Why Nanopolar Regions Matter in Tunable Dielectrics, Flexoelectrics, and Photovoltaics

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Nanopolar regions can have consequences disproportionate to their size when present in a paraelectric material. This talk focuses on identifying and understanding the impact of nanopolar regions on nominally paraelectric applications including: tunable dielectrics, flexoelectrics, and photovoltaic devices.

Nanopolar regions can be difficult to differentiate from a lossy paraelectric material through polarizationelectric field hysteresis loops. Thus temperature dependent Rayleigh analysis was repurposed as an indicator of the presence of nanopolar regions in addition to temperature dependent dielectric measurements, second harmonic generation, and piezoresponse force microscopy. Using these methods in tunable dielectrics, nanopolar regions were shown to persist up to 65 °C above the ostensible paraelectric transition temperature in Bao.7Sro.3TiO3 films, with relative tunabilities of 86% at 250 kV/cm and 100 kHz. The dielectric loss in these films doubled for AC electric field over 10 kV/cm at room temperature.(*1*) In addition to increasing dielectric loss, persistent nanopolar regions can also enhance the flexoelectric response in paraelectrics due to strain gradient induced poling (flexoelectric poling). Flexoelectric poling in BST ceramics leads to remnant polarization in flexoelectric measurements, an induced d₃₃ piezoelectric response after the removal of the strain gradient, and the production of a persistent internal bias.(*2*)

Many of the methods used to track nanopolar regions, such as Rayleigh analysis, have the added benefit of requiring low voltages, which is useful in tracking nanopolar regions in semiconducting photovoltaic materials. Using the aforementioned methodologies, relaxor ferroelectricity was identified in methylammonium lead iodide at temperatures up to 57 °C, which is consistent with the tetragonal-to-cubic phase transition temperature. Large signal poling greater than $1.6 \times 10^{-2} \text{ kV/cm}$ induced permanent macroscopic ferroelectric domains, which show preferential stabilization and a distinguishable electrical response, indicating routes to increased device stability and improved photovoltaic performance through domain engineering.

References:

- 1. L. M. Garten, P. Lam, D. Harris, J.-P. Maria, S. Trolier-McKinstry, *Journal of Applied Physics* **116**, 044104 (2014).
- 2. L. M. Garten, S. Trolier-McKinstry, *Journal of Applied Physics* 117, 094102 (2015).