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A NOVEL APPROACH TO THE APPLICATION OF FERROELECTRIC THIN FILMS TO MICRO-ACTUATION

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Summary A micro-actuator capable of significant force and displacement remains an outstanding challenge in the development of micromachines. Active materials are attractive for their large work per unit volume, and specifically ferroelectrics since they are electrically activated. However, conventional piezoelectric materials display limited strains (0.1%), and conventional configurations like bi-morph cantilevers are too constrained to deliver the necessary performance. This paper describes an alternative strategy that combines a new mode of electrostriction in ferroelectrics that explicitly use domain switching to deliver extremely large strains (1-6%) at moderate forces and electrical fields along with a new approach to microactuators that use partially released thin films. Together this strategy enables micro-actuators with large force and displacement. This paper describes the theoretical analysis of the domain patterns in bulk and thin film ferroelectric perovskites that led to this strategy, detailed computational studies for specific designs and the subsequent experimental validation.

INTRODUCTION

Ferroelectric crystals are widely used in a variety of applications including sensors, actuators, capacitors and non-volatile data storage elements. In particular, poled ceramics of ferroelectric materials are used commonly for their piezoelectric property in actuator applications. However their application as microactuators raises two difficult challenges. First, the strains of ferroelectric ceramics are limited (about 0.1%). Second, these materials have to be adapted to micromachinable configurations and processes. This paper describes a strategy to address these difficulties developed through a theoretical understanding of ferroelectric perovskites. It combines a new mode of electrostriction in ferroelectrics that explicitly use domain switching to deliver extremely large strains (1-6%) at moderate forces and electrical fields along with a new approach to microactuators that use partially released thin films.

DOMAIN SWITCHING AND LARGE ELECTROSTRICTION

Ferroelectric materials are spontaneously electrically polarized and mechanically distorted. A variety of materials display ferroelectricty, but we focus on perovskites like $BaTiO_3$ and $PbTiO_3$. They are nonpolar and cubic at high temperature, but tetragonal and electrically polarized in the $\langle 001 \rangle_c$ at room temperature. The transformation from the non-polar cubic to the polarized tetragonal state can proceed along any of the $\langle 001 \rangle_c$ directions giving rise to in six symmetry-related variants at room temperature. Switching from one variant to another by the application of electric fields can potentially generate strains equal to the tetragonal distorsion which range from 1-6% depending on the material. However, homogeneous switching has prohibitive barriers, and one has to affect this switching by nucleation and growth. This requires the ability to form large domains of uniform polarization domains and low energy boundaries (domain walls) between them.

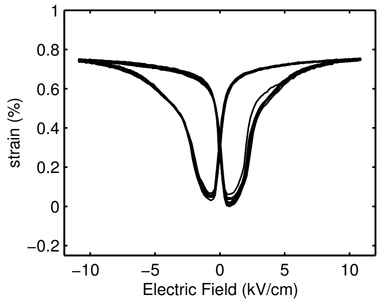
Consider a ferroelectric crystal occupying a region Ω in the reference configuration, and undergoing a deformation y and with polarization density $p(y)$ in the current configuration. The total energy of the system at temperature θ is given by [1]

$$\mathcal{E}[y,p;\theta] \quad = \quad \int_\Omega \left\{ \alpha |\nabla_x P|^2 + W(\nabla_x y, P, \theta) - (\det \nabla_x y) E_o \cdot P \right\} dx - \int_{\partial_1 \Omega} t_0 \cdot y dA_x + \frac{1}{2} \int_{\mathbb{R}^3} |\nabla_y \phi|^2 dy \; , \quad (1)$$

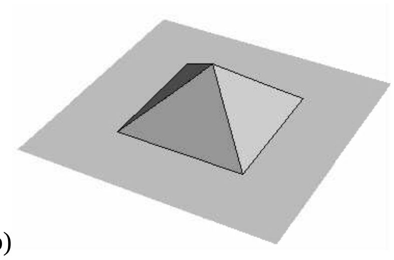
where $P(x) = p(y(x))$ is the pull-back of the polarization density to the reference configuration and the electric potential ϕ is determined by solving Maxwell's equation, $\nabla_y \cdot (-\nabla_y \phi + p) = \rho$ on $\mathbb{R}^3$ subject to appropriate boundary conditions. The first term represents a domain wall energy. The second term is the free energy density W which depends on the deformation gradient, polarization, and temperature. It encodes all information about the crystallography, spontaneous polarization and spontaneous strain. The third term is the potential energy of the applied electric field. The second integral is the potential energy of the applied mechanical load, and the third integral is the electrostatic energy associated with the electric field generated by the spontaneous polarization of the crystal. The equilibrium deformation and polarization can be found by minimizing the total energy over all possible deformations, y, and polarizations, p.

Since there are multiple variants of the ferroelectric state at room temperature, the free energy density W has multiple wells. Therefore, energy minimizers consist of domains of (approximately) uniform polarization and deformation gradient. However, the boundaries between the domains can not be arbitrary; instead, low elastic and electric field energy require that the jump in the spontaneous distortion and polarization be simultaneously compatible across it. This is not satisfied generically, and thus many ferroelectrics are not suited for large electrostriction. However, It turns out that the conditions are simultaneously satisfied in materials which undergo a phase change involving a loss of two-fold symmetry[1]. This is true in materials like $BaTiO_3$ and $PbTiO_3$ and gives rise to gives rise to 180 and 90 degree domain walls. Further, the 90 domain walls provide the low energy pathways for switching with large strain.

However, the electrostatic field energy often forces the formation of very fine domains. Therefore it is important to design configurations and electrical boundary conditions (through the placement of electrodes) that allow large domains. One



(a)



(b)

Figure 1. (a) Large electrostriction in $BaTiO_3$. (b) A tent-like actuated shape of a large displacement actuator.

such configuration is the flat plate configuration with electrodes on top and bottom. If the thickness of the plate is small compared to the lateral extent, then the non-local term, the third integral in (1), becomes local[1] and one obtains large domains. Further, if the flat plate is made of a single crystal of $BaTiO_3$ with normal in the $\langle 001 \rangle_c$ direction and subjected to a fixed compressive load and a cyclic electric field across the thickness, then stable (energy minimizing) variant switches between those with in-plane and out-of-plane directions. 90 degree domain walls provide a pathway between these states and one obtains electrostriction of approximately 1% [1]. Figure 1(a) shows the experimentally measured (electrostrictive) strain[2, 3] as a function of applied field verifying the theory. Similar considerations in $PbTiO_3$ predicts strains of about 6.5% and strains of up to 5% have been experimentally obtained.

The considerations above have recently been extended to ceramics or polycrystals[4]. A theory that describes the effective behavior has been derived and has been used to show that cooperative domain switching and consequently large electrostriction is possible if and only if the polycrystal has a $\langle 001 \rangle_c$ fiber texture.

THIN FILMS

An application of ferroelectrics to micromachines calls for the integration of these materials with silicon and in the form of thin films. The traditional method is to make bimaterial cantilevers by depositing ferroelectrics on silicon and micromachinig. Unfortunately, silicon constrains the large strain materials, energy is expended in bending the silicon and it has poor bending scaling (third power of thickness). An alternative is to use partially released films motivated by a theory of thin films of martensitic films [5, 6]. The idea is to deposit a film of active material like ferroelectrics on a substrate, and then back-etch the substrate to release a portion of the substrate. The behavior of the partially released film is described by a rigorously derived membrane-type theory. This theory shows that thin films can indeed form domains. Further, it is possible to form large displacement actuators by carefully matching the geometry of the released region with the crystallography of the material. One such device can be made of a $\langle 001 \rangle_c$ film of $BaTiO_3$ by releasing it along a square region aligned with the pseudocubic direction. Such a device can be made to a cycle between a flat shape and a tent-like shape enclosing a large volume (Figure 1(b)) by domain switching, and thus form the active element of a micropump. Similar strategies can be designed to make linear motors.

CONCLUDING REMARKS

The discussion above was based on a theory of energy minimization. It is possible to derive a time-dependant theory by considering the gradient flow of (1). Finite-difference simulations of the resulting equations validate the discussion above and provide insights into the evolution of domains and the resulting hysteresis[7]. Such simulations also provide insights into the stress and electric field concentrations that can arise were the film not a single crystal or perfectly textured polycrystal. Finally, a program of synthesis of thin films, fabrication of microactuators and experimental evaluation is currently underway at the California Institute of Technology (USA), and the preliminary results are encouraging [8].

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