Polarizability of Biased Ferroelectric Particles of Different Shapes

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Ferroelectric materials exhibit nonlinear polarization with hysteresis effects, meaning that a remanent polarization can be obtained in the material after subjecting it to a bias field. When subjecting a biased ferroelectric particle to an incident electromagnetic wave, the linearized scattering is proportional to the linearized polarizability, which in turn depends on the remanent polarization. In this contribution, we show how this linearized polarizability can be computed using an open source finite elements code based on FEniCSx (`https://fenicsproject.org/`). The starting point is the fully nonlinear phase-field model based on Landau-Ginzburg theory [1], where the free energy is written

$$G = a^{(1)}_{ij} P_i P_j + a^{(2)}_{ijkl} P_i P_j P_k P_l + a^{(3)}_{ijklmn} P_i P_j P_k P_l P_m P_n + \frac{1}{2} g_{ijkl} P_{k,i} P_{l,j} \\ - P_i E_i - \frac{1}{2}\varepsilon_0 \kappa_{ij} E_i E_j + \frac{1}{2} c_{ijkl}(\varepsilon_{ij} - Q_{ijmn} P_m P_n)(\varepsilon_{kl} - Q_{klmn} P_m P_n) \tag{1}$$

Here, we use the Einstein notation where summation over repeated indices is assumed, and an index with a comma indicates differentiation. Hence, it is seen that this model takes into account nonlinear interactions (terms multiplied by $a^{(2)}_{ijkl}$ and $a^{(3)}_{ijklmn}$), gradients of the polarization (term multiplied by g_{ijkl}), linear background permittivity (term multiplied by κ_{ij}), and material strain (term multiplied by c_{ijkl}). The solution is characterized by a minimum of the energy functional G, which can be written (the i:th component of $\partial G/\partial \boldsymbol{P}$ is $\partial G/\partial P_i$)

$$0 = -\frac{\partial G}{\partial \boldsymbol{P}}, \quad 0 = \nabla\cdot\boldsymbol{D} = -\nabla\cdot\frac{\partial G}{\partial \boldsymbol{E}}, \quad \boldsymbol{0} = \nabla\cdot\boldsymbol{\sigma} = \nabla\cdot\frac{\partial G}{\partial \boldsymbol{\varepsilon}} \tag{2}$$

which represents a coupled system of polarization, electrostatics, and elasticity. This set of equations is solved using FEniCSx for a static bias field $\boldsymbol{E}_\mathrm{b}$, and the corresponding static polarization distribution in the particle, $\boldsymbol{P}_0(\boldsymbol{r})$, is computed. When considering a weak incident electric field $\Delta\boldsymbol{E}\mathrm{e}^{\mathrm{j}\omega t}$ and assuming all material processes are fast enough to maintain the condition $\partial G/\partial \boldsymbol{P} = \boldsymbol{0}$ to first order, we obtain the time harmonic polarization perturbation $\Delta\boldsymbol{P}\mathrm{e}^{\mathrm{j}\omega t}$ as

$$\Delta\boldsymbol{P}\mathrm{e}^{\mathrm{j}\omega t} = \left(\left.\frac{\partial^2 G}{\partial \boldsymbol{P}^2}\right|_{\boldsymbol{P}_0}\right)^{-1} \cdot \Delta\boldsymbol{E}\mathrm{e}^{\mathrm{j}\omega t} = \varepsilon_0 \boldsymbol{\chi}\cdot\Delta\boldsymbol{E}\mathrm{e}^{\mathrm{j}\omega t} \tag{3}$$

Taking the background relative permittivity $\boldsymbol{\kappa}$ into account, the total linearized permittivity is $\boldsymbol{\kappa}(\boldsymbol{r}) + \boldsymbol{\chi}(\boldsymbol{r})$. It is now straightforward to insert this permittivity in a traditional linear problem and compute the linearized polarizability $\boldsymbol{\gamma}$ of the particle:

$$\nabla\cdot[\varepsilon_0(\boldsymbol{\kappa}(\boldsymbol{r}) + \boldsymbol{\chi}(\boldsymbol{r}))\cdot(\boldsymbol{E}_0 - \nabla u)] = 0 \quad\Rightarrow\quad \boldsymbol{p} = \varepsilon_0 \int (\boldsymbol{\kappa}(\boldsymbol{r}) + \boldsymbol{\chi}(\boldsymbol{r}) - \mathbf{I})\cdot(\boldsymbol{E}_0 - \nabla u)\,\mathrm{d}V = \varepsilon_0 \boldsymbol{\gamma}\cdot\boldsymbol{E}_0 \tag{4}$$

In the presentation, I will demonstrate how the polarizability $\boldsymbol{\gamma}$ depends on the shape and bias of the ferroelectric particle. Shapes with high symmetry such as spheres and cubes will be considered, where it is seen that the bias introduces anisotropy in the polarizbility. I will also consider shapes as rods and discs with finite thickness, where the shape induced anisotropy interacts with the bias induced anisotropy.

References

[1] K. M. Rabe, C. H. Ahn, and J.-M. Triscone, editors. *Physics of Ferroelectrics—A Modern Perspective*. Springer, 2007.