** = piezo-electric co-efficients; $\epsilon_{\mathbf{T}}$ = permittivity

We will be working with two such piezo-electric materials, namely PZT-5A (*Lead zirconate titanate*) and PVDF (Polyvinylidene fluoride).

3 Simulation Setup

We will configure the following setup in COMSOL to perform the required simulations.



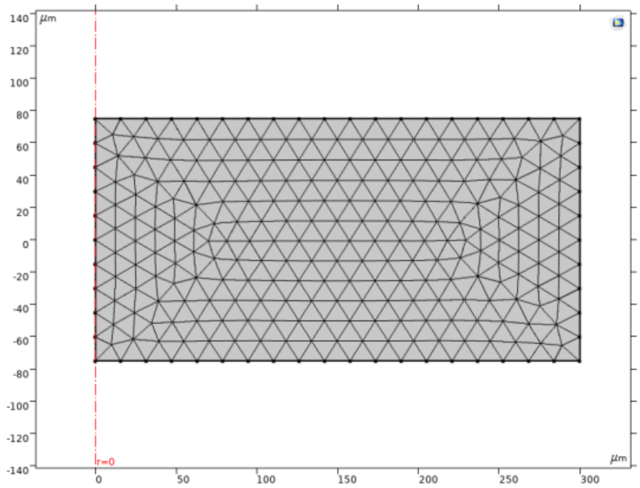
(a) Measuring charge density (b) Measuring induced current

We use the Piezo-electricity Multiphysics setup in COMSOL, by interfacing the *Structural Mechanics* and *Electrostatics* modules. The piezo-electric material is a simple cylindrical mesh, with the following boundary conditions: (let the top and bottom circular faces be A and B resp.)

- **Structural Mechanics:** Face B is set to a *fixed constraint*, and the force is applied on the material on Face A as a *boundary load*.
- **Electrostatics:** Face B is set to *ground potential*, and Face A is set to *floating potential*, which acts as a perfectly conducting electrode (this can also be interfaced with Electrical Circuits module for the second aim).

3.1 Model Parameters

The model geometry and applied loads are radially symmetric, so we utilise the symmetry by using a 2D Axi-Symmetric model in COMSOL. The 2D mesh is revolved around the $r = 0$ axis to produce 3D visualizations.

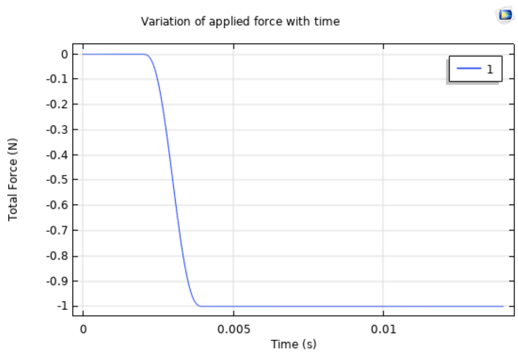


(a) 2D Axi-Symmetric Mesh

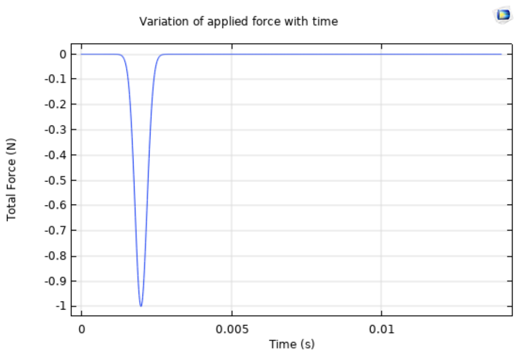
- The radius of the cylinder is set to 300 μm for all the simulations.
- The time range for simulations is $t \in range(0, 10^{-5}, 7.5 \cdot 10^{-2})$ (or smaller, depending on convergence of solution).

3.2 Applied Load

The load is specified by setting the total force on the material (along the $-ve\ z$ direction). We will use a smooth step (sigmoid) and a delta (gaussian) variation of the force with time, as shown below.



(a) Step load



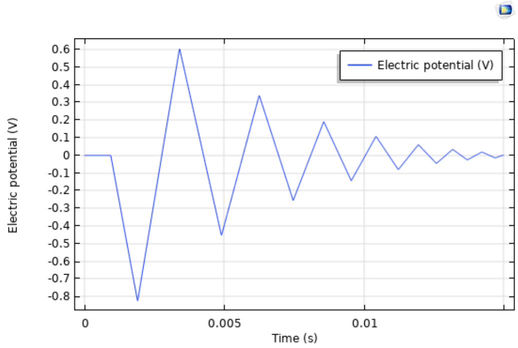
(b) Gaussian load

4 Results

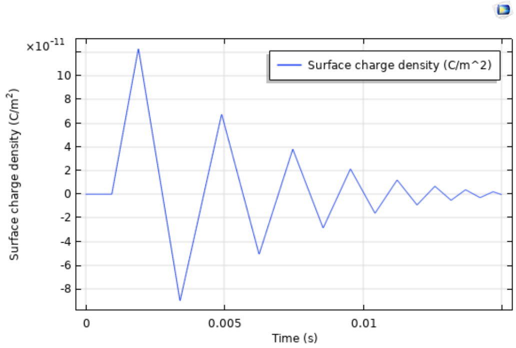
4.1 Part-1 (Measure time response of charge density)

4.1.1 Material: PZT-5A, 150 μm

- **Gaussian Load**



(a) Average potential vs. time

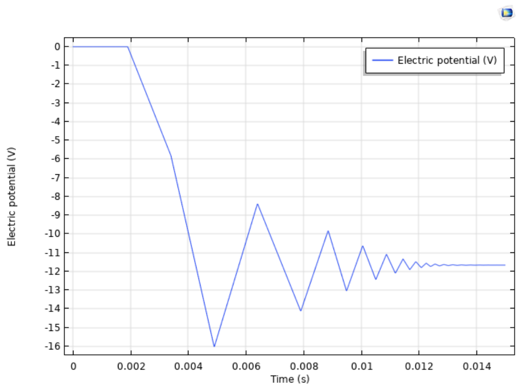


(b) Average charge density vs. time

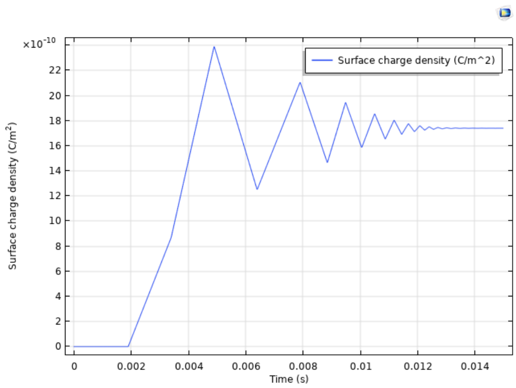
Figure 4: PZT-5A, 150 μm, Gaussian Load

We see that there are oscillations in the average surface charge density and induced potential, which damp out over time. This may be due to the stress co-efficients of the PZT material which cause reverberations of the applied load. This can be damped out faster by attaching a hard surface such as aluminium at the bottom plate of the cylindrical PZT geometry. **We note that the initial response of the charge density to the applied load, is a positive valued peak.**

- **Step Load**



(a) Average potential vs. time



(b) Average charge density vs. time

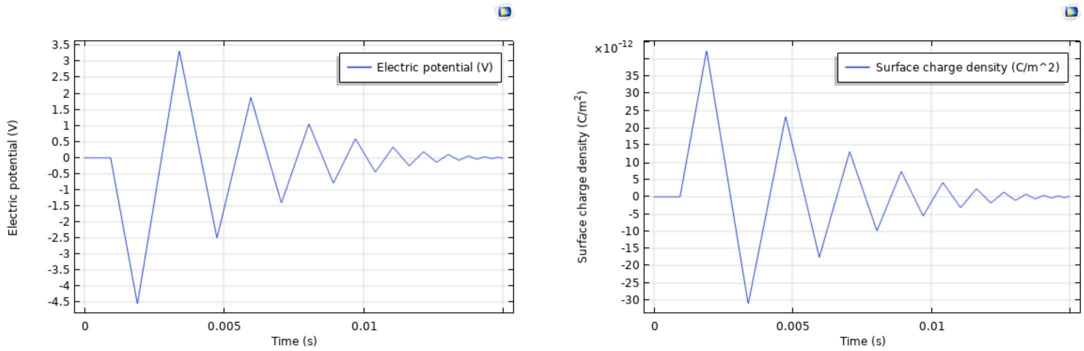
Figure 5: PZT-5A, 150 μm, Step Load

In this case also, we see a sudden change in the quantities, which then oscillate and settle into a non-zero equilibrium value corresponding to the applied load.

Note: The GIF files for these simulations can be viewed in the presentation found here: `https://20akshay00.github.io/PHY312-Project/presentation/PHY312.html`

4.1.2 Material: PZT-5A, 750 μm

- **Gaussian Load**



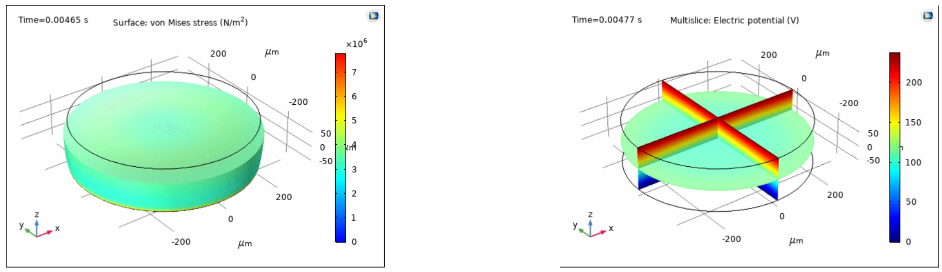
(a) Average potential vs. time (b) Average charge density vs. time

Figure 6: PZT-5A, 750 μm, Gaussian Load

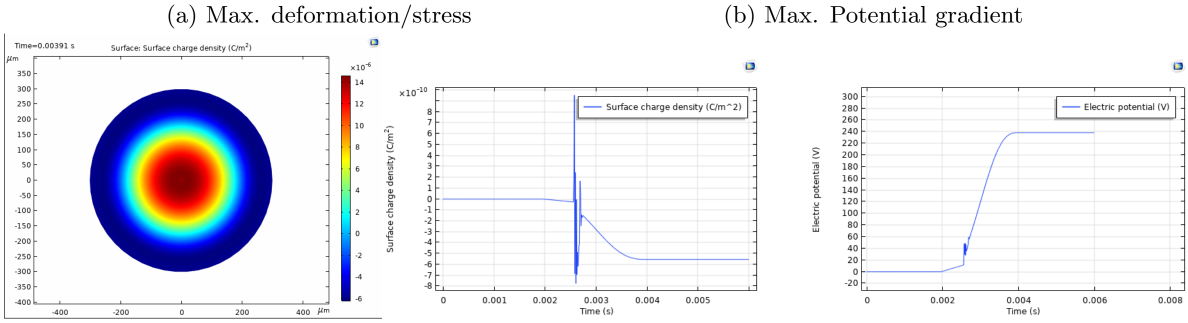
In this case, the qualitative shape of the time-response is same as the 150 μm simulation, however the magnitude of voltage/charge density is 2-5 times larger than the 150 μm values. The frequency of the damped oscillations is also slightly higher (noticeable after t = 0.01 secs).

4.1.3 Material: PVDF, 150 μm

- **Step Load**



(a) Max. deformation/stress (b) Max. Potential gradient

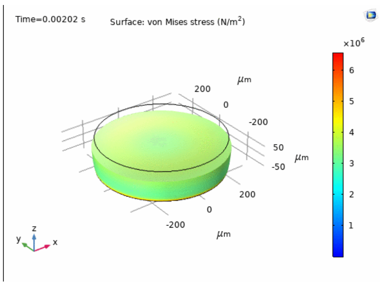


(c) Surface charge density (d) Average charge density vs. time (e) Average potential vs. time

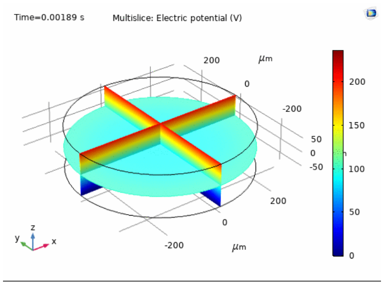
Figure 7: PVDF, 150 μm, Step Load

Unlike in PZT, PVDF seems to be a stiff material, so the applied load results in a smooth deformation of the geometry into the equilibrium position. As a result, the induced potential and charge density also smoothly settle into a stable configuration. The irregular bump observed in (d) might be from reverberations of the load which reflect back. **We note that the initial response of the charge density to the applied load, is a negative valued peak.**

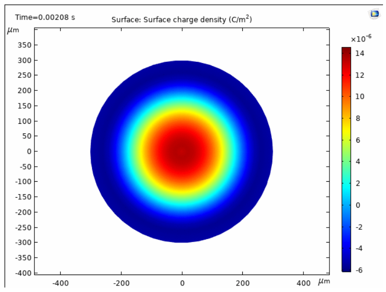
- **Gaussian Load**



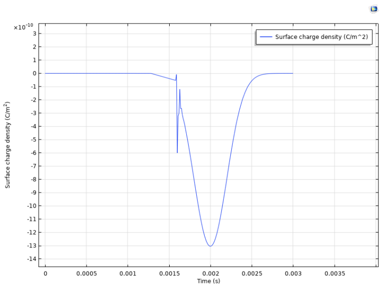
(a) Max. deformation/stress



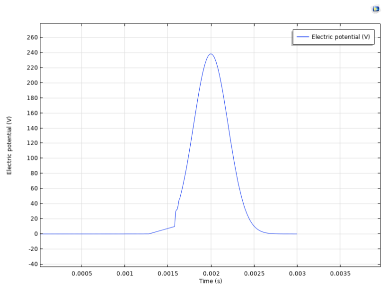
(b) Max. Potential gradient



(c) Surface charge density



(d) Average charge density vs. time



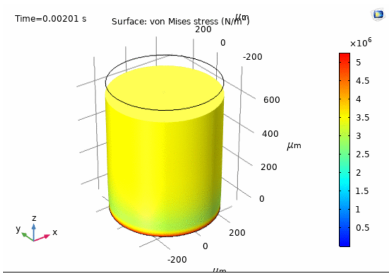
(e) Average potential vs. time

Figure 8: PVDF, 150 μm, Gaussian Load

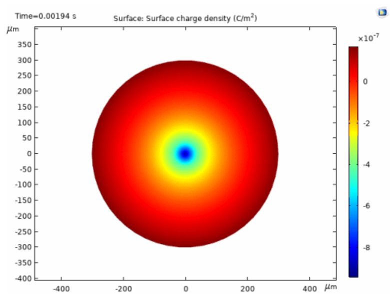
Under a gaussian load too, we observe a smooth gaussian shaped response of the average potential and charge density as seen in the figures.

4.1.4 Material: PVDF, 750 μm

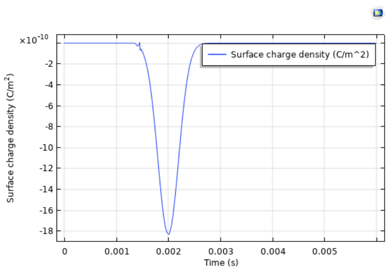
- **Gaussian Load**



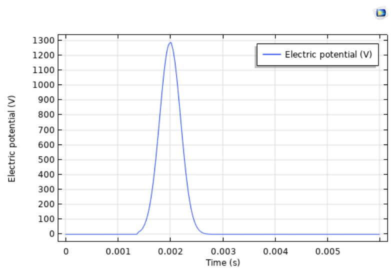
(a) Max. deformation/stress



(b) Surface charge density



(c) Average charge density vs. time



(d) Average potential vs. time

Figure 9: PVDF, 750 μm, Gaussian Load

In this case the response has the same qualitative shape, but the induced charge density distribution is much more narrow, and most of the surface has near-zero charge density as seen in (b).

4.2 Part 2 (Measuring current through resistor)

4.2.1 Setup

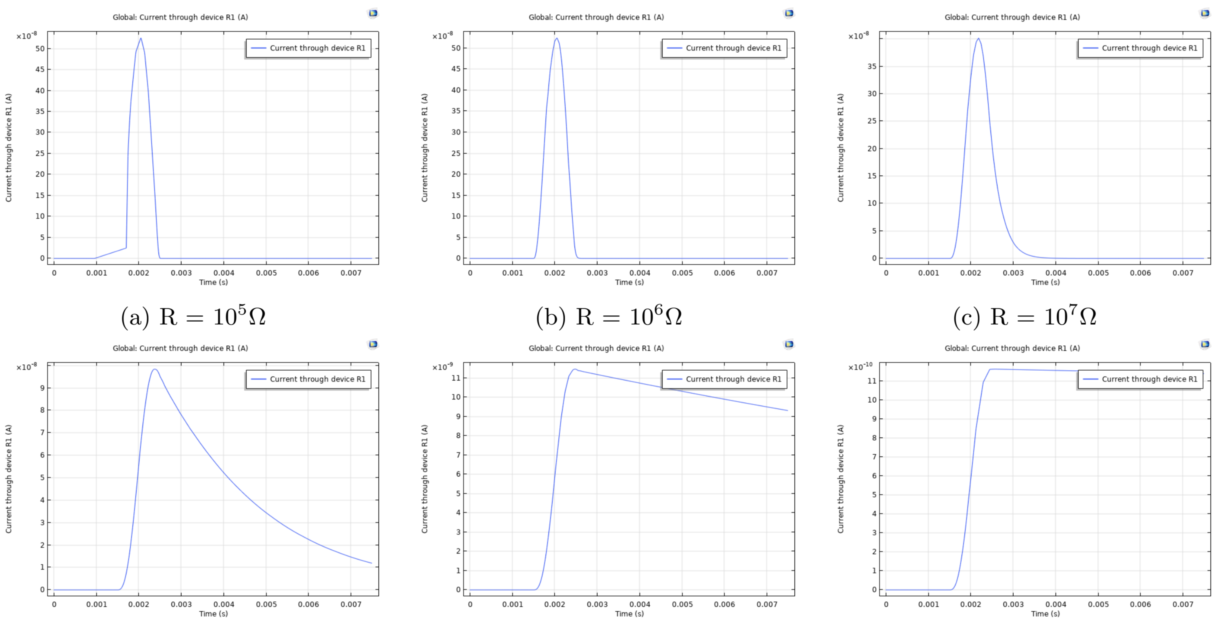
This involves building a SPICE circuit, however we also want to connect our non-component piezo-electric geometry to the circuit. This involves coupling the Electrostatics and Electric Circuit MultiPhysics modules in COMSOL. We do this in the following way:

- Set the floating potential on Face B to *Circuit*.
- Create SPICE circuit, add a *External I-terminal* component and link it to the floating potential terminal.

This will couple the two interfaces and our geometry will be substituted for a voltage source with same voltage response from the piezo-electric material. We then measure the current across the resistance R.

4.2.2 Material: PZT-5A, 150 μm

- **Step Load**



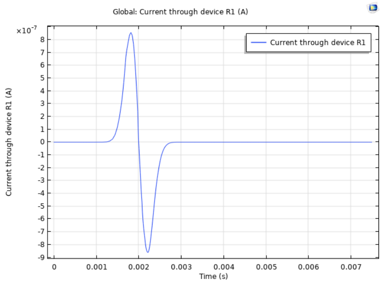
(a) R = $10^5\Omega$ (b) R = $10^6\Omega$ (c) R = $10^7\Omega$

(d) R = $10^8\Omega$ (e) R = $10^9\Omega$ (f) R = $10^10\Omega$

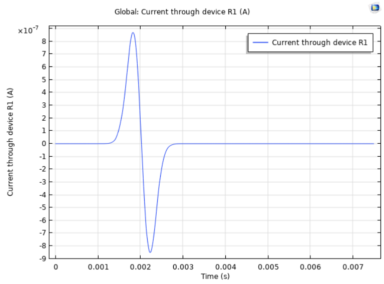
Figure 10: Current through resistor R

For small resistance the current turns out to be ill-defined, so we have performed the simulations for larger resistance value ($> 10^5\Omega$). We see that as the resistance increases, the gaussian response falls of slower till it ideally becomes a sigmoid response (saturation).

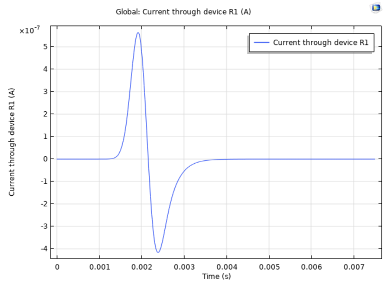
- **Gaussian Load**



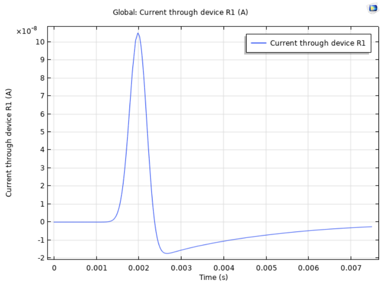
(a) R = $10^5\Omega$



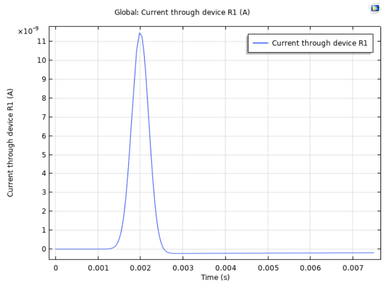
(b) R = $10^6\Omega$



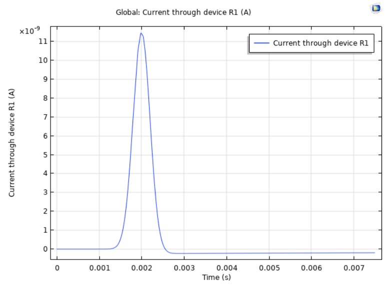
(c) R = $10^7\Omega$



(d) R = $10^8\Omega$



(e) R = $10^9\Omega$



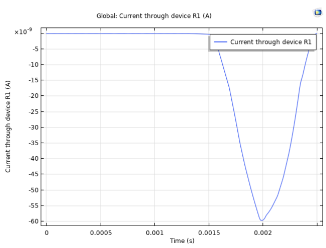
(f) R = $10^10\Omega$

Figure 11: Current through resistor R

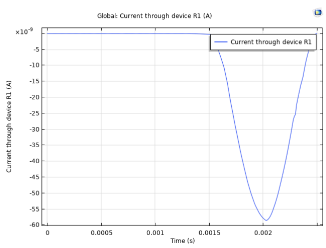
In case of the gaussian load, we observe an AC response with positive and negative peaks, which disappears into a single positive peak as the resistance increases.

4.2.3 Material PVDF, 150 μm

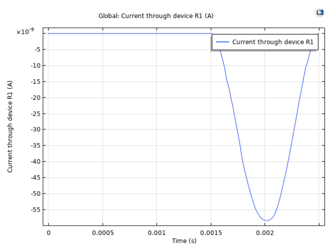
- **Step Load**



(a) R = $10^5\Omega$



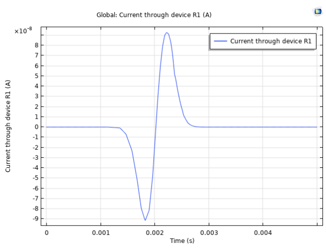
(b) R = $10^6\Omega$



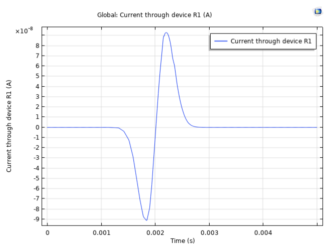
(c) R = $10^7\Omega$

Figure 12: Current through resistor R

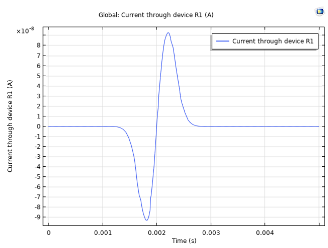
- **Gaussian Load**



(a) R = $10^3\Omega$



(b) R = $10^4\Omega$



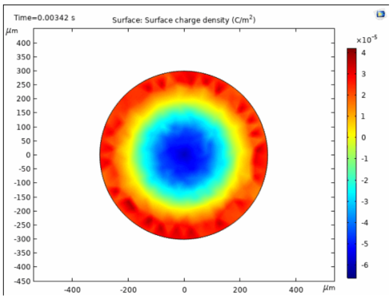
(c) R = $10^5\Omega$

Figure 13: Current through resistor R

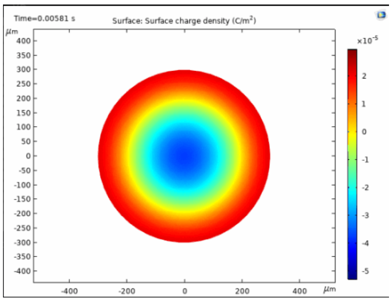
In case of PVDF we note that step load produces a single gaussian shaped current response, which does not vary much with increasing resistance. In case of the gaussian load, we once again observe an AC current response. An interesting observation is that the current response of PVDF is opposite polarity to that of PZT-5A for the same applied load. We can then conclude that the poling voltage for the two materials are of opposite polarities.

5 Failed Attempts

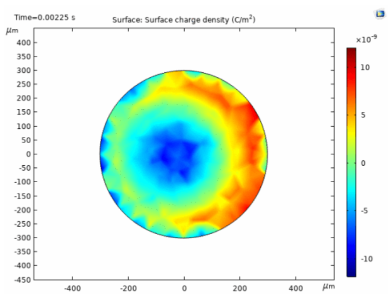
Initially we had performed the simulation with 3D geometry, however due to improper meshing, we produced unphysical symmetry (such as loss of radial symmetry), and computation times were long. Below is a comparison between the 3D and 2D Axi-symmetric results for the charge density of PZT-5A.



(a) 3D result (150μm)



(b) 2D Axi-symmetric result (150 μm)



(c) 3D result (750 μm)

This became evidently incorrect for thicker geometries as seen above, so we re-evaluated and gathered data from a 2D Axi-symmetric setup instead.

6 Conclusion

We have used COMSOL to observe and study induced charge distribution, potential gradient and current generation due to applied load on two different materials. Some issues are present in the current generation simulations due to incorrect matching of impedance while interfacing the Electrostatics and Electric Circuit modules, but we were unable to correct this.

References

[1] *Solving an electrical spice circuit using Comsol Multiphysics*; https://arxiv.org/abs/1907.01316

[2] *Comsol Multiphysics Playlist*; https://youtube.com/playlist?list=PLEfHDND8UieDX4l4n-vB8VFqrHpMAOa2t

[3] *Model Piezoelectric Devices as Both Transmitters and Receivers*; https://www.comsol.com/blogs/how-to-model-piezoelectric-devices-as-both-transmitters-and-receivers/