**Electrostatic Energy**

<http://repository.ust.hk/ir/bitstream/1783.1-19649/1/PhysRevB.73.144107.pdf>

<http://www.mmm.psu.edu/SC2005ActaMater.pdf>

<http://repository.ust.hk/ir/bitstream/1783.1-3525/1/ApplPhysLett_92_1629051.pdf>

<http://aip.scitation.org/doi/pdf/10.1063/1.1707211>

There are two main contributions to the electrostatic energy: depolarization energy and externally applied electric field energy. The depolarization energy is due to the long-range electrostatic spontaneous polarization interactions. The externally applied electric field energy is due to an externally applied electric field. <https://www.researchgate.net/profile/Jie_Wang20/publication/228999664_Phase_Field_Simulations_of_Polarization_Switching-Induced_Toughening_in_Ferroelectric_Eramics/links/54b3cd720cf26833efcf5be3.pdf>

**Depolarization Energy**

In a linear dielectric (), the displacement field is:

Now what happens if we have permanent dipoles in our material? The displacement field is given by:

with representing the permanent dipoles (the ferroelectric domains) present in our material, and is the background permittivity. Let us simply write the electric displacement field as:

is the spontaneous polarization, which is also the order parameter in our other energy terms. is the depolarization field. We have the electrical equilibrium which is governed by:

The divergence of the electric displacement field gives the amount of free charge. We assume there are no space charges within our sample.

The electric field is related to the electric potential by:

We must therefore solve:

Assume for ,

Or, in terms of the electric potential,

If we assume

We can solve via Fourier transform techniques.

The electric field is then:

This is the inhomogeneous electric field.

Boundary conditions for …follow the same 2D method as YuLuanLi’s Susbtrate method. Let us apply short circuit conditions, where . The actual value of is unimportant because we use the electric field, the derivative of potential, in our free energy equation.

We separate the solution such that,

We solve the first equation using 3D Fourier transforms:

We solve the second equation using 2D Fourier transforms. is the 2D (in-plane) Fourier transform of

To apply boundary conditions:

Recasting into a matrix,

is an arbitrary constant such as

At the 2D Fourier space origin

The matrix for determining the coefficients is:

Boundary condition:

To apply:

Recasting into a matrix,

is an arbitrary constant such as

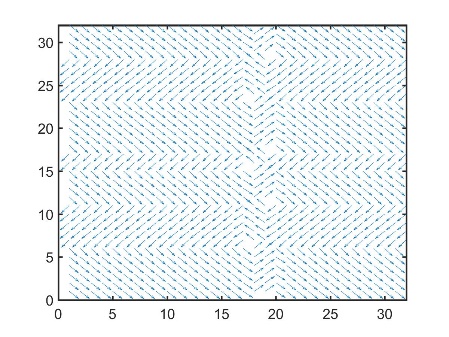
At the 2D Fourier space origin

When calculating the electric field, the is neglected: . Mathematically the Fourier space origin leads to a divergence. Physically, the point is due to surface polarization (???).

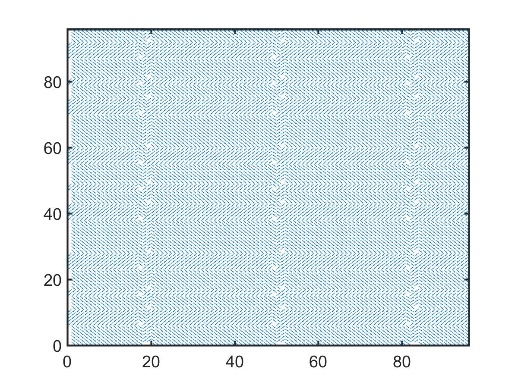
**is used for macroscopic boundary conditions**

**is a constant**

The Fourier transform automatically imposes periodic boundary conditions on our simulation volume. So in reality, when our simulation volume looks like:



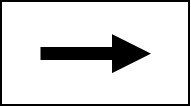
Our actual sample volume being simulated looks like (repeated infinitely more times):



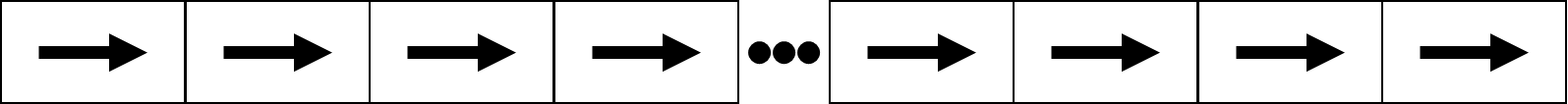
So in our actual physical representation, we have uncompensated surface polarizations that can create an additional electric field component. This surface polarization field component can be approximated using <http://www.mmm.psu.edu/SC2005ActaMater.pdf> :

This surface polarization contribution needs to be accounted for along the directions in which we apply periodic boundary conditions. When we apply alternate boundary conditions such as short circuit (potential is constant at the film surface and film/substrate interface) do we still need to account for this? Also when we apply open circuit boundary conditions as open circuit (displacement field is zero at the film surface and film/substrate interface) do we need to account for this.

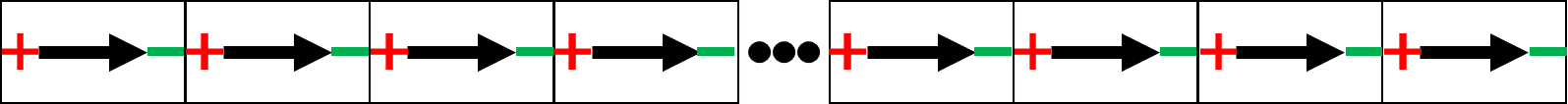
Our simulation volume is:



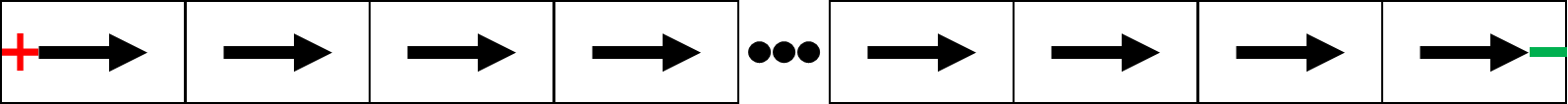
But because we used Fourier transform techniques to solve the electrostatic equilibrium, the physical representation of our simulation is an infinitely repeating pattern. In fact, within the Fourier transform technique there is no surface because our simulation volume infinitely repeats.



The Fourier transform technique does not account for surface effects because the physical representation of our simulation is infinitely repeating, with no surface. A dipole moment creates bound charges. In our example, the bound charges take the below form:



The charges within the sample volume cancel each other, and only the surface charges are uncompensated:



These surface charges create an electric field, which we can approximate with:

Mathematically, this field is due to the Fourier space origin.

Regardless, in the case of an infinitely periodic sample, the surface polarization can be neglected (our simulation volume is solely within the center of the film such that the surface polarization electric field is weak (E~V/d, d>>1) or screened by the bulk of the material). We can also neglect surface polarization when we assume charges compensate the surface polarization.

The total energy is then:

**External Electric Field**

The externally applied electric field is .

**Electric Energy**

The LGD functional for electrical energy is:

We assume electrical equilibrium is established instantaneously. We also ignore the surface polarization electric field effect. The functional derivative is therefore: