

NUMERICAL PROCEDURE FOR POLYCRYSTALLINE FERROELECTRICS USING LANDAU'S POTENTIAL AND VECTOR-NODAL FINITE ELEMENT

*Gakuji Nagai¹ and Takamasa Hayashi¹

¹ Dept. of Mathematical and Design Engineering, Faculty of Engineering, Gifu University
Yanagido 1-1, Gifu City, Gifu 501-1193, JAPAN
E-mail: gakuji@gifu-u.ac.jp

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ABSTRACT

Ferroelectricity/ferroelasticity is a coupling problem of mechanics and electrostatics. For the analyses of linear behaviours in the electro-mechanical problem, conventional FEM[1] has been widely used. In the FEM, displacement and electric voltage, scalar potential, are chosen as independent variables. On the other hand, for the material-nonlinear analyses of the ferroelectric/ferroelastic problem, this FEM would not be appropriate because of the possibility of numerical or physical instabilities in constitutive law level. Various numerical approaches for the material nonlinearity still have been studying [2].

Recently, an alternative FEM[3] has been proposed to overcome these difficulties. In this FEM, displacement and vector potential, instead of the scalar potential in conventional one, are chosen as independent variables. Ordinal nodal interpolation is used for the discretization of displacement but edge interpolation should be used for the discretization of vector potential in 3-D case. Note that in 2-D case nodal interpolation is used for both independent variables. These two FEMs are dual each other in terms of electrics. In conjunction with the alternative FEM, Landau's constitutive law models[3] based on energetically local minimum potential functions can be utilized for the description of the material nonlinearity. In solid-state physics these models are common and they are usually used for describing phase transitions phenomenologically. This class of the models is well-suited for the alternative FEM. The resulting computational procedure is very similar to the one for the buckling analyses of structures like shallow arches.

We present that the combinational approach of the alternative FEM and the Landau's potentials is advantageous to the material-nonlinear analyses in polycrystalline ferroelectric/ferroelastic problem. Using a potential in the literature[5] with dielectric relaxation, dynamic analyses of polycrystalline BaTiO₃ ceramics will be demonstrated. For example, Fig. 1 shows the dynamic behaviours of electric remnant polarization in a randomly-oriented 2-D polycrystalline in the case that upper and lower faces are subjected to electric voltage.

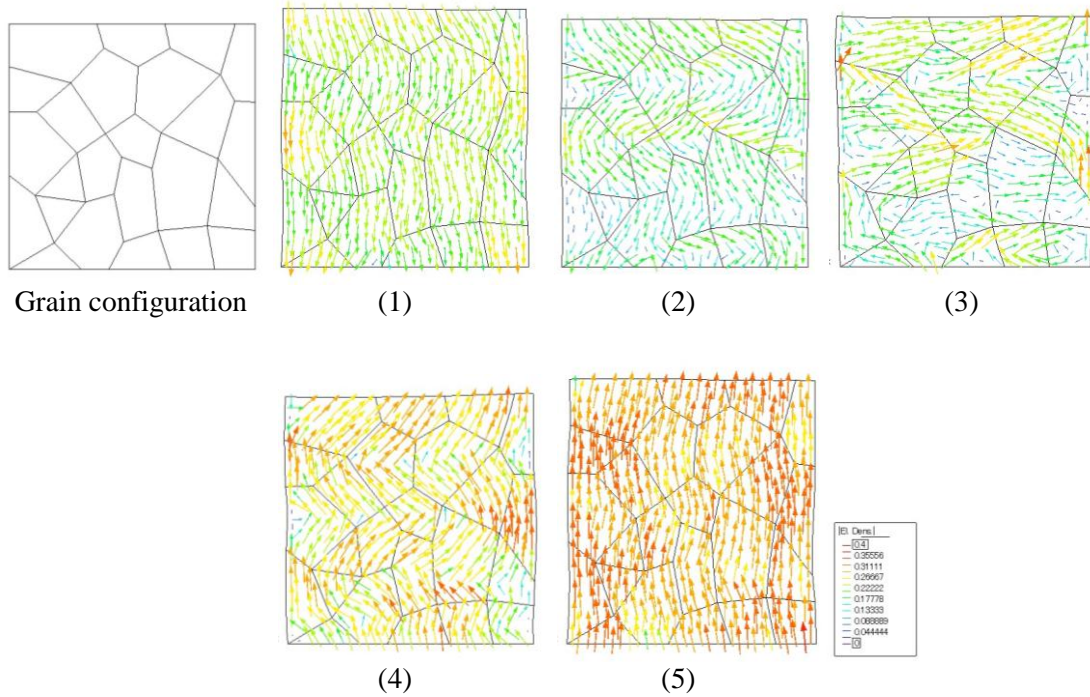


Fig. 1 Process of domain switching in 2-D polycrystalline

REFERENCES

- [1] H. Allik, T. J. R. Hughes, *Finite element method for piezoelectric vibration*, Int. J. Num. Meth. Eng., 2, (1970), 151-157.
- [2] M. Kamlah, *Ferroelectric and ferroelastic piezoceramics – modeling of electromechanical hysteresis phenomena*, Continuum Mech. Thermodyn. 13, (2001), 219-268.
- [3] C. M. Landis, *A new finite-element formulation for electromechanical boundary value problems*, Int. J. Num. Meth. Eng., 55, (2002), 613-628.
- [4] P. Chandra, P. B. Littlewood, *A Landau primer for ferroelectrics*, arXiv:cond-mat/0609347v1 [cond-mat.mtrl-sci], (2006)
- [5] N. A. Pertsev, A. G. Zembilgotov, and A. K. Tagantsev, *Effect of mechanical boundary conditions on phase diagrams of epitaxial ferroelectric thin films*, Physical review letters, 80(9), (1998), 1988-1991.