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Ferroelectricity in $(BaTiO_3)_n/(SrTiO_3)_m$ Superlattices Containing as Few as one $BaTiO_3$ Layer (n=1)[1]

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The question of how thin a ferroelectric can be and still be ferroelectric has been the source of an intensive research effort over the past decade. Several studies, both theoretical and experimental, have concluded that with appropriate boundary conditions ferroelectricity can exist in superlattices containing $BaTiO_3$ or $PbTiO_3$ layers as thin as one unit cell. In this talk I will show the results of experiment and theory for $BaTiO_3/SrTiO_3$ superlattices grown by reactive molecular-beam epitaxy (MBE) on three different substrates: TiO_2-terminated (001) $SrTiO_3$, (110) $DyScO_3$, and (110) $GdScO_3$. With the aid of reflection high-energy electron diffraction (RHEED), precise single-monolayer doses of BaO, SrO, and TiO_2 were deposited sequentially to create commensurate $BaTiO_3/SrTiO_3$ superlattices with a variety of periodicities. The superlattices consist of an n unit-cell-thick slab of $BaTiO_3$ followed by an m unit-cell-thick slab of $SrTiO_3$, which are designated $[(BaTiO_3)_n/(SrTiO_3)_m]_q$, where q is the number of times the bilayer is repeated. X-ray diffraction (XRD) measurements exhibit clear superlattice peaks and the narrowest rocking curves ever reported for oxide superlattices. High-resolution transmission electron microscopy reveals nearly atomically abrupt interfaces. UV Raman results show that the $BaTiO_3$ in these $[(BaTiO_3)_n/(SrTiO_3)_m]_q$ superlattices is tetragonal and the $SrTiO_3$ is polar due to strain. Temperature-dependent UV Raman and XRD reveal the paraelectric-to-ferroelectric transition temperature (T_C). Our results* demonstrate (1) that $[(BaTiO_3)_n/(SrTiO_3)_m]_q$ superlattices containing as few as one strained $BaTiO_3$ layer (n=1) are ferroelectric and (2) the sensitivity of T_C to the boundary conditions. Comparisons to *ab initio* and phase-field modeling of the properties of these $[(BaTiO_3)_n/(SrTiO_3)_m]_q$ ferroelectric superlattices will be made and the importance of strain demonstrated. In addition to probing finite size effects and the importance of mechanical boundary conditions, these heterostructures may be relevant for novel phonon devices, including mirrors, filters, and cavities for coherent phonon generation and control. * D.A. Tenne, A. Bruchhausen, N.D. Lanzillotti-Kimura, A. Fainstein, R.S. Katiyar, A. Cantarero, A. Soukiassian, V. Vaithyanathan, J.H. Haeni, W. Tian, D.G. Schlom, K.J. Choi, D.M. Kim, C.B. Eom, H.P. Sun, X.Q. Pan, Y.L. Li, L.Q. Chen, Q.X. Jia, S.M. Nakhmanson, K.M. Rabe, and X.X. Xi, “Probing Nanoscale Ferroelectricity by Ultraviolet Raman Spectroscopy,” *Science* **313** (2006) 1614-1616.

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