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Electromechanical Grain Boundary Model with Formation Mechanism in Polycrystalline Ferroelectrics

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ABSTRACT

Grain boundaries (GBs) are transitional, defective, and anisotropic interfaces between adjacent grains with different orientations. However, most models assume that the GB is an isotropic dielectric determined by itself and lacks formation information; these assumptions hinder the theoretical investigation of the effect GBs have on polycrystalline ferroelectrics at the mesoscopic scale. Here, a novel GB model based on the formation mechanism is established for ferroelectric polycrystals. It has been found that the Curie-Weiss temperature range, elastic coefficient, and permittivity of GBs are related to the orientation of adjacent grains and the polarization state. The shielding effect, polarization enhancement, domain continuity, and spontaneous polarization on the GBs are obtained in mesoscopic simulations based on this model. In addition, the proportion of GBs can significantly affect the electric field distribution in grains. It provides a mechanistic explanation for the relationship between the coercive electric field and the proportion of GBs in the previous experiment. By achieving a better mesoscopic description of GBs, the GB model proposed in this work provides an effective investigation tool for electromechanical, electro-caloric, and energy storage of polycrystalline functional materials.

KEYWORDS

Grain Boundary; polycrystalline ferroelectrics; domain switching; formation mechanism

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