Texture and eco-piezoceramics

L. E. Fuentes-Cobas[1], J. R. Narváez-Monroy[1], A. Campos-Rodríguez[1], M. E. Montero-Cabrera[1], R. Domínguez-García[1], E. E. Villalobos-Portillo[2], L. Fuentes-Montero[3], B. Batista-Fierro[4], M. S. Luévano-Jáquez[4], L. Pardo[5]

[1]Centro de Investigación en Materiales Avanzados, Chih., México, [2]European Synchrotron Radiation Facility, Grenoble, France, [3]Diamond Light Source, Didcot, UK, [4]Universidad Autónoma de Chihuahua, Chih., México, [5]Instituto de Ciencia de Materiales de Madrid, Madrid, Spain

luis.fuentes@cimav.edu.mx

Research on lead-free piezoceramics is a trending topic [1]. A significant component of this search is the characterization of the effect of texture on the properties of polycrystalline electroceramics. The present contribution describes an integrated methodology, systematized in a software package, to solve the following tasks: (a) interpretation by numerical simulation of XRD patterns produced by textured samples; (b) forecast of the effective elasto-electrical properties of piezoceramics, starting from the knowledge of the corresponding single-crystal tensors and the texture determined in (a).

Part (a) considers 1D and 2D diffraction experiments, with Bragg-Brentano, grazing incidence and transmission geometries. The inverse pole figure of the symmetry axis of fiber-textured piezoceramics is proposed and refined by a Rietveld-type procedure [2].

The calculations in part (b) are performed using a variant of the Voigt-Reuss-Hill approximations. Particular precautions are taken with regard to the selection of the quantities considered as independent variables [3].

The computer programs developed to solve the proposed tasks are shown, the use of the MPOD database [4] in this type of work is described, and representative case studies are presented.

Fig. 1 shows as an example the computerized modelling of the variation of the representative longitudinal surfaces of the elastic compliance $s(\mathbf{h})$ and the charge constant $d(\mathbf{h})$ of the lead-free piezoceramic $0.95(Na_{0.5}Bi_{0.5})TiO_3$-$0.05BaTiO_3$ (BNBT5) as the texture evolves from relatively sharp to a random distribution.

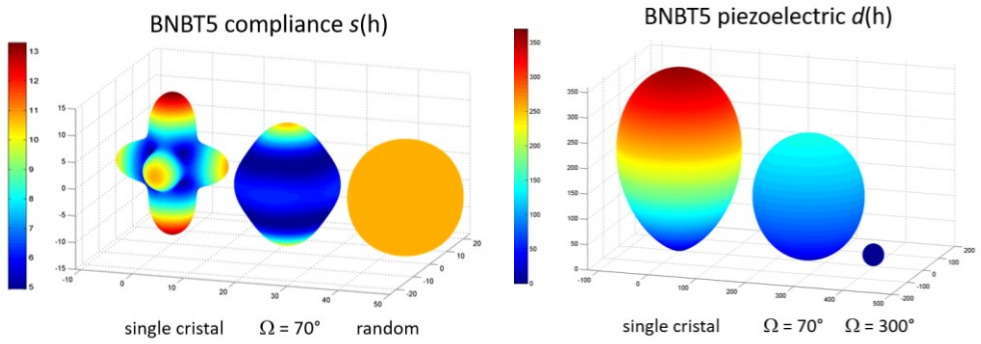

Figure 1. Modelled effect of axial texture on elastic compliance and piezoelectric charge constant of lead-free BNBT5 piezoceramic. As the width of the orientation distribution (Ω) increases, the elasticity tends to isotropic and the piezoelectricity collapses to zero.

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