A Phenomenological Micromechanical Constitutive Model for General Ferroelectric Materials: 95/5 PZT

<u>W.D. Dong</u>^{1*} and J. Robbins² ¹Computational Materials and Data Science, Sandia National Laboratories, Albuquerque, New Mexico, 87185 ²Multiscale Science, Sandia National Laboratories, Albuquerque, New Mexico, 87185 *Corresponding Author: wdong@sandia.gov

A rate-independent phenomenological micromechanical constitutive model applicable for single and polycrystalline ferroelectric/ferroelastic materials is presented. The model captures the domain-switching and phase-transformation phenomena which are the leading cause of nonlinearity and hysteresis within ferroelectric materials. A new type of energy based switching criteria is formulated to allow for both step-like and diffuse transitions through the use of continuous mapping functions between the free energy of the transitions and the relative volume-fraction ratios of the domain-variants. These switching criteria are used to govern both domain-switching and phase-transformation phenomena. The distributed transitions are associated with compositional fluctuations and defects within the ferroelectric. They also have the added benefits of reducing the crystal grain count required to approximate a ceramic material and capturing minor hysteresis loop phenomenon. Corrections to the electrical and mechanical loads were developed to account for inter-granular interactions caused by electrical and mechanical incompatibility between neighboring grains. This was necessary to capture the correct hysteresis shape for certain materials. A fitting of the ferroelectric model to experimental results of 95/5 PZT electrically loaded under varying pressures is presented to demonstrate the high level of fidelity achievable using this technique.