MAR05-2005-020132

Abstract for an Invited Paper for the MAR05 Meeting of the American Physical Society

Enhancing Ferroelectrics using Strain

DARRELL SCHLOM, Penn State University

We have used epitaxy and the misfit strain imposed by an underlying substrate to shift the paraelectric-to-ferroelectric transition temperature (T_c) by hundreds of degrees and to enhance the ferroelectric properties of SrTiO₃ and BaTiO₃. Although SrTiO₃ is normally not ferroelectric at any temperature, predictions based on thermodynamic analysis imply that a biaxial strain of order 1% will shift its T_c to the vicinity of room temperature. Such strains are also predicted to elevate the T_c of BaTiO₃ by comparable amounts. In practice, the synthesis of uniformly strained ferroelectric films is challenging. Epitaxial ferroelectric films are often grown to thicknesses greatly exceeding their critical values, resulting in undesirable relaxation toward a zero-strain state by the introduction of dislocations. Dislocation densities of $\sim 10^{11}$ cm⁻² are common in epitaxial ferroelectric films grown on lattice-mismatched substrates, and the resulting inhomogeneous strain smears out the ferroelectric phase transition. Our approach to controlling the properties of ferroelectric $SrTiO_3$ and $BaTiO_3$ films centers on the development of new substrates $(DyScO_3 \text{ and } GdScO_3)$ that enable the growth of uniformly strained films below, or at least far closer to, the critical thickness for relaxation. Our results^{1,2} demonstrate not only the largest strain-induced shift in T_c ever achieved, but also manifest a paradigm shift in how to manipulate the properties of ferroelectric thin films. Strain is a viable alternative to the traditional method of chemical substitutions for shifting T_c by large amounts. These strained $SrTiO_3$ and $BaTiO_3$ films have better structural perfection (narrower rocking curve widths) than $SrTiO_3$ and $BaTiO_3$ single crystals. An unexpected surprise is that the strained SrTiO₃ films exhibit a frequency dependence of their dielectric constant consistent with relaxor ferroelectricity. ¹J.H. Haeni, P. Irvin, W. Chang, R. Uecker, P. Reiche, Y.L. Li, S. Choudhury, W. Tian, M.E. Hawley, B. Craigo, A.K. Tagantsev, X.Q. Pan, S.K. Streiffer, L.Q. Chen, S.W. Kirchoefer, J. Levy, and D.G. Schlom, Nature 430 (2004) 758-761. ²K.J. Choi, M. Biegalski, Y.L. Li, A. Sharan, J. Schubert, R. Uecker, P. Reiche, Y.B. Chen, X.Q. Pan, V. Gopalan, L.-Q. Chen, D.G. Schlom, and C.B. Eom, *Science* **306** (2004) 1005-1009.