

Modelling needle domains with dislocations: a dislocation pile-up model and comparison with synchrotron experiment

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ABSTRACT

The shape and strain field of a needle domain in a barium titanate single crystal are modelled using a distribution of dislocations and line charges. The arrangement of these dislocations and charges is a result of the balance of modified Peach-Koehler forces acting among the dislocations and a lattice friction assumed to act at each dislocation site. Based on measurements of needle shape by synchrotron X-ray diffraction, dislocation pile-up theory is used to compute the distribution of discrete dislocations along the needle and hence estimate the lattice friction. It is found that the lattice friction in this model is proportional to the opening angle of a wedge-shape needle domain and consistent with the observed magnitude of stress required to mobilize needle domains. The microstrain distribution around an a-a needle domain tip, obtained from X-ray diffraction measurement, is further used to test the dislocation model, with a similar pattern and magnitude of strains identified in the model and the experiment.

1. Introduction

The term ‘needle domain’ (also *needle-shaped* domain, *needle-like* domain, see Harrison and Salje (2010); Tagantsev, Cross and Fousek (2010)), has been used to describe thin, plate-like domains in ferroic crystals, terminating at a wedge-shaped end within the crystal. The appearance of such needle domains in ferroelectric crystals commonly accompanies the manufacturing process, polarization switching, or crack growth (Salje and Ishibashi (1996); Fang, Xu, He and Luo (2002); Matsumoto and Okamoto (2010); Carka and Landis (2012)). The generation of needle domains is driven by stress or electric fields which induce local polarization switching, and these driving fields can be due to inhomogeneous temperature distribution, or external mechanical and electrical loading, with nucleation commonly occurring at an inhomogeneity. Understanding the distribution and evolution of needle domains is of significance in determining the macroscopic response of ferroelectric crystals, and the ability to control their evolution is desirable to enable a range of next-generation devices.

Theoretical studies of domains in ferroelectrics commonly adopt a phase-field methodology based on the Ginzburg-Landau theory to simulate the evolution of microstructure. Several researchers (Li and Landis (2011, 2010); Carka and Landis (2012); Lich and Dinh (2019); Indergand, Vidyasagar, Nadkarni and Kochmann (2020)) have applied this method to needle domains to explore their formation, stability, and dynamic interactions. These studies have shown that configurations with groups of needle domains can be unstable, while the needles can also grow rapidly along their length direction. Typically some kind of stabilizing force or stress is needed in the models, such as a lattice friction, suggesting that this may be present in the real crystals. Furthermore, the stresses and electric fields due to incompatibility near the needle tips appear to play an important role in their interaction with each other and with nearby crystal defects or surfaces. Simulations suggest that needle domains play an important role as a mechanism for switching processes in both single crystals and polycrystals, while thermal fluctuations may also be important in facilitating these switching processes. The phase-field methodology has provided a powerful way of representing domain wall motion in simulations. However, a disadvantage of the approach is that simulations are generally limited to small length scales – of order micrometres or less – due to the need to resolve domain walls in the simulation. This leaves the simulation of device-scale regions of material beyond reach.

For the simulation of multiple needle domains in larger regions of material, the interaction between the needle domains is dominated by the stress and electric fields arising around each needle. An approximation of the fields due

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to each needle can be gained by representing the needle domain as a set of dislocations. This approach goes back more than half a century to early studies of ferroelectric crystals, which indicated that the needle tips behaved like groups of dislocations (Bornarel (1972)). Recently, Sui and Huber (2020) showed that the fields due to a needle tip could be approximated by a combination of an effective edge dislocation and a line of effective charge, accounting for material anisotropy and electromechanical coupling by using a formulation due to Barnett and Lothe (Barnett and Lothe (1975)). The resulting modified Peach-Koehler forces on the effective dislocations, and the accompanying electrostatic forces on the effective charges were used to investigate the stability and evolution of various patterns of needle domains, both in extended crystals, and in the vicinity of boundaries (Sui and Huber (2020); Sui, Huber and Zhou (2021)). In these studies, the interaction and evolution of simplified ‘blunt’ needle domains were investigated using an equivalent dislocation and line charge model, however, details of the wedge-shaped needle tip were neglected.

The above studies of needle domains by dislocation modelling lacked detailed evidence for the lattice resistance (or friction) that was assumed to determine the stability of needle domains by resisting the motion of the needle tips. However, the observed shape of the tips of needle domains provides some evidence for the relative mobility of the effective dislocations themselves. As Bornarel (1972) pointed out, the short range interactions of dislocations near a needle tip tend to make the tip acutely wedge shaped; no quantitative evaluation of this statement appears to have been given in the literature. Yet, measurements of the shape of the needle tip, combined with observations of the surrounding strain fields, provide an opportunity to test and calibrate the dislocation model. X-ray diffraction experiments have the potential to provide the necessary measurements of both needle shape and strain fields so as to verify a dislocation model and provide a quantitative measure of the lattice friction that has been assumed in some prior works. X-ray methods are well-established in the investigation of domain structures and the measurement of local strain in ferroelectrics (Niizeki and Hasegawa (1964); Hruszkewycz, Highland, Holt, Kim, Folkman, Thompson, Tripathi, Stephenson, Hong and Fuoss (2013); Fitzpatrick, Fry, Holdway, Kandil, Shackleton and Suominen (2005); Nittala, Mhin, Jones, Robinson, Ihlefeld and Brennecke (2012)). Compared with optical microscopy, X-ray diffraction has the advantages of clearly distinguishing and identifying crystal structure and domain types, as well as the ability to map lattice strains. Several authors (Kim, Gopalan and Steiner (2000); Birkhol (2006); Park and Chung (1997); Fogarty, Steiner, Cronin-Golomb, Laor, Garrett, Martin and Uhrin (1996)) have employed X-ray methods in the study of BaTiO₃ single crystals, obtaining high-resolution measurements of the shape and distribution of domains.

In this paper, the shape of a needle domain is observed using synchrotron X-ray reflection topography and the local strain field is mapped using diffraction measurements. Using the needle shape measurement, a model of an assembly of edge dislocations and line charges distributed along the incompatible domain wall is calibrated. We discuss the criterion for needle domain evolution, based on the evidence of the equilibrium shape of the needle domain. An equilibrium arrangement of repelling dislocations and line charges, counterbalanced by lattice friction, is identified. This is then used to make a numerical prediction of the strain field around a needle tip based on superposition of the anisotropic fields of individual dislocations. The result is compared with experimental measurements of the strain field, demonstrating the utility of the dislocation representation of a needle domain.

2. Experiment

Synchrotron X-ray measurements were performed at beamline B16, Diamond Light Source, using reflection topography. Unfocussed, monochromatic light of energy 18.6 keV ($\lambda = 0.67 \text{ \AA}$) was used to illuminate a BaTiO₃ [1 0 0] oriented single crystal plate of size $10 \times 4 \text{ mm}$ and 0.55 mm thickness with polished surfaces, see Figs. 1(a) and 1(b). Reflected light was measured by a Photonic Science X-ray eye MiniFDI camera at detector distance 115 mm, with 1392×1040 pixels (pixel size = $6.5 \text{ \mu m}$). X-ray diffraction enabled discrimination between a^1 , a^2 and c domains through the $\{2\ 4\ 0\}$ family of reflections, see Fig. 1(c), with the sample rotation angle χ' used to identify each domain type, as listed in table 1. An optical micrograph, Fig. 1(d), showed many needle domains within the crystal plate and was used to identify an isolated a -a needle domain.

2.1. Measurement of needle domain shape

The shape of the fine a^1 needle domain marked in Fig. 1(d) was imaged by integrating measurements over a rocking angle range $21.66^\circ < \omega < 21.72^\circ$ with steps of 0.001° . The resulting image was projected into the sample surface plane after removal of dark-field, resulting in a 400×500 pixel representation of a region of the sample surface, revealing the needle tip as a sharp wedge, Fig. 2(a). The shape profile of the needle domain was obtained by computing the variation of the total intensity of collected light with distance x from the needle's tip. The opening angle at the tip

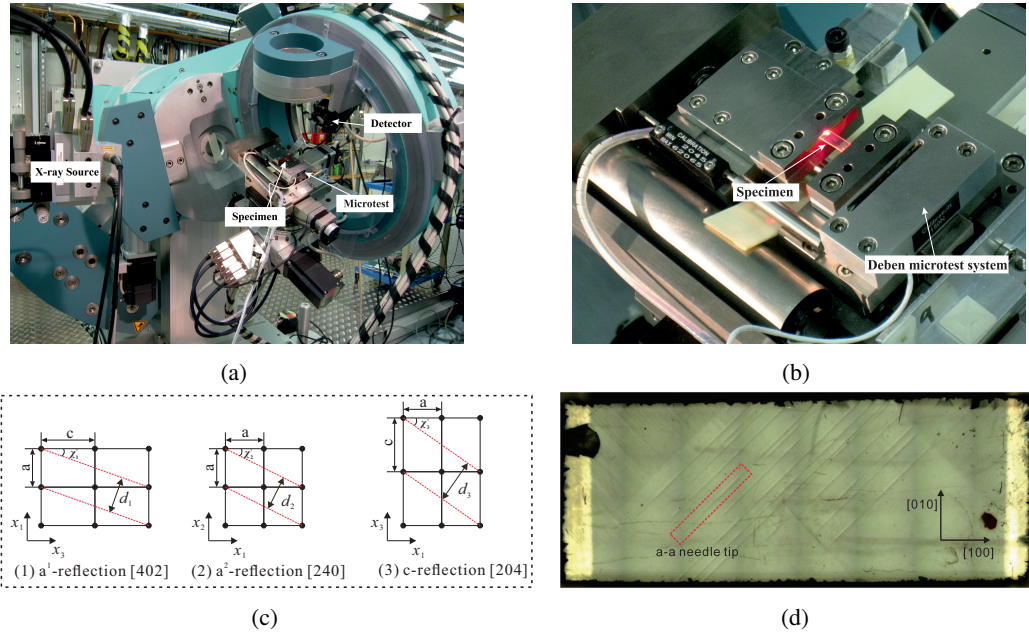


Figure 1: X-ray observation (a) experimental set up of X-ray observation showing X-ray source, with BaTiO_3 specimen and detector mounted in a 5-circle diffractometer; (b) close up of the specimen held in a Deben microtest system for load application; (c) lattice spacings, d , and sample rotations χ' for the $\{2\ 4\ 0\}$ reflections of tetragonal BaTiO_3 ; (d) Optical micrograph of the BaTiO_3 crystal plate showing multiple needle domains, and highlighting the observed needle tip.

Table 1

The diffraction spacing and the second order reflection angles used to distinguish the domains a^1 , a^2 and c (Lattice parameters: $a = 3.985 \text{ \AA}$ and $c = 4.029 \text{ \AA}$; wavelength $\lambda = 0.67 \text{ \AA}$)

	Spacing (d)	χ'	2θ
a^1 -reflection $[402]$	1.7860 ($\text{\AA}$)	26.314°	44.065°
a^2 -reflection $[240]$	1.7821 ($\text{\AA}$)	26.565°	44.166°
c -reflection $[204]$	1.7978 ($\text{\AA}$)	26.818°	43.761°

was estimated from the intensity data to be about 0.8° . Fig. 2(b) shows the variation of normalized total intensity with distance from the needle tip, indicating an approximately linear wedge-shaped profile extending for over a millimetre, while the needle width is about $14 \mu\text{m}$ at 1 mm from the tip. Some variations in intensity along the profile are observed in fig. 2(b), which may be due to surface polishing defects. Based on the observation of a sharp wedge shape of needle domain in this experiment, we can develop a model of the needle domain as a group of discrete dislocations coupled with line charge, spread over the whole wedge length.

2.2. Measurement of the strain field around the needle tip

The existence of a needle domain causes distortion of a crystal that generates local mechanical and electrical fields in the surrounding domain. X-ray diffraction was used to detect strain in the vicinity of the needle tip according to the variation in d -spacing between crystallographic planes. A region of approximately $200 \mu\text{m} \times 200 \mu\text{m}$ on the crystal surface was scanned with the X-ray beam slitted to a $10 \mu\text{m} \times 10 \mu\text{m}$ size, and the crystal position incremented in $10 \mu\text{m}$ steps. At each location on the crystal, the corresponding a^2 $[240]$ reflection of the surrounding domain was detected. The location of this reflection in the MiniFDI camera varied by a few pixels, corresponding to variations $\Delta\theta$ in the Bragg reflection angle. A reference measurement taken at a corner of the scanned region, see Fig. 3, was used as a datum for strain, defining a reference spacing d_0 .

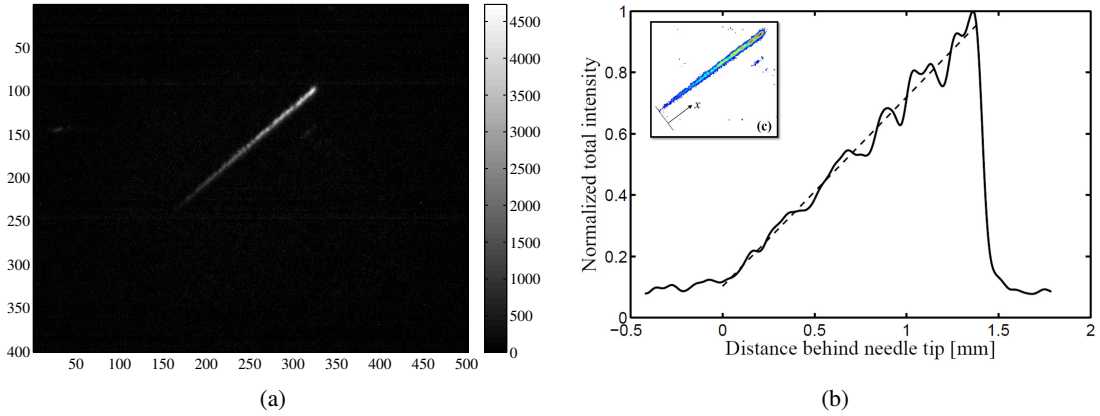


Figure 2: The shape of the needle domain, (a) Integrated image of a needle domain showing pixel intensity; (b) Variation of the normalized total intensity with distance x from the needle tip. Solid line: intensity data; Dashed line: linear fit; (c) inset: wedge shape of needle domain.

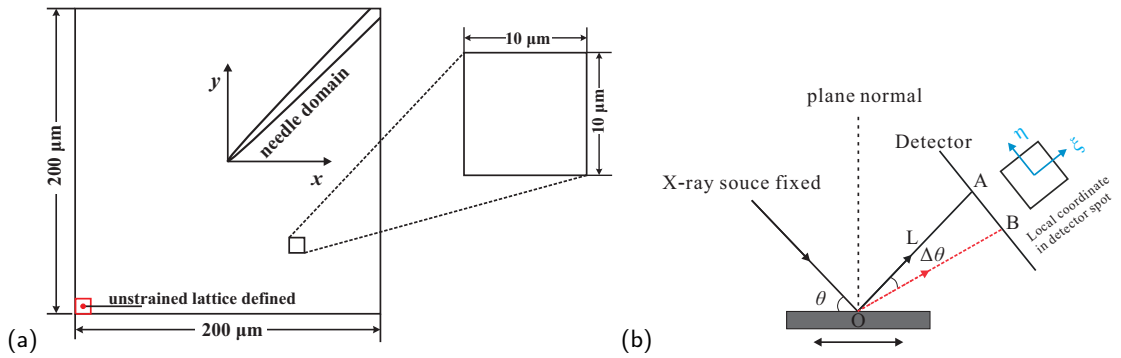


Figure 3: (a) The $200\ \mu\text{m} \times 200\ \mu\text{m}$ scanned region around the needle tip, and reference point for strain measurement. (b) Variation of the reflection position in detector co-ordinates ξ, η .

When a region of the sample surface is strained, the change in the d -spacing, $\Delta d = d - d_0$, for a fixed wavelength of light, is given by

$$2(\Delta d \sin \theta + d \cos \theta \Delta \theta) = \Delta \lambda = 0 \quad (1)$$

Hence the direct strain component ϵ along the scattering vector is

$$\epsilon = \Delta d / d = -\cot \theta \Delta \theta \quad (2)$$

As the movements in the detected light spot were comparable to the size of the spot, spot location was identified using the mass center $(\bar{\xi}, \bar{\eta})$ of the detected intensity $I(\xi, \eta)$ for each spot in ξ - η detector coordinates:

$$\bar{\xi} = \frac{\iint \xi \cdot I(\xi, \eta) d\xi d\eta}{\iint I(\xi, \eta) d\xi d\eta}, \quad \bar{\eta} = \frac{\iint \eta \cdot I(\xi, \eta) d\xi d\eta}{\iint I(\xi, \eta) d\xi d\eta} \quad (3)$$

Variations in $\bar{\eta}$ were used to calculate the corresponding $\Delta \theta$ and hence strain. The resulting map of strains $\epsilon_{[2\ 4\ 0]}$ is shown in fig. 4. The resolution of strain measurement is approximately ± 25 microstrain, limited by the detector pixel size, but it should also be noted that a uniform offset in the range ± 50 microstrain may reasonably be expected due to an unknown strain at the reference point. The general pattern of strain around the needle tip is asymmetric with a region of mostly tensile strains of magnitude 200-300 microstrain directly below the needle, and a region of mostly compressive strains of magnitude 100-200 microstrain above the needle and towards the left of the scanned region. A transition from tensile to compressive strains (hence low microstrain values) appears to occur ahead of the needle. These observations will subsequently be compared with a model based on effective dislocations and line charges.

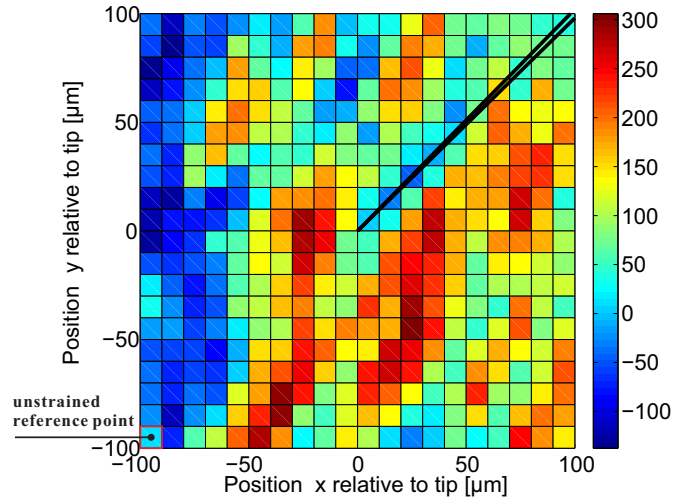


Figure 4: Microstrain field around the needle tip in the [240] direction measured by X-ray diffraction. Dark lines indicate the approximate position of the needle domain tip.

3. Model using dislocations with friction

Needle domains are generated by non-uniform stress and electric fields which induce polarization switching, typically nucleating at an existing boundary or defect. The needle domains grow into the crystal, extending in their length direction, while remaining narrow in the width direction. Their growth stops when there is balance between the forces driving needle extension and any resistance to movement of the needle tip, which may take the form of a lattice friction resisting local rearrangement of the polar domain. The resistance to needle domain extension may be estimated by considering a model of the fields around the needle tip based on effective dislocations. In previous work, Sui and Huber (2020), adopted an effective edge dislocation of Burgers vector b accompanied by a line charge of density q per unit length to model the fields produced by a blunt a-a needle domain, as shown in Fig. 5. The magnitude of the Burgers vector of the equivalent dislocation $b = 3\varepsilon_0 w$ is proportional to the width of the needle domain and the lattice strain $\varepsilon_0 = 2(c - a)/3a$. The magnitude of the corresponding line charge density $q = \sqrt{2}p_0 w$ is proportional to the needle domain width and the spontaneous polarization p_0 . Taking into account a charge screening effect due to limited conduction in the region of the needle-tip, an effective line charge of density $0.48q$ was used to represent electrostatic forces at the needle-tip – see Sui and Huber (2020) for details. This simplified model facilitated the study of interaction of needle domains. However, in practice, the needle domain tip is not blunt, as verified by the experimental observations in section 2. The detailed shape of the needle tip can be represented using a spatial distribution of discrete edge dislocations, each with Burgers vector b_s coupled to line charge density q_s , distributed over the needle tip. The summation of b_s and q_s over the needle tip is then equal to the total effective dislocation b and total line charge density $0.48q$ associated with the needle tip.

Referring to Fig. 6(a) a group of dislocations and charges distributed around the needle tip can define the shape of the tip. These dislocations locally repel each other: in the absence of lattice friction or other forces limiting their motion, they would separate, resulting in the formation of a compatible domain wall. Conversely, having measured the width w and length L of a needle tip (or equivalently the wedge opening angle $\varphi \approx w/L$), it is possible to infer the lattice friction using the theory of dislocation pile-up.

To do this, the total Burgers vector b and line charge $0.48q$ are distributed among N dislocations, with individual Burgers vectors $b_s = b/N$ and line charge $q_s = 0.48q/N$. Considering the small opening angle $\varphi \approx 0.8^\circ$ of the needle tip, the model was simplified by locating all the equivalent dislocations and charges along a straight line aligned with the length direction of the needle domain, see Fig. 6(b). Fixing the first dislocation at the tip and defining this as the origin of the x -axis, other dislocations are successively placed at positions x_i , as shown in Fig. 6(c), with $x_N = L$. The discrete dislocation and line charge located at position x_i are labelled d_i . Each discrete dislocation is assumed to be acted upon by a lattice resistance force f , as marked in Fig. 6(c), which depends on Burger's vector b and a friction

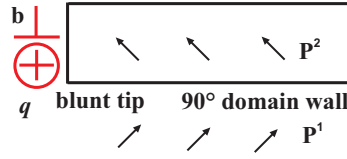


Figure 5: The blunt needle tip modelled as the coupling fields of an effective dislocation b and line charge q .

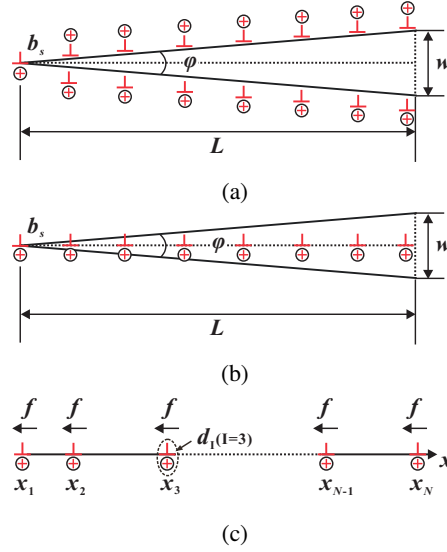


Figure 6: Needle domain tip with a distribution of dislocations and line charges (a) Wedge-shaped tip with distributed dislocations and line charges. (b) Approximation using a straight line distribution. (c) Positions x_I of dislocations d_I , and net forces f acting on individual dislocations in a pile-up along the x -axis.

stress τ_0 that is equivalent to the Peierls stress

$$f = \tau_0 |\mathbf{b}| \quad (4)$$

To compute the cumulative modified Peach-Koehler force acting on each dislocation, the generalized displacement gradient for an edge dislocation and line charge in an anisotropic piezoelectric medium, due to Barnett and Lothe (1975), was used:

$$u_{K,m} = (2\pi |\mathbf{x}|)^{-1} \left\{ -m_m (S_{KS} b_S + Q_{KS} q_S) + n_m (nn)^{-1}_{KJ} [(4\pi B_{JS} + (nm)_{JP} S_{PS}) b_S + (S_{SJ} + (nm)_{JP} Q_{PS}) q_S] \right\} \quad (5)$$

where lower-case indices run from 1 to 3 while upper-case indices run from 1 to 4, such that u_K ($K = 1 \dots 3$) is the displacement vector and u_4 is equal to the electric potential ϕ . The 4×4 matrices $\mathbf{S}$, $\mathbf{Q}$ and $\mathbf{B}$ are related to the piezoelectric material constants, see Appendix I. Plane basis vectors $\mathbf{m}$ and $\mathbf{n}$ are defined such that $\mathbf{m} \cdot \mathbf{x} = |\mathbf{x}|$ and $\mathbf{n} \cdot \mathbf{x} = 0$; the components of the 4×4 matrices $(\mathbf{nn})$ and $(\mathbf{nm})$ are defined in Appendix I. Having computed strain and electric field using Eq. (5), the corresponding stress and electric displacement fields are directly obtained from the piezoelectric constitutive equations:

$$\sigma_{ij} = C_{ijkm} u_{k,m} + e_{mij} \phi_{,m} \quad (6)$$

$$D_i = e_{ikm} u_{k,m} - \kappa_{im} \phi_{,m} \quad (7)$$

where C_{ijkm} , e_{mij} , and κ_{im} are the plane-stress tensors of elastic, piezoelectric, and dielectric constants, respectively. The constitutive equations relate mechanical stress σ_{ij} and electric displacement D_i to the displacement gradients $u_{k,m}$ and the electric potential gradient $\phi_{,m}$. The cumulative Peach-Koehler force on dislocation d_I is then:

$$F_m^I = \sum_{J=1, J \neq I}^N \sigma_{ij}^J b_j^I \epsilon_{ilm} k_l + \sum_{J=1, J \neq I}^N E_m^J q^I \quad (8)$$

where, the stress σ_{ij}^J and electric field E_m^J are those due to dislocation d_J located at position x_J and the summation for the I th dislocation includes contributions from all dislocations other than itself. ϵ_{ilm} is the rank 3 permutation symbol, and $\mathbf{k} = \mathbf{m} \times \mathbf{n}$. The location of each dislocation x_I was varied to ensure that the force F_m^I on the dislocation was counterbalanced by the lattice friction $\tau_0 b^I$, with the constraint that all N dislocations would fit into the given length of the wedge, such that $x_N = L$. This constraint enabled a consistent value of the lattice friction stress τ_0 to be inferred.

3.1. Relation of lattice friction to the wedge opening angle

The selection of the number, N , of discrete dislocations influences the computation of lattice friction and the cumulative modified Peach-Koehler force acting at the tip of the needle domain. In order to choose N in such a way as to obtain a consistent estimate of the friction stress τ_0 , the theory of dislocation pile-up was employed. Each discrete dislocation at position x_I experiences the modified Peach-Koehler force from all the other dislocations, in equilibrium with the lattice friction. The modified Peach-Koehler force on each discrete dislocation is computed using Eq. (5-8). Noting that the discrete burgers vectors b_s and line charge densities q_s in Eq. (8) scale linearly with needle width w/N , it can be seen that the modified Peach-Koehler force acting on each dislocation scales with the square of the needle width and inversely with the distance between dislocations and N^2 :

$$F^I = \frac{A'w^2}{N^2} \sum_{J=1, J \neq I}^N \frac{1}{x_J - x_I} \quad (9)$$

where A' is only dependent on the material constants. Thus each discrete dislocation in equilibrium satisfies a balance equation,

$$\tau_0 |b_s| = \frac{A'w^2}{N^2} \sum_{J=1, J \neq I}^N \frac{1}{x_J - x_I} \quad (10)$$

Substituting for b_s gives

$$\tau_0 = \frac{Aw}{N} \sum_{J=1, J \neq I}^N \frac{1}{x_J - x_I} \quad (11)$$

where, $A = A'/3\epsilon_0$. An approximate solution of x_I for large N is given by Wang, Chen and Tong (2007):

$$x_I = \frac{Aw\pi^2}{8\tau_0 N^2} (I - 1)^2 \quad (12)$$

The length of needle tip is $L \approx x_N$. Noting that $\varphi = w/L$ gives, finally

$$\tau_0 = \varphi \frac{A\pi^2}{8} \frac{(N - 1)^2}{N^2} \quad (13)$$

indicating that the inferred lattice friction stress τ_0 in this model is proportional to the measured wedge angle at the needle tip.

In the above argument the number N of dislocations representing the needle tip could be chosen arbitrarily. By varying N and recomputing stable dislocation pile-ups, the relationship between N and the inferred lattice friction stress τ_0 was computed, see fig. 7(a). We set the spontaneous polarization p_0 and the spontaneous strain ϵ_0 to 0.25 C/m² and 0.0073, respectively; other material constants match those used in previous calculations by Sui and Huber (2020). The number N of discrete dislocations was varied from 2 to 300. Nondimensionalization using characteristic parameters was applied to make the results independent of the influence of physical dimensions, and to help avoid numerical instability during the computing process. The characteristic parameters were the spontaneous polarization p_0 , spontaneous strain ϵ_0 , the width of needle domain w , and the coercive electric field E_0 (0.1×10^6 V/m). Then stress τ_0 was normalized by $\sigma_0 = E_0 p_0 / \epsilon_0$.

Fig. 7(a) shows that the inferred lattice friction stress τ_0 is insensitive to the chosen number of dislocations representing the wedge provided $N > 50$. Using $N = 150$, the friction stress τ_0 is estimated to be $\tau_0 = 0.81\sigma_0 \approx 2.9$ MPa.

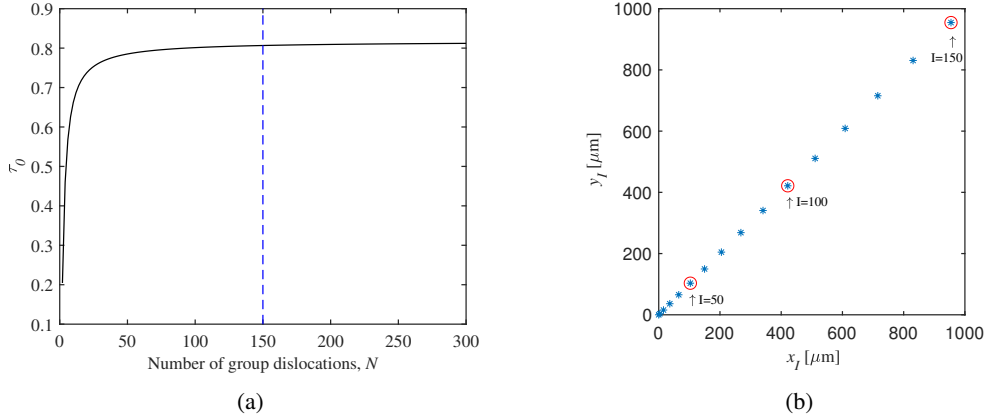


Figure 7: (a) Variation of the inferred lattice friction stress τ_0 with the number N of distributed dislocations. τ_0 is normalized by $\sigma_0 = E_0 p_0 / \varepsilon_0$. (b) The corresponding equilibrium positions of selected dislocations $I = 1, 10, 20, 30, \dots, 150$ distributed along the needle.

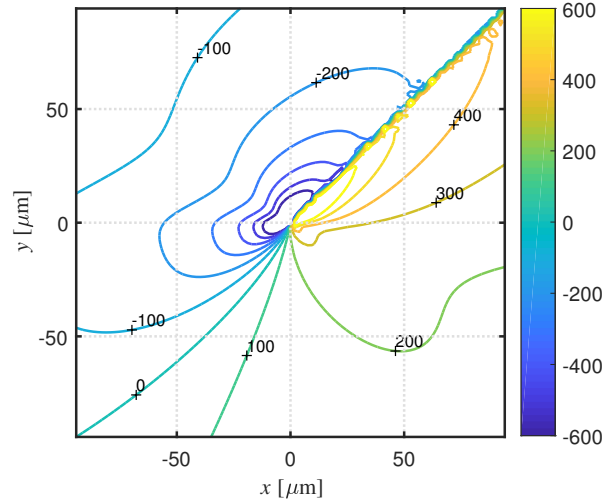


Figure 8: Microstrain field ε_{240} around the needle tip calculated using dislocation pile-up theory.

This estimate compares well with the measured stress for mobilising needles in similar BaTiO_3 crystal plates (approximately 1-4 MPa, Potnis and Huber (2013)). The resulting equilibrium positions of selected dislocations for the $N = 150$ case are shown in Fig. 7(b); the spacing between the adjacent dislocations increases with distance from the needle tip.

3.2. Strain field near the needle tip

The strain field near the needle tip can be simulated using the dislocation model. For this calculation, the strain fields due to a set of $N = 150$ dislocations and line charges with total Burgers vector and line charge density equivalent to that of a $1350\mu\text{m}$ length needle domain with the opening angle $\varphi = 0.8^\circ$ were superimposed. The 150 dislocations were located in equilibrium positions along the line $y = x$ with $x > 0$, and lattice friction set to $\tau_0 = 2.9\text{ MPa}$. Fig. 8 shows a contour map of the direct strain component parallel to the $[240]$ direction, ε_{240} due to a single needle domain in a large crystal plate, under plane stress conditions. For comparison with the experimental data in fig. 4, the microstrain values are given relative to the value at location $(-100\mu\text{m}, -100\mu\text{m})$ which was taken as a datum for strain measurement in the experiment.

Comparing figs 4 and 8, it can be seen that the numerical and experimental results have a similar magnitude and pattern of strain. In particular, there are generally tensile strains in the region below the needle, and compressive strains towards the left of the region modelled. There is a transition between tensile and compressive regions ahead of the needle. Some differences between the experimental measurements and the theoretical calculation may be expected due to the assumption of a perfect crystal adopted in the simulation, or inaccuracies in material parameters, which were taken from the literature. Furthermore, the calculation neglects the presence of nearby boundaries and other needle domains which are present in the experimental measurements. Despite these sources of error, there is a generally satisfactory agreement between the measured data and the calculations, suggesting that the dislocation model may have utility in understanding needle domains.

4. Conclusions

The electromechanical fields produced by a 90° a-a needle domain in a BaTiO₃ single crystal plate were modelled using an assembly of equivalent edge dislocations and line charges distributed over the needle tip. Analytical solutions to the problem of a dislocation and line charge in an anisotropic piezoelectric medium were used, along with superposition of fields, to enable calculation of the stress, strain and electric field distribution around a wedge-shaped domain needle tip. Using this model, the lattice friction resisting motion of the dislocations (and hence resisting needle tip motion) was related to the wedge opening angle at the needle tip. Hence, using a measured opening angle, the lattice friction was estimated and found to be roughly consistent with measurements of the stress necessary to mobilise needle domains in crystal plates. More generally, the lattice resistance was shown to be proportional to the equilibrium wedge opening angle of needle domains.

A synchrotron X-ray experiment was used to measure a needle domain in BaTiO₃ and obtain its wedge-shaped profile. Using diffraction of a scanned microbeam, strain in the domain surrounding the needle was mapped. The pattern of strain in the vicinity of the needle was found to be asymmetric, consistent with the anisotropic nature of the crystal. The experimental data was in general agreement with a model based on superposition of the fields of an assembly of dislocations and line charges held in equilibrium by lattice friction. The results suggest that the dislocation model may be a suitable way to simulate certain aspects of the behaviour of needle domains, with the advantage that analytical expressions for the electromechanical fields exist, enabling the efficient modelling of large regions of material.

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Appendix I

Material matrices in the Barnett and Lothe integral formalism: Barnett and Lothe (1975) provided a convenient integral formalism using the material matrices Q_{KS} , S_{KS} , and B_{KS} where

$$Q_{KS} = -\frac{1}{2\pi} \int_0^{2\pi} (nn)_{SK}^{-1} d\theta \quad (14)$$

$$S_{KS} = -\frac{1}{2\pi} \int_0^{2\pi} (nn)_{KJ}^{-1} (nm)_{JS} d\theta \quad (15)$$

$$B_{KS} = \frac{1}{8\pi^2} \int_0^{2\pi} \{ (mm)_{KS} - (mn)_{KJ} (nn)_{JR}^{-1} (nm)_{RS} \} d\theta \quad (16)$$

The components of the 4×4 matrices (nn) and (nm) are defined by

$$(ab)_{JK} = a_i E_{iJKm} b_m \quad (17)$$

where, a and b any are real three-dimensional vectors. Here lower-case indices run from 1 to 3 while upper-case indices run from 1 to 4. The group of tensors E_{iJKm} is:

$$E_{iJKm} = C_{ijkm} \quad (J, K = 1, 2, 3)$$

$$\begin{aligned}
&= e_{mij} \quad (J = 1, 2, 3; K = 4) \\
&= e_{ikm} \quad (J = 4; K = 1, 2, 3) \\
&= -\kappa_{im} \quad (J = K = 4)
\end{aligned} \tag{18}$$

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