TEM studies of polarization nanodomains in (BaTiO3/SrTiO3)10 superlattices on silicon

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Over the last decade, it has been recognized that different topological structures formed in ferroelectrics significantly influence the physical properties of the material system. Ferroelectric oxides deposited on a semiconductor substrate are of particular interest for applications in nanoelectronics or photonics. A particularly attractive candidate of ferroelectric materials is $BaTiO_3$.

We investigated the crystalline structure, defects and the polarization patterns in $(BaTiO_3/SrTiO_3)_{10}$ superlattices epitaxially grown by molecular beam epitaxy (MBE) on a silicon substrate. A thin epitaxial $SrTiO_3$ template directly grown on the substrate is mainly used to compensate for the lattice mismatch between $BaTiO_3$ and Si.

To determine the spontaneous polarization within the $(BaTiO_3/SrTiO_3)_{10}$ superlattice, the in-plane and out-of-plane strain components of the lattice were determined using Geometrical Phase Analysis (GPA) and using a direct peak finding method. Furthermore, a more refined peak finding algorithm was used to analyze the displacements of the Ti atoms relative to the center of their respective unit cells in real space. Therefore, high-resolution HAADF-STEM images, which show a direct visualization of the atom columns in a crystal, were recorded. The analyses resulted in two-dimensional displacement maps of the Ti atoms, in which the areas of the $BaTiO_3$ layers revealed periodic, wave-like polarization patterns. These patterns are also partially continued in the $SrTiO_3$ layer. The two-dimensional strain maps show a strong modulation of the out-of-plane strain component and a periodic variation of the in-plane strain component in the region of the $BaTiO_3$ layers. The combination of the displacement maps and the strain maps shows a significant correlation between the two. These investigations of $(BaTiO_3/SrTiO_3)_{10}$ superlattices contribute to the understanding of two-dimensional oxide ferroelectrics for the future integration of topological polar nanostructures in devices.

Keywords:

$BaTiO_3$, ferroelectrics, HAADF-STEM

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