Structural and orientational optimization for ferroelectric materials

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Polycrystalline ferroelectric materials differ significantly from single crystals because of the presence of variously oriented grains or crystallites [1]. The orientation of ferroelectric crystals plays a critical role in the anisotropy of their piezoelectric properties [2]. Another aspect of ferroelectric materials is their crystallizing in different crystallographic structures depending on the poling of the sample. For instance, the relaxor ferroelectric PMN-PT or (1-x) $(PbMg_{1/3}Nb_{2/3})O_3$-$xPbTiO_3$ exhibits pseudo-tetragonal symmetry when poled along [001] direction and exhibits rhombohedral symmetry while poled along [111] direction. The set of combination of variables, known as solution space, which dictates the orientation distribution of grains is unlimited. Besides orientation distribution parameters we would choose the crystallographic structure as another design variable. An optimization procedure incorporating a continuum modelling is used to identify the optimal structure and orientation distribution of ferroelectrics for piezoelectric applications. Crystallographic orientation is inextricably related to the piezoelectric properties of ferroelectrics. This suggests that piezoelectric properties can be tailored by a proper choice of crystallographic structure and the parameters which control the orientation distribution. Nevertheless, this choice is complicated and it is impossible to analyze all possible combinations of the structure and distribution parameters or the angles themselves [3]. Stochastic optimization combined with a generalized Monte Carlo scheme optimizes the objective functions, the effective piezoelectric coefficients. Global piezoelectric properties are calculated using the homogenization method at each structure and orientation configuration chosen by the optimization algorithm. A modified simulated annealing is employed to identify the objective functions of the optimization. Optimal design variables which would generate polycrystalline configurations that enhance the macroscopic piezoelectricity are identified.

References

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