The 12th International Congress on Mesomechanics
21-25 June 2010, Taipei, Taiwan

A Multiscale Nonlinear Finite Element Simulation of Domain Switching Behaviors in Piezoelectric Materials

Yasutomo Uetsuji,
Department of Mechanical Engineering, Osaka Institute of Technology

Tetsuya Hata,
Graduate School of Engineering, Osaka Institute of Technology

Hiroyuki Kuramae,
Department of Technology Management, Osaka Institute of Technology

Kazuyoshi Tsuchiya
Department of Precision Engineering, Tokai University

Marc Kamlah
Institute for Materials Research II, Forschunzentrum Karlsruhe

Ferroelectric piezoceramics, which are being increasingly used in various electronic and mechanical device applications for actuators, sensors and information storage, consist of many grains at a microscopic scale. Each grain is subdivided into domains which are characterized by asymmetric lattice with spontaneous polarization. High electric or mechanical loading conditions result in a change of spontaneous polarization direction within individual domains, which is commonly referred to as domain switching. In poling process the domain switching can produce the macroscopic polarization and it leads polycrystalline materials into a large piezoelectricity. In order to predict the performance and reliability of such devices, it is necessary to understand the nonlinear behavior of ferroelectric materials. In particular, we must clarify the relation between the global electronic and mechanical properties of macrostructure and the local ferroelectric behaviors in microstructure to design polycrystalline piezoelectric materials.

In this paper, a multiscale nonlinear finite element simulation based on

homogenization theory is presented for domain switching behaviors in ferroelectric piezoceramics. Crystal morphologies, which are characterized as an inhomogeneous structure composed of many grains and domains with individual orientations, are modeled in a microstructure. Then the homogenized properties of macrostructure can be estimated with perfect correlation to microscopic switching behaviors. We utilized an incremental form of fundamental constitutive law in consideration with changes of elastic stiffness, dielectric, piezoelectric stress constants and spontaneous polarization cased by domain switching. A multiscale nonlinear formulation was devised by employing the homogenization approach based on perturbation method and it was implemented into our original finite element method code.

The developed simulation was applied to a polycrystalline material. A computational example was presented for a typical ferroelectric material, barium titanate ($BaTiO_3$). A virtual distribution of crystal orientations, which satisfied transversely isotropy and poled perfectly along one direction, was generated and introduced into integral points of a regular-devised finite element model of microstructure. Each integral point represents a single grain in polycrystal. An external uniform electric field was applied to a macrostructure and then the domain switching behavior was investigated for the above microstructure. In order to determine a representative volume element (RVE), we addressed the influence of number of mesh division on the homogenized properties of macrostructure before and after poling process. By employing a RVE, the macroscopic hysteresis and butterfly curves were estimated and the change of crystal orientation distribution was revealed in response to domain switching in microstructure.