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Obtaining an Energy Function for Relaxor Rhombohedral Crystals and its use in Phase Field Modeling

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ABSTRACT

Rhombohedral relaxor single crystals are finding increasing use in medical ultrasound, in accelerometers, and as sensors and actuators for smart structures. Recently they have been used extensively to produce strain to study magnetostrictive heterostructures at the nanoscale. The large strain and low dielectric loss are the result of an engineered domain state where there is little or no driving force for domain wall motion. This includes crystals cut and poled in the [001] and [011] orientation. When these crystals are driven at higher stress and electric field values, they undergo field driven phase transformations. In applications such as ultrasound that require linear response, temperature dependence and the non-linearity associated with these phase transformations are to be avoided. In other applications such as energy harvesting and large deflection producing miniature robots, these phase transformations can be used to increase the available electric field generated strain by a significant factor.

This talk will begin with an overview of recent applications of relaxor ferroelectric crystals. The effect of material composition on the non-linear crystal behavior will be presented to set the stage for the development of an energy function capable of reproducing the observed material behavior. The challenges of developing a 10^{th} order Landau-Devonshire energy function will be discussed and a function capable of describing the dielectric, piezoelectric and ferroelectric properties of these crystals will be presented. Coefficients of the energy function were determined based on the results of many experimental measurements in our laboratory and from published work. The resulting energy function reproduces temperature induced phase transformations as well as *PE* and *SE* hysteresis loops of the domain engineered rhombohedral crystals at multiple temperatures. This energy function has been implemented in a phase field model to investigate the evolution of rhombohedral domain structures. Computational simulations of these domain structures will be presented.