Finite Element Model of a Ferroelectric

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Abstract: Ferroelectric technology continues attracting significant interest due to its wide range of applications (capacitors, nonvolatile memories, accelerometers ...). In this work we present a finite element model of a simple ferroelectric structure. Piezoelectric and ferroelectric matrices are included. The coupling between the piezoelectric and ferroelectric parameters will be introduced formally using a thermodynamic approach. Using the Comsol finite element nonlinear analysis, the ferroelectric loop (polarization versus electric field) and butterfly loop (strain versus electric field) in ferroelectric materials is obtained and discussed. The experimental results are compared to the finite element simulations

Keywords: Ferroelectric, piezoelectric, finite element, ferroelectric loop, butterfly loop.

1. Introduction

Ferroelectric materials are characterized by having permanent electric polarization vectors, which can be oriented in opposite directions by applying an external electric field, being able to switch between both states (figure 1).

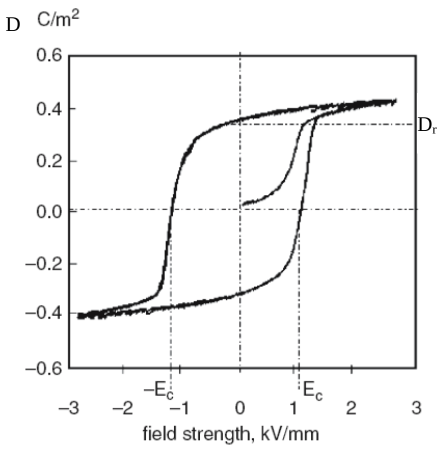

Figure 1. Hysteresis cycle of a ferroelectric material.

Moreover, the two opposite directions of the polarization vectors are stable. This property, known as bistability, allows the use of ferroelectric materials as nonvolatile memory elements [1].

In addition to its application in computer memories [2], [3], ferroelectric materials can be used in the fabrication of many novel devices that can take advantage of the special properties of ferroelectric materials. A large number of these devices have a potential commercial development; figure 2 shows several applications of thin film ferroelectric materials.

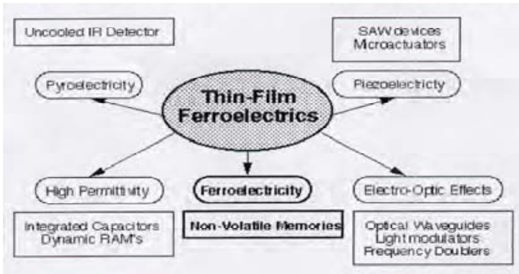

Figure 2: Several applications of ferroelectric materials.

Piezoelectricity is one of the special properties present in ferroelectric materials. It can be applied in the manufacture of micromachines, such as accelerometers and in the manufacturing of several types of control devices.

There are two kinds of piezoelectricity: direct and indirect. In direct piezoelectricity the ferroelectric layer expands or contracts when a certain voltage is applied across it.

On the other hand, when the ferroelectric layer is compressed, a voltage appears between the opposite sides of the ferroelectric layer. This type of piezoelectricity, known as indirect piezoelectricity, is applied in the construction of pressure sensors.

Pyroelectricity is another particular property of ferroelectric materials. When a heating process is applied to a ferroelectric crystal, positive and negative ions are created in the opposite sides of the ferroelectric layer. This effect involves the apparition of electric voltage between both sides of the crystal that can be used in infrared temperature sensors.

There are ferroelectric materials that also exhibit electro-optic activity. This means that the refractive index of a ferroelectric material changes when a voltage is applied across it. This property is used in color-filtering devices, displays, image recording systems.

In this work, we have performed a finite element model of ferroelectric materials with Comsol Multiphysics, linked to the model of a piezoelectric material present in the program. The characteristic curves of the material were simulated, verifying the proper operation of the model.

2. Ferroelectric Model

Ferroelectric materials have two states of polarization (p^+ and p^-) and can switch between them when an external electric field is applied. In Figure 3 it can be seen that there is no tendency towards one of the two polarization states in the absence of applied voltage. Figure 4 shows the evolution when an external electric field is applied. In this case, applying a positive voltage V, a resulting positive state of polarization (p^+), is obtained, because some of the dipoles switch their orientation. Applying a negative voltage -V, a ferroelectric state in opposite polarization (p^-) would be established.

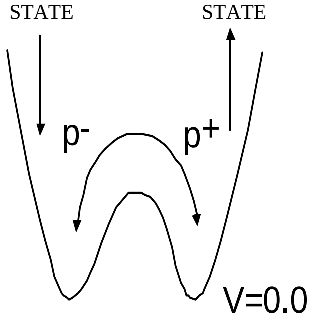

Figure 3: Polarization states in the absence of applied of electric field.

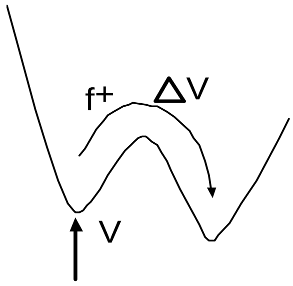

Figure 4: Effect in the polarization states when a positive voltage is applied.

When an external electric field is applied to a ferroelectric capacitor, the polarization state of the capacitor changes, if the applied electric field direction is the opposite to the previous one. The amount of negative polarization (p^-) which becomes positive tendency (p^+) when applying a positive voltage V, ie, the increasing of the p^+ polarization state, is given by the following equation [4]:

$$\Delta p^+ = (1 - p^+) \cdot f^+ \cdot \Delta V \qquad (1)$$

where $\mathbf{\Delta p^+}$ is the increment of the positive polarization state, ΔV is the increment of the applied voltage and **($\mathbf{f^+ \cdot \Delta V}$)** is the probability of the occurrence of a switching of polarization state due to an increment in the applied voltage ΔV.

In this equation, f^+ is obtained as:

$$f^+ = \frac{1}{1 + e^{\frac{-(V - V_C)}{V_0}}} \cdot \frac{1}{Vo} \qquad (2)$$

where **Vc** y **Vo** are the coercitive and thermal voltages respectively. These two voltages are very relevant parameters in ferroelectric capacitors.

The thermal voltage is defined by the next equation:

$$Vo = \frac{K.T}{q} \qquad (3)$$

where **K** is the Boltzmann constant ($1{,}38047.10^{-23}$ J/K), **T** is the temperature (K) and **q** is the electron charge ($1{,}601864.10^{-19}$ C).

From the previous expressions we can obtain an expression for p^+ as follows:

$$p^+ = 1 - (1 - p^+{}_i).\frac{1 + e^{\frac{(Vi - Vc)}{Vo}}}{1 + e^{\frac{(V - Vc)}{Vo}}} \qquad (4)$$

where $\mathbf{V_i}$ is the initial voltage and $\mathbf{p^+{}_i}$ is the initial positive polarization.

Finally, the electric displacement (D^+), obtained for positive applied voltages has the value:

$$D^+ = Ps \cdot (2 \cdot p^+ - 1) \qquad (5)$$

In a similar way, we can obtain for negative voltages:

$$D^- = -Ps \cdot (2 \cdot p^- - 1) \qquad (6)$$

where

$$p^- = 1 - (1 - p^-{}_i).\frac{1 + e^{\frac{(Vi - Vc)}{Vo}}}{1 + e^{\frac{(-V - Vc)}{Vo}}} \qquad (7)$$

3. FEM model

The employed geometry in the model is a plane capacitor with cylindrical shape (figure 5). It is defined as an element of *electric currents* inside AC/DC physics and as a piezoelectric material inside the *Piezoelectric Device* physics.

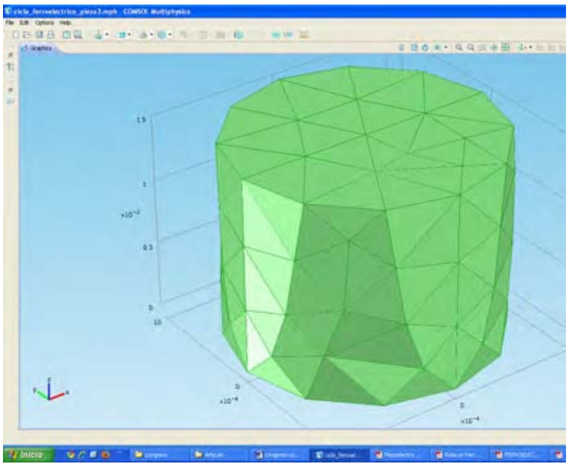

Figure 5: Geometry used in the model.

In the first case, in *the electric field*, the value of $D^{+/-}$ is introduced as a parameter of *remanent displacement*.

In the second one, the existing theoretical relationship between d_{33} and the value of $D^{+/-}$, obtained from the thermodynamic behavior of ferroelectric materials, is introduced in the piezoelectric matrix [5].

$$d_{33}^{+/-} = 2 \cdot Q_{33} \cdot \varepsilon_{33}^T \cdot D^{+/-} \qquad (9)$$

$$d_{33}^{+/-} = d_{32}^{+/-} = 2 \cdot Q_{12} \cdot \varepsilon_{33}^T \cdot D^{+/-} \qquad (10)$$

As expected result, when introducing this non linearity, we should obtain a shape of s_{33} vs E as shown in figure 6, known as butterfly cycle of a piezoelectric material [5].

The electrical boundary conditions have been defined. A sinusoidal voltage is applied to the upper electrode. The lower electrode remains connected to ground. The perimeter of the structure is electrically isolated.

We have employed a triangular mesh with *time dependent* resolution. In both physics, a non lineal solver is used.

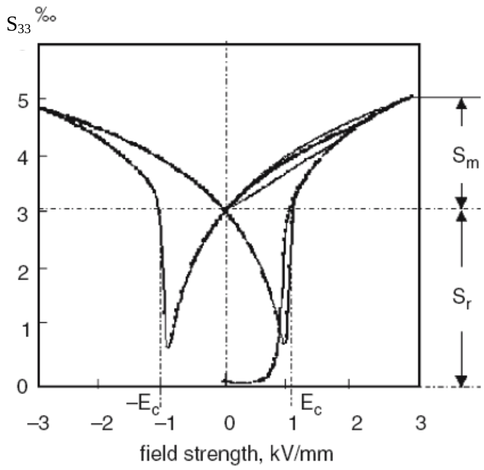

Figure 6. Butterfly cycle of a piezoelectric material [5].

4. Simulation result and discussion.

The obtained results were simulated for the upper part of the structure, were the sinusoidal voltage is applied. We evaluated the D_{33} vs E_{33} in *AC/DC* physics and S_{33} vs E_{33} in *Piezoelectric Device* physics.

First, an electrical field below the coercitive field was applied, obtaining a lineal response of a dielectric material (figure 7) and the typical response of a piezoelectric material (figure 8) for a lineal material described in Comsol.

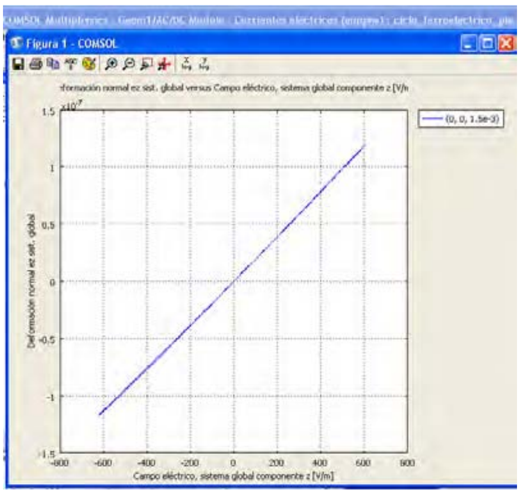

Figure 7. Response of a ferroelectric material for E<Ec.

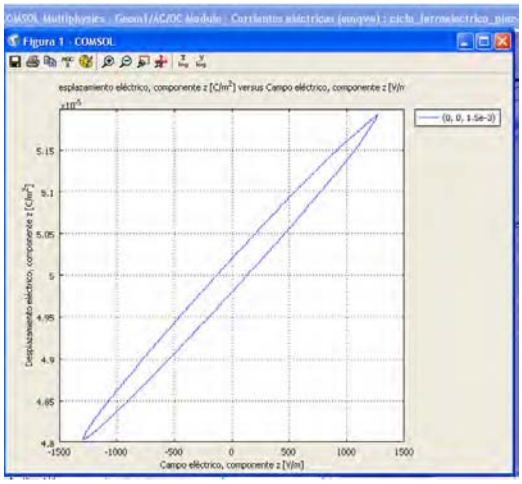

Figure 8. Response of a piezoelectric material for E<Ec.

Once the linear response was obtained, we simulated the response for an electrical field higher than Ec, obtaining the typical non linear response of a ferroelectric material and the effect of this nonlinearity in the piezoelectric response (figures 9 and 10). Comparing those graphs with the expected from theory (graphs 1 and 6), we can conclude that the model performs the behavior of a ferroelectric material from both points of view, electrical and mechanical.

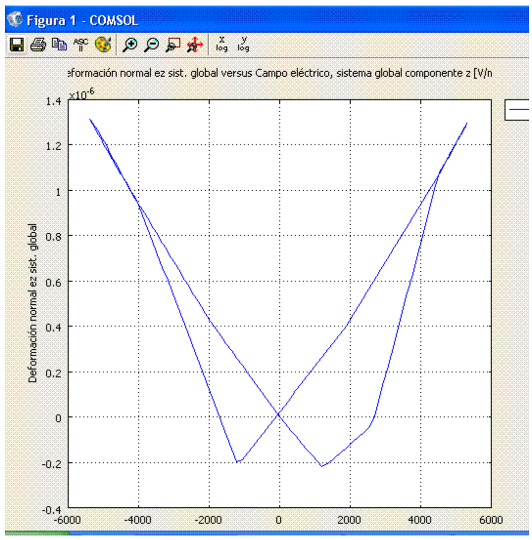

Figure 9. Simulated butterfly cycle.

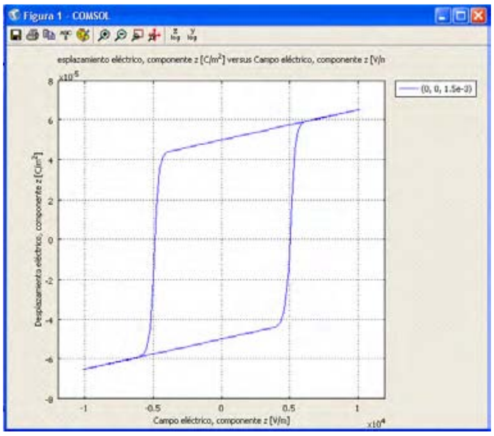

Figure 10. Simulated ferroelectric cycle.

5. Conclusions

The developed model allows to adequately describing ferroelectric materials, not included in the Comsol material libraries. The predicted electrical and mechanical responses of the materials are confirmed, this shows than the piezoelectric and ferroelectric characteristics have been well described with this model.

This will allow developing models for more complex structures with relevant technological interest, such as multiferroic materials.

6. References

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