

## **Infrared-active Phonons in $(\text{CaTiO}_3)_1/(\text{SrTiO}_3)_1$ , $(\text{BaTiO}_3)_1/(\text{SrTiO}_3)_1$ , $(\text{CaTiO}_3)_1/(\text{BaTiO}_3)_1$ Perovskite Superlattices.**

**S. S. A. Seo<sup>1\*</sup>, H. N. Lee<sup>2</sup>, H. M. Christen<sup>2</sup>, and T. W. Noh<sup>1</sup>**

<sup>1</sup> Research Center for Oxide Electronics and School of Physics, Seoul National University,  
Seoul, 151-747, Korea

<sup>2</sup> Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge,  
TN 37831, USA

\*E-mail of the corresponding author: [sseo@phya.snu.ac.kr](mailto:sseo@phya.snu.ac.kr)

Many artificial structures of solid-state materials have useful and interesting properties, which are usually unattainable in single-phase materials. Among them, superlattices of titanate perovskites have received a lot of attention due to enhanced dielectric and ferroelectric properties. For progress toward practical application, physical information of phonon dynamics is indispensable to understand the electric characteristics of the materials.

Three kinds of unit-cell controlled  $(\text{CaTiO}_3)_1/(\text{SrTiO}_3)_1$ ,  $(\text{BaTiO}_3)_1/(\text{SrTiO}_3)_1$ , and  $(\text{CaTiO}_3)_1/(\text{BaTiO}_3)_1$  superlattices are grown by pulsed laser deposition equipped with reflection high-energy electron diffraction for *in-situ* surface monitoring. Single-stepped  $\text{SrTiO}_3$  (001) substrates are used for atomic layer-aligned interfaces. Between the substrate and the superlattices,  $\text{SrRuO}_3$  (100nm) bottom-electrode layer is deposited for screening the phonons of  $\text{SrTiO}_3$  substrates as well as electric characterization. X-ray diffraction reciprocal space mapping shows that in-plane lattices of the superlattices are fully strained to coincide with those of  $\text{SrTiO}_3$  substrates.

Far-infrared spectra of the superlattices are measured by grazing angle ( $48^\circ$ ) reflectance method at various temperatures using Fourier-transform infrared spectrometer. Due to electric selection rules, three longitudinal optic phonons are clearly seen in raw reflectance spectra. By model-fitting the spectra, frequencies and relaxations of the phonons are extracted. Soft-mode frequencies of the superlattices are red-shifted, which give physical clues of the enhanced dielectric properties by Lyddane-Sachs-Teller relations. In addition, anomalous zone-folded behaviors of stretching mode and bending mode phonons of titanium and oxygen ions are observed. As lattice mismatch between the layers increases (1.7% in  $(\text{CaTiO}_3)_1/(\text{SrTiO}_3)_1$ , 2.1% in  $(\text{BaTiO}_3)_1/(\text{SrTiO}_3)_1$ , 3.7% in  $(\text{CaTiO}_3)_1/(\text{BaTiO}_3)_1$ ), splitting of the phonon frequencies increases and the phonon shapes become asymmetric. These observations are understood by changes of electrical bonding strength between ions, due to lattice distortions and interfacial strains in the superlattices.