



A Computational Model of the Piezoelectric Effect

Joshua Milem¹ and Anna Turnbull^{1,2}

¹Laboratory for Hybrid Quantum Systems, Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824

²Lyman Briggs College, Michigan State University, East Lansing, MI 48824



Piezoelectric Effect – What is it?

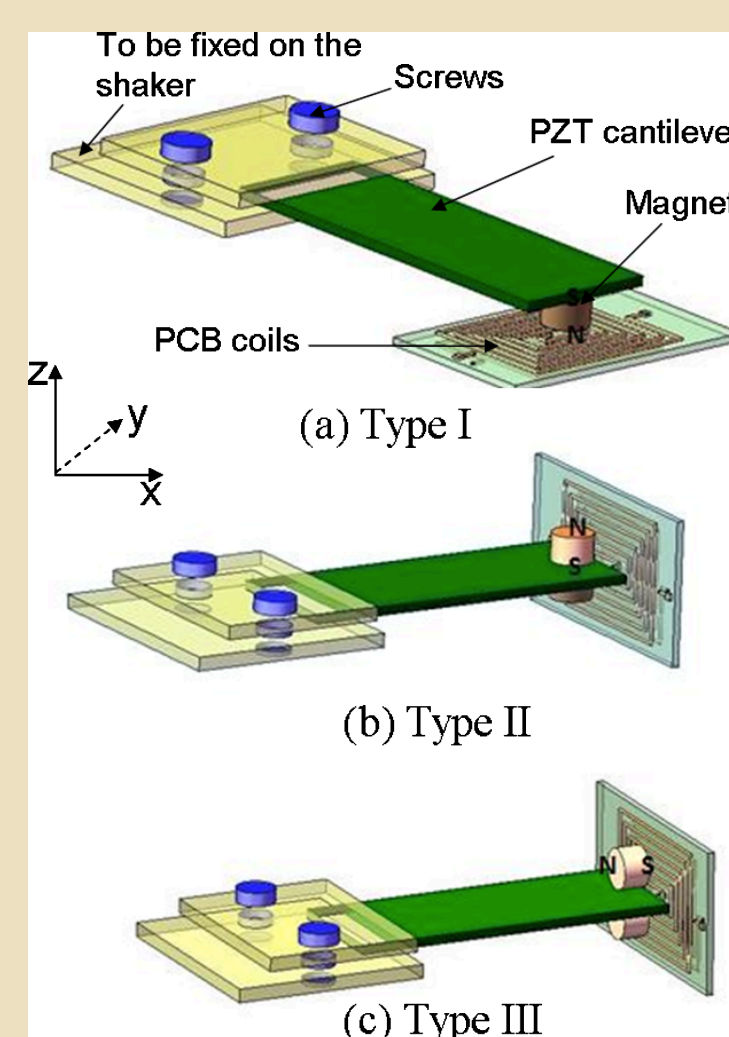
Original figure of piezoelectric effect in picture form because the internet sucks
(compression = voltage, voltage = compression)—**IN PROGRESS**

Motivation in SAW and LiNbO₃

SAW pic from Johannes or Justin—**IN JP'S THESIS?**

Uses of Piezoelectric Crystals

Piezoelectric Energy Harvesting Devices, sensors, etc



References

Computational and Theoretical Model of Piezoelectric Materials

Computational Model

The Tools: Monte Carlo Simulation (hoomd)

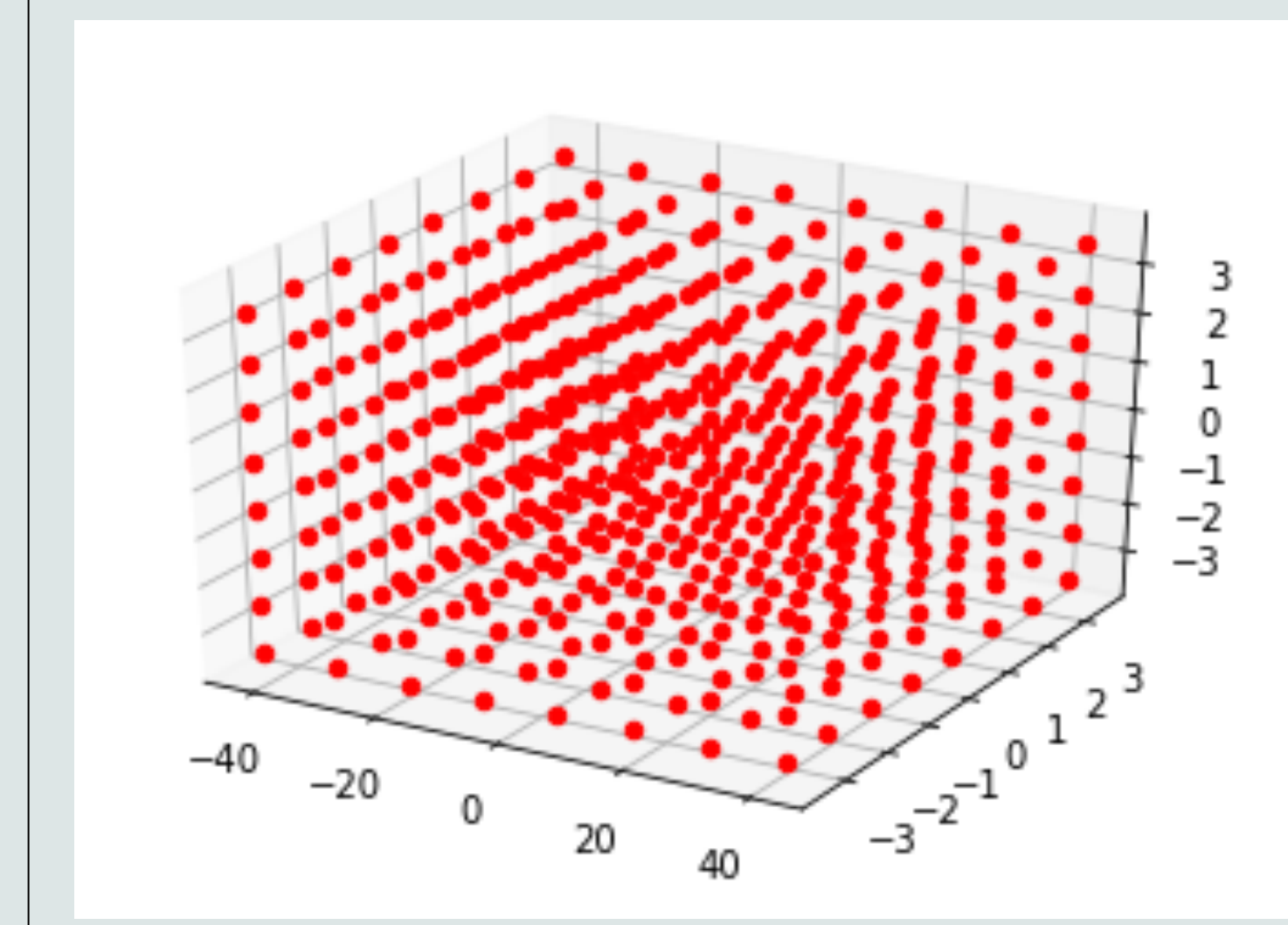
Creating a Lattice of Interacting Atoms

Pieces of our code will be used in our description of our model all in this column

Applying an Electric Field and Seeing a Change

Problems with the Model

Output of Code Initially (No E applied) – A lattice of particles representing the crystalline structure & Energy stored in lattice vs. time plot



Output of Code Shortly after E field applied (several hundred counts) – Initial Lattice Deformation & Energy Plot – **IN PROGRESS**

Output of Code a while after E field applied (a thousand counts) – Visible Lattice Deformation & Energy Plot – **IN PROGRESS**

Theoretical Model

Derivation of equations that describe piezoelectricity and what they mean