Quantitative Modeling of High-response Piezoelectricity near a Phase Boundary

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The giant electromechanical responses of the relaxor piezoelectrics such as PMN-PT and PZN-PT continue to pose a theoretical challenge both in terms of fundamental understanding and in mediating between data and applications. Here [1] we adapt the empirical Landau-Devonshire (LD) approach in a study of the widely used “engineered domain” samples, finding that we can give a quantitative description of the properties of five samples of these materials lying close to the Morphotropic Phase Boundary (MPB).

The MPB separates the Rhombohedral (R) and Tetragonal (T) phases (with an intercalated mixed phase), and the physics around the MPB is that of a soft rotational degree of freedom of the polarization. It has been shown that an LD model with terms up to only fourth order in the polarization can describe the R-to-T transition because the magnitude of the polarization is relatively constant while its angle changes facilely. In the engineered-domain R phase the polarization is domainwise locally R but globally T; the distortion from cubic leads to non-cubic deviations in the electromechanical responses by large factors. We introduce a globally-T LD model to describe the system. Key details are, a) that the system is approximated as close to the MPB, and b) care has been taken in averaging out the local polarization components perpendicular to the global polarization axis. The resulting description accounts for extreme piezoelectric response, its observation at compositions near the MPB, accompanied by ultrahigh dielectric constant and mechanical compliances with rather large anisotropies, while maintaining analytic simplicity. We also identify new sum rules in the data which are obeyed by the theory. Both the sum rules and a 4-parameter fit to 10 experimental quantities are accurate to a few percent in this theory; it therefore offers a general and powerful means of accounting for the full set of signature characteristics in these functional materials.

1] D.M. Newns, M. Kuroda, F. Cipcigan, J. Crane, and G.J. Martyna, Appl. Phys. Lett., **110**, 022904 (2017).