

# Materials Science and Engineering Doctoral Defense

## Characterization of Perovskite Oxide/Semiconductor Heterostructures

School for Engineering of Matter, Transport and Energy

HsinWei Wu

Advisor: David Smith

### abstract

Integrated oxide/semiconductor heterostructures have attracted intense interest for device applications which require sharp interfaces and controlled defects. The research of this dissertation has focused on the characterization of perovskite oxide/oxide and oxide/semiconductor heterostructures, and the analysis of interfaces and defect structures, using scanning transmission electron microscopy (STEM) and related techniques. The SrTiO<sub>3</sub>/Si system was initially studied to develop a basic understanding of the integration of perovskite oxides with semiconductors, and successful integration with abrupt interfaces was demonstrated. Defect analysis showed no misfit dislocations but only anti-phase boundaries (APBs) in the SrTiO<sub>3</sub> (STO) films. Similar defects were later observed in other perovskite oxide heterostructures. Ferroelectric BaTiO<sub>3</sub> (BTO) thin films deposited directly onto STO substrates, or STO buffer layers with Ge substrates, were grown by molecular beam epitaxy (MBE) in order to control the polarization orientation for field-effect transistors (FETs). STEM imaging and elemental mapping by electron energy-loss spectroscopy (EELS) showed structurally and chemically abrupt interfaces, and the BTO films retained the c-axis-oriented tetragonal structure for both BTO/STO and BTO/STO/Ge heterostructures. The polarization displacement in the BTO films of TiN/BTO/STO heterostructures was investigated. The Ti<sup>4+</sup> atomic column displacements and lattice parameters were measured directly using HAADF images. A polarization gradient, which switched from upwards to downwards, was observed in the BTO thin film, and evidence was found for positively-charged oxygen vacancies. Heterostructures grown on Ge substrates by atomic layer deposition (ALD) were characterized and compared with MBE-grown samples. A two-step process was needed to overcome interlayer reaction at the beginning of ALD growth. A-site-rich oxide films with thicknesses of at least 2-nm had to be deposited and then crystallized before initiating deposition of the following perovskite oxide layer in order to suppress the formation of amorphous oxide layers on the Ge surface. BTO/STO/Ge, BTO/Ge, SrHfTiO<sub>3</sub>/Ge and SrZrO<sub>3</sub>/Ge thin films with excellent crystallinity were grown using this process. Metal-insulator-metal (MIM) heterostructures were fabricated as ferroelectric capacitors and then electrically stressed to the point of breakdown to correlate structural changes with electrical and physical properties. BaTiO<sub>3</sub> on Nb:STO was patterned with different top metal electrodes by focused-ion-beam milling, Au/Ni liftoff, and an isolation-defined approach.

December 13, 2017; 9:00 AM; PSF 306