Effect of different electric inclusions on large electrocaloric effect in ferroelectric nanoparticle

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Abstract

The electrocaloric effect (ECE)is the temperature change in a material with a varying electrical field under adiabatic conditions. The influence of different electric inclusions on large electrocaloric effect in ferroelectric nanoparticle are investigated based on the phase field approach containing the time-dependent Ginzburg-Landau equation. To capture a clear physical picture with the simulation, the crack area is considered to be filled with liquid, such as water, oil or air. When the electric inclusion is air or oil, the simulations exhibit a macroscopic electric field concentration and a significant influence on the domain evolution, while little influence is obtained when the electric inclusion is water. Thus the applied electric field, which switches the polarization from multi-domain to mono-domain of a ferroelectric crystal, is much larger for air/oil inclusion than water inclusion. Meanwhile, the numerical calculations indicated that the electrocaloric efficiency $\Delta T / \Delta E$ undergoes a dramatic decrease with increasing applied electric field, which is consistent with experimental observations. Furthermore, for a ferroelectric crystal with a water inclusion under relatively lower applied electric field, a large negative ECE (about -5.835K) is obtained near room temperature (about 40°C), a good result that enlarges the temperature range of large ECE exhibits in ferroelectrics. The results indicates that the non-uniform distributions of the stress-electric fields induced by different electric inclusions play an importation role in ECE. Because the domain transition takes place to minimum total free energy, which involves the course of the electric field, strain, temperature and polarization interaction. The results may provide a better phenomenological explanation for ECE in ferroelectric materials with defects.

Keywords: Electrocaloric effect; Ferroelectrics; Phase field model; Electric inclusion; Multi-domain to mono-domain transition;