Phase field simulation of temperature dependent dielectric and piezoelectric properties in $BaTiO_3$ polycrystalline ceramics: potentials of temperature energy harvesting

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Abstract

Piezoelectric materials have been recognized for their potential utility in sensors, actuators, and energy harvesting devices. Barium titanate ($BaTiO_3$) is one of the basic and widely applied lead-free ferroelectric materials [1], and can be used for temperature energy harvesting. On the other hand, it is well known that the microstructures and electromechanical properties of $BaTiO_3$ ceramics depend on temperature, and that it is difficult to measure the dielectric and piezoelectric properties of $BaTiO_3$ ceramics experimentally. Phase field approach can serve as an efficient tool for the purpose of microstructural analysis of ferroelectric materials [2]. Recently, Shindo et al. [3] developed a phase field model for BaTiO3 polycristalline ceramics with oxygen vacancies, and investigated the electromechanical response of poled $BaTiO_3$ ceramics. Narita et al. [4] also studied the electromechanical response of unpoled and poled $BaTiO_3$ ceramics, and discussed the effects of grain size and oxygen vacancy density on the dielectric and piezoelectric properties.

The purpose of this work is to investigate the effect of temperature on the dielectric and piezoelectric properties of poled $BaTiO_3$ ceramics with oxygen vacancies and to examine the potential of temperature energy harvesting. First, a phase field model is used for ferroelectric polycrystals, coupled with the time-dependent Ginzburg-Landau theory and the oxygen vacancies diffusion, to demonstrate the interaction between oxygen vacancies and domain evolutions. To generate grain structures, the phase field model for grain growth is also employed. The polarization vs electric field curve and strain vs electric field curve are calculated from cryogenic to high temperatures, and the dielectric and piezoelectric properties of the $BaTiO_3$ ceramics at various temperatures are evaluated. Next, output voltage of the $BaTiO_3$ ceramics with temperature dependent dielectric and piezoelectric properties is predicted using one-dimensional beam theory and finite element method.

References

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