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Defects in flexoelectric solids

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ABSTRACT

A solid is said to be flexoelectric when it polarizes in proportion to strain gradients. Since strain gradients are large near defects, we expect the flexoelectric effect to be prominent there and decay away at distances much larger than a flexoelectric length scale. Here, we quantify this expectation by computing displacement, stress and polarization fields near defects in flexoelectric solids. For point defects we recover some well known results from strain gradient elasticity and non-local piezoelectric theories, but with different length scales in the final expressions. For edge dislocations we show that the electric potential is a maximum in the vicinity of the dislocation core. We also estimate the polarized line charge density of an edge dislocation in an isotropic flexoelectric solid which is in agreement with some measurements in ice. We perform an asymptotic analysis of the crack tip fields in flexoelectric solids and show that our results share some features from solutions in strain gradient elasticity and piezoelectricity. We also compute the energy release rate for cracks using simple crack face boundary conditions and use them in classical criteria for crack growth to make predictions. Our analysis can serve as a starting point for more sophisticated analytic and computational treatments of defects in flexoelectric solids which are gaining increasing prominence in the field of nanoscience and nanotechnology.

1. Introduction

Flexoelectricity refers to the coupling of electric polarization to strain gradients. It has been studied in-depth in liquid crystals (Meyer, 1969; Harden et al., 2010; Buka and Eber, 2012) and biomembranes (Raphael et al., 2010; Petrov, 2006). However, in recent years there has been a surge in interest in flexoelectric phenomena in harder materials, such as lead zirconate titanate (PZT) and other perovskites (Nguyen et al., 2013; Zubko et al., 2013). The primary reason for this development is the advent of accurate probes that can detect polarizations and stresses at the nano-scale (Ma and Cross, 2001, 2002; Zubko et al., 2007; Catalan et al., 2011; Chin et al., 2015). Concurrent developments have also taken place in the theoretical interpretations of the experiments. Atomistic simulations, such as lattice dynamics (Maranganti and Sharma, 2009) and first principles calculation (Hong and Vanderbilt, 2011, 2013) have shed some light on the microscopic origins of flexoelectric phenomena in solids and given estimates for the magnitude of the flexoelectric constants. On the other hand, computational methods based on finite elements have been used to study stress and polarization fields in macroscopic solids (Abdollahi et al., 2014). Recently, we presented analytic solutions to some boundary value problems in flexoelectric solids in one and two dimensions (Mao and Purohit, 2014). Our goal in this paper is to utilize that framework to describe the

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stress and polarization fields near defects in flexoelectric solids. Defects are the spots where the effects of flexoelectricity are expected to be prominent due to the large strain gradients in their vicinity. Our analysis will enable better interpretation of experimental data since most specimens inevitably have defects in them.

Flexoelectricity also offers a simpler alternative explanation to some phenomena that have been discovered before. In the 1960s and 1970s a series of experiments (Koehler et al., 1962; Turchányi et al., 1973; Whitworth, 1975) were performed to study charged dislocations in cubic crystals, i.e. alkali halides. These solids have centrosymmetric lattices which rule out piezoelectricity as the cause for the charge carried by dislocations in them, but this symmetry does not rule out flexoelectricity. In fact, flexoelectric phenomena can be observed in dielectrics of any symmetry group, including isotropic ones. We show in this paper that some of the results for charged dislocations can be qualitatively understood in terms of flexoelectricity. Charged dislocations were also observed in experiments on ice by Petrenko and co-workers in 1980s (Petrenko and Whitworth, 1983). They conducted a thorough study of the electromechanical properties of ice and attributed charged dislocations and other phenomena to a so-called "pseudo-piezoelectricity" (Petrenko and Whitworth, 1999). This phenomenon assumed that the polarization in ice is proportional to the pressure gradient. This is a natural result of what is known today as flexoelectricity (Mao and Purohit, 2014). Indeed, Petrenko and co-workers studied point defects, dislocations and cracks in ice and arrived at their conclusions about pressure gradient dependent polarization from a microscopic view point (Petrenko, 1996). We show here that the results from our formulation based on a strain-gradient coupled polarization agree quite well with the findings of Petrenko and co-workers.

The study of cracks and other defects in closely related piezoelectric solids has a long history (Kuna, 2010). A primary motivation for these studies was to better understand damage and failure of piezoelectric devices. In particular, mathematical techniques from linear elastic fracture mechanics (LEFM) were used to find analytic solutions for a variety of crack problems in piezoelectric solids (Sosa, 1992; Suo et al., 1992; Pak, 1992) which are now referred to as linear piezoelectric fracture mechanics (LPFM). Parallel experimental studies were also conducted, as summarized in Schneider (2007). It was realized that both mechanical failure and electric breakdown are responsible for damage in piezoelectric devices due to the singular nature of the stress and electric fields near a crack tip. For example, an "electric-yielded" zone in ferroelectrics was proposed (Gao et al., 1997; Wang, 2000), which is analogous to the plastic zone in fracture mechanics. Other important developments in this field involve treatment of boundary conditions, anisotropy, mode mixing etc., as summarized in Kuna (2010). All these studies have led to the development of a powerful continuum framework to study electromechanical effects in cracks. Some insights from this literature are used in our analysis. Also, since strain gradient elasticity (SGE) is an important ingredient of flexoelectricity, we draw upon the literature on asymptotic solutions of crack tip fields in gradient elasticity (Zhang et al., 1998; Aravas and Giannakopoulos, 2009).

This paper is organized as follows. First, we construct Green's function for a flexoelectric boundary value problem. We use it in our studies of point defects and dislocations. Second, we give an analytic solution to the problem of a single point defect in an isotropic flexoelectric solid. Third, we solve for the polarization fields of screw and edge dislocations and connect our analysis to various experiments. Fourth, we obtain asymptotic solutions to crack tip fields for Mode I and II cracks in flexoelectric solids with both conducting and insulating conditions, as well as Mode III, Mode D and Mode E cracks. We also give solutions for some mixed mode cracks. Finally, we discuss new fracture criteria that could be used for predicting failure in flexoelectric solids.

2. Flexoelectric Green's function

We consider an isotropic flexoelectric solid in which the displacement field is $u_k(x_1, x_2, x_3)$, $k = 1, 2, 3$ and the electric potential is $\varphi(x_1, x_2, x_3)$. Such a solid is characterized by the Lame constants, λ and μ, an SGE length scale l, two flexoelectric constants f_1 and f_2 and the dielectric permittivity ϵ. If the deformation and charge separation are sufficiently small then we can use a linearized theory and derive a Navier-type equation for the displacement field and the electric potential. The governing equations obtained in Mao and Purohit (2014) are as follows:

$$\nabla^2(a\epsilon\varphi + fu_{k,k}) = 0, \tag{1}$$

$$(\lambda+\mu)(1 - l_1^2\nabla^2)u_{k,kj} + \mu(1 - l_2^2\nabla^2)u_{j,kk} = 0, \tag{2}$$

where $\nabla^2 = \partial_{ii}$ is the Laplacian operator and l_1, l_2 and l_0 are some material length scales given by

$$l_1^2 = l^2 - \frac{\epsilon_0 f^2}{(\lambda+\mu)a\epsilon} + \frac{f_2^2}{(\lambda+\mu)a}, \quad l_2^2 = l^2 - \frac{f_2^2}{a\mu}, \quad l_0^2 = l^2 - \frac{\epsilon_0 f^2}{(\lambda+2\mu)a\epsilon}, \tag{3}$$

with $f = f_1 + 2f_2$ and $a^{-1} = \epsilon - \epsilon_0$, where ϵ_0 is the permittivity of vacuum.

Now, let $\mathcal{L}_i = (1 - l_i^2\nabla^2)$, then the flexoelectric Green's function for displacement G_{ij} can be obtained by solving the following equation:

$$(\lambda+\mu)\mathcal{L}_1 G_{ik,kj} + \mu\mathcal{L}_2 G_{ij,kk} + \delta_{ij}\delta(\boldsymbol{r}) = 0, \tag{4}$$