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Published in:
Applied Physics Letters

Document Version:
Peer reviewed version

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Download date: 13. Oct. 2020
The influence of notches on domain dynamics in ferroelectric nanowires


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(Received 26 November 2009; accepted 16 December 2009; published online 29 January 2010)

The extent to which notches inhibit axial switching of polarization in ferroelectric nanowires was investigated by monitoring the switching behavior of single crystal BaTiO$_3$ wires before and after patterning triangular notches along their lengths. Static zero-field domain patterns suggested a strong domain-notch interaction, implying that notches should act as pinning sites for domain wall propagation. Surprisingly though, notches appeared to assist, rather than inhibit, polar switching. The origin of this effect was rationalized using finite element modeling of the electric field distribution along the notched wire; it was found that the air gap associated with the notch acted to enhance the local field, both in the air, and in the adjacent region of the ferroelectric. It seems that this local field enhancement outweighs any pinning interactions. © 2010 American Institute of Physics. [doi:10.1063/1.3300638]

There is a great disparity in the extent to which the behavior of ferromagnetic and ferroelectric domains have been mapped and understood in nanoscale structures and devices. For example, in mesoscale disks and nanoscale rings of soft ferromagnetic materials, it has been known for some time that demagnetizing fields cause the formation of vortex domains. For example, in mesoscale disks and nanoscale rings of soft ferromagnetic materials, it has been known for some time that demagnetizing fields cause the formation of vortex domains. Not only have these magnetic vortices been imaged, but the dynamic modes of vortex switching have also been examined. By contrast, in ferroelectrics, while atomistic simulations have suggested that analogous polarization vortices should exist, only circumstantial evidence for their presence has ever been found.

Of particular relevance to the work presented herein, is the extent to which interactions between domain walls and perturbations in surface morphology are understood within the two ferroic subgroups. In magnetics research, as part of the development of “race-track” memory, Parkin and co-workers have pioneered an understanding of the pinning potentials associated with notches and a variety of domain wall types. Physics relating to controlled domain wall migration, from notch to notch, has been developed; in addition, elegant concepts such as “resonant amplification,” where current pulses cause domain walls to resonate within their pinning potential wells, have not only been conceived of, but also experimentally realized. In ferroelectrics, however, relatively little has been done to explore the behavior of domains in nanowires and the nature of the interactions between domains and local variations in nanowire morphology is almost totally unexplored. While ferroelectric race-tracks are not of technological interest, basic mapping of the manner in which domain walls migrate in small scale ferroelectric objects is highly important; switching of smaller and more morphologically complex capacitors, planned for future ferroelectric random access memory chips, relies critically on domain wall propagation.

In this letter, the influence that notches have on the behavior of ferroelectric domains has been studied in single crystal wires of BaTiO$_3$. While static domain patterns suggested a strong domain-notch interaction, the dynamics of polar switching were not found to be inhibited by notches. If anything, notches were found to assist switching. Finite element (FE) modeling suggested that increased switchability arose from localized “hot-spots” in the electric field.

The wires examined in this study were directly machined from commercially obtained single crystal BaTiO$_3$, using a single beam FEI200TEM focused ion beam microscope (FIB). Patterning methodologies employed were similar to those used in previous work. Initially, thin lamellae (~150 nm in thickness, ~10 μm wide, and ~6 μm deep) were cut perpendicular to the single crystal BaTiO$_3$ crystal. Then either the host crystal was tilted in the FIB to allow the ion beam to pattern notched wires directly into the face of the lamella, or the lamella was lifted out of the bulk crystal, placed on a 3 mm holey carbon-coated copper grid, and returned to the FIB for wire and notch patterning.

Figure 1 shows transmission electron microscopy images of notched wires, and the patterns adopted by the domains that form on cooling through the Curie temperature. In most cases, either a herringbone pattern was seen, or simple parallel stripe domains persisted, but the domain periodicity noticeably decreased on moving from the main body of the wire to the notch center. Both these observations suggest that the notch has had an influence over the manner in which domains have formed.

The observed change in domain periodicity is of particular interest, as prior work, on single crystal BaTiO$_3$ nanoshapes, has consistently seen that the domain periodicity decreases as the ferroelectric becomes smaller, in abeyance of a Landau–Kittel energy expression of the form

$$G(d, w) = Uw + \frac{\gamma d}{w},$$

suggesting that, under equilibrium conditions, the domain width scales as the square root of size.
energy cost for a given local change in domain density ($\delta \nu$) is greatest in the notched region, because the curvature of the free energy function around the equilibrium point is greater there than elsewhere on the wire.

$$\frac{\delta^2 G(d,w)}{\delta \nu^2} = 2 \frac{\gamma d}{w^3} = 2 \sqrt{\frac{U}{\gamma d}} \text{ at the equilibrium point.}$$

Both of the above features of the energy landscape should lead to the inhibition of domain wall movement through the notched region, reducing switchability.

To investigate this further, FIB-milled lamellae (~300 nm in thickness) were placed onto functionally passive single crystal MgO carriers and incorporated into capacitor structures with coplanar Pt electrodes, as had been done in previous work.36,37 The BaTiO3 in the interelectrode gap was then FIB-milled to form short sections of wires, ~900 nm wide by ~2 $\mu$m long. After thermal annealing,38 the switching properties of these short wires were monitored by measuring capacitance-voltage (C-V) characteristics, taking particular care in the evaluation and subtraction of background capacitance signals.36,37 Notches were then FIB-milled into the wires, creating the structures shown schematically, and in plan-view secondary electron images in Fig. 2. After a further anneal, the switching characteristics were again measured, and compared to those obtained prior to milling the notches. The C-V response of the notched and prenotched wires, imaged in Fig. 2, are shown in Fig. 3 at two different temperatures. Since the capacitance at a given
bias voltage is a measure of the alteration in polarization with field at that bias \( (C \propto \chi = dP/dE) \), the C-V measurement effectively maps the population of local switching events (per unit field) occurring at each value of applied voltage. Even though the overall capacitance signal decreases in the notched sample, it is clear from Fig. 3 that the distribution of voltage, across which switching events occur, is less diffuse in notched wires than in prenotched wires. This is strongly accentuated in Fig. 3(a), but was generally true in all the C-V data sets obtained. Thus, even though imaging of the static domain configurations showed that notches should inhibit the migration of domain walls, electrical switching measurements indicated the opposite.

In an attempt to rationalize this, FE modeling (using “QUICKFIELD”) was performed to see how the presence of the notch might alter local electric fields when bias voltage is applied. The outline of the array of three notched wires shown in Fig. 2(c) was traced and used to define the geometry for the modeling. To gain an overall impression of field distribution, BaTiO\(_3\) was assigned an isotropic relative permittivity of 1000 (acknowledging the multidomain nature of the ferroelectric during most of the switching cycle). What is immediately evident from Fig. 4(a), is that a great deal of field is dropped across the air-filled regions at the notches. This is expected as large fractions of applied bias are often dropped across areas of low permittivity. More unexpected was the knock-on consequence of field enhancement within the ferroelectric adjacent to the notches. It appears that the effects of field focusing associated with the notch geometry outweigh any pinning interactions between the notch and the domain walls, resulting in the overall increase in switchability observed. An obvious next step is to examine the manner in which antinotches alter axial switching behavior. As can be seen in Fig. 4(b), FE modeling suggests that antinotches are associated with field minima under applied bias.

In summary, an attempt has been made to study the influence that notches have on the static and dynamic behavior of ferroelectric domains. While static domain configurations suggested a notch-domain wall interaction that should inhibit domain wall motion during axial switching, direct functional measurement found switching to be accelerated in the presence of notches. FE modeling suggests that this counterintuitive observation is related to the unusual field focusing effect that the notch geometry creates.

The authors acknowledge useful discussions with J. F. Scott, G. Catalan, F. D. Morrison, and A. J. Bell.