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Interaction of domain walls with defects in ferroelectric materials

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Abstract

A thermodynamic approach is used to derive the driving force on a domain wall in a piezoelectric material. Using 2D finite element simulations, the influence of different kinds of defects on the kinetics of a domain wall in ferroelectric–ferroelastic gadolinium molybdate, $Gd_2(MoO_4)_3$ (GMO), is studied. Results are compared with experiments conducted on single crystal GMO containing extensive bulk defects. It is found that domain wall movement is impeded for certain defects while it is virtually unaffected for others. Qualitatively, results are in good agreement with experimental findings.

Keywords: Piezoelectric material; Domain wall; Defects; Driving force; Material force; Configurational force; Energy–momentum tensor; Eshelby tensor

1. Introduction

Experimental studies suggest that domain wall movement in ferroelectric materials is strongly influenced by the presence of certain kinds of defects. The intention of this paper is to study this phenomenon using concepts of continuum mechanics to describe ferroelectric material behavior. Closely following the concept introduced in Mueller et al. (2006), a 180° domain wall is modeled as a singular surface at which a jump in the spontaneous polarization occurs. The domain wall can be thought of as an inhomogeneity which allows for the application of configurational or driving forces (Maugin, 1993; Gurtin, 2000; Kienzler and Herrman, 2000; Gross et al., 2003). We will however not emphasize the general use of configurational forces here but rather derive the driving force on a domain wall from thermodynamic considerations. Knowing the driving force, it will be possible to establish a relation to the domain wall velocity. Experimental background for the domain wall kinetics can be found in Flippen (1975), where domain wall velocities were measured. Numerical simulations will be used to study some basic configurations and to gain some fundamental knowledge about the interaction of defects and domain walls. Three types of defects are considered. The first one is a surface defect, reflecting an imperfect electrode. The second one

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is a hole in one side of a sample where the electrodes remain intact. The third type involves a defect in the polarization in one domain.

Results will be compared with experimental studies on GMO (Kumada, 1969; Newnham et al., 1969; Keve et al., 1971; Lupascu et al., 2002). Artificial macroscopic defects were implemented in macroscopic single crystals containing a single planar domain wall. The domain wall is moved over such a defect by applying electric fields. The influence of a defect on the domain wall motion was examined by optical observations, measurements of the switching current, and acoustic emissions.

The domain wall in GMO is intrinsically rigid due to the orthorhombic symmetry of the crystal. The primary ordering parameter, i.e., the primary reordering of atoms in the unit cell during the phase transition to the ferroelectric phase, confines the domain wall to the [1 1 0] crystal plane (Xu, 1991).

2. Theory

2.1. Field equations

The piezoelectric body under consideration $\mathscr{B}$ is assumed to be separated into two domains by a domain wall $\mathscr{S}$. The normal vector $\boldsymbol{n}_{\mathscr{S}}$ to the domain wall points from the sub-body $\mathscr{B}^-$ into $\mathscr{B}^+$, refer to Fig. 1 for details. Including volume forces $\boldsymbol{f}$, the mechanical equilibrium condition for the bulk and the domain wall reads

$$\begin{aligned} &\operatorname{div}\boldsymbol{\sigma} + \boldsymbol{f} = \boldsymbol{0} \quad \text{in } \mathscr{B}^{+/-}, \\ &[\![\boldsymbol{\sigma}]\!]\boldsymbol{n}_{\mathscr{S}} = \boldsymbol{0} \quad \text{on } \mathscr{S}, \end{aligned} \tag{1}$$

where $\boldsymbol{\sigma}$ is the stress tensor. The jump operator $[\![(\cdot)]\!]$ is defined in Appendix A. Prescribing either the displacements $\boldsymbol{u}$ on the boundary $\partial\mathscr{B}_u$ or tractions $\boldsymbol{\sigma n}$ on the boundary $\partial\mathscr{B}_t$, the boundary conditions for the mechanical problem are

$$\begin{aligned} &\boldsymbol{u} = \boldsymbol{u}^* \quad \text{on } \partial\mathscr{B}_u, \\ &\boldsymbol{\sigma n} = \boldsymbol{t}^* \quad \text{on } \partial\mathscr{B}_t. \end{aligned} \tag{2}$$

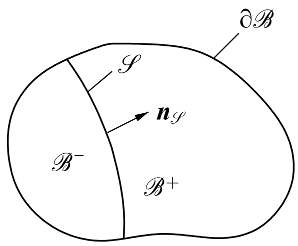

Fig. 1. Body containing a domain wall.

Analogously, the electro-static relations (Gauss law) for the electric displacement $\boldsymbol{D}$ read

$$\begin{aligned} &\operatorname{div}\boldsymbol{D} - q = 0 \quad \text{in } \mathscr{B}^{+/-}, \\ &[\![\boldsymbol{D}]\!] \cdot \boldsymbol{n}_{\mathscr{S}} = 0 \quad \text{on } \mathscr{S}, \end{aligned} \tag{3}$$

with volume charge density q. The corresponding boundary conditions for the electric potential φ and the surface charge density $\boldsymbol{D} \cdot \boldsymbol{n}$ on the boundary $\partial\mathscr{B}_\varphi$ or $\partial\mathscr{B}_Q$ respectively are

$$\begin{aligned} &\varphi = \varphi^* \quad \text{on } \partial\mathscr{B}_\varphi, \\ &\boldsymbol{Dn} = -Q^* \quad \text{on } \partial\mathscr{B}_Q. \end{aligned} \tag{4}$$

The kinematic relations in the bulk and on the domain wall are given by

$$\begin{aligned} &\boldsymbol{\varepsilon} = \frac{1}{2}\left(\operatorname{grad}\boldsymbol{u} + (\operatorname{grad}\boldsymbol{u})^{\mathrm{T}}\right) \quad \text{in } \mathscr{B}^{+/-}, \\ &[\![\boldsymbol{u}]\!] = \boldsymbol{0} \quad \text{on } \mathscr{S}, \end{aligned} \tag{5}$$

where $\boldsymbol{\varepsilon}$ is the strain tensor. Analogously, the relations

$$\begin{aligned} &\boldsymbol{E} = -\operatorname{grad}\varphi \quad \text{in } \mathscr{B}^{+/-}, \\ &[\![\varphi]\!] = 0 \quad \text{on } \mathscr{S} \end{aligned} \tag{6}$$

are valid. Here, $\boldsymbol{E}$ is the electric field, and φ is the electric potential.

In order to provide a closed system of equations, the following constitutive equations are assumed in the bulk:

$$\begin{aligned} &\boldsymbol{\sigma} = \mathbb{C}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^0) - \mathbb{b}^{\mathrm{T}}\boldsymbol{E}, \\ &\boldsymbol{D} = \mathbb{b}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^0) + \boldsymbol{KE} + \boldsymbol{P}^0. \end{aligned} \tag{7}$$

The material behavior is characterized by the stiffness tensor $\mathbb{C}$, the piezoelectric tensor $\mathbb{b}$ (more commonly denoted by $\boldsymbol{e}$) and the dielectric tensor $\boldsymbol{K}$. The different lattice parameters and the different remanent polarizations of the unit cells in different domains are taken into account by irreversible strains $\boldsymbol{\varepsilon}^0$ and irreversible polarizations $\boldsymbol{P}^0$.

2.2. Thermodynamic approach

In contrast to Mueller et al. (2006), where a variational principle was used to introduce a driving force on the domain wall, a thermodynamic approach is presented here that yields the same result. For the isothermal case, the second law of thermodynamics can be expressed as

$$\int_{\partial\mathscr{B}} ((\boldsymbol{\sigma n}) \cdot \dot{\boldsymbol{u}} + (\boldsymbol{D} \cdot \boldsymbol{n})\dot{\varphi})\,\mathrm{d}A + \int_{\mathscr{B}^{+/-}} (\boldsymbol{f} \cdot \dot{\boldsymbol{u}} - q\dot{\varphi})\,\mathrm{d}V - \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathscr{B}^{+/-}} H\,\mathrm{d}V \geqslant 0 \tag{8}$$