Dependence of e31,f on Polar Axis Texture for Tetragonal Pb(Zrx,Ti12x)O3 Thin Films

Charles B. Yeager[1], Yoshitaka Ehara[2], Naoya Oshima[2],
Hiroshi Funakubo[2],and Susan Trolier-McKinstry[1]
[1]Department of Materials Science and Engineering and Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania 16802, USA
[2]Department of Innovative and Engineered Materials,Tokyo Institute of Technology, 4259 Nagatsuta-cho, Midori-ku, Yokohama 226-8502, Japan

It was shown by Ouyang et al. [Appl. Phys. Lett. 86, 152901 (2005)] that the piezoelectric e31,f coefficient is largest parallel to the spontaneous polarization in tetragonal PbZrxTi1xO3 (PZT) films. However, the expected piezoelectric data are typically calculated from phenomenological constants derived from data on ceramic PZT. In this work, the dependence of e31,f on c-axis texture fraction, f001, for {001}PZT thin films was measured by growing films with systematically changed f001 using CaF2, MgO, SrTiO3, and Si substrates. An approximately linear increase in e31,f with f001 was observed for compositions up to 43 mol.% Zr, and 100% c-domain properties were extrapolated. It was demonstrated that c-axis PZT films can achieve e31,f exceeding 12 C/m2 for many tetragonal compositions. The energy harvesting figure of merit, e31,f
2/er, for c-axis PZT films
surpassed 0.8 C2/m4. This is larger than the figure of merit of gradient-free PZT films grown on Si substrates by a factor of four.