Translational Covariance of Flexoelectricity at Ferroelectric Domain Walls

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Abstract

Macroscopic descriptions of ferroelectrics have an obvious appeal in terms of efficiency and physical intuition. Their predictive power, however, has often been thwarted by the lack of a systematic procedure to extract the relevant materials parameters from the microscopics. Here we address this limitation by establishing an unambiguous two-way mapping between spatially inhomogeneous fields and discrete lattice modes. This yields a natural treatment of gradient couplings in the macroscopic regime via a long-wavelength expansion of the crystal Hamiltonian. Our analysis reveals an inherent arbitrariness in both the flexoelectric and polarization gradient coefficients, which we ascribe to a translational freedom in the definition of the polar distortion pattern. Remarkably, such arbitrariness cancels out in all physically measurable properties (relaxed atomic structure and energetics) derived from the model, pointing to a generalized translational covariance in the continuum description of inhomogeneous ferroelectric structures. We demonstrate our claims with extensive numerical tests on 180° domain walls in common ferroelectric perovskites, finding excellent agreement between the continuum model and direct first-principles calculations.

Short Biography

Oswaldo Diéguez is an Associate Professor at the Department of Materials Science and Engineering of Tel Aviv University, where he heads the Atomistic Simulation of Materials group. The group aims at understanding the properties of materials from the atomistic picture, at characterizing materials by performing numerical experiments, and at discovering new materials. Most of this work relates to the family of perovskite oxides with ferroelectric properties, although other current projects involve rare-earth layered MAX materials and the computation of the mean inner potential of solids.