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Revealing atomic structure and composition in ultrahigh energy storage density ferroelectric thin-films

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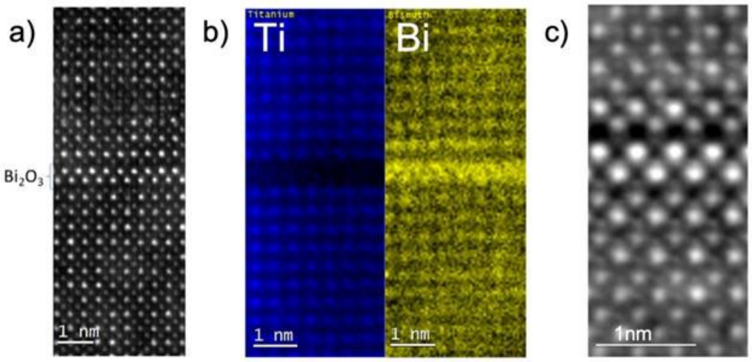
Ferroelectric thin film material is positioned to be a strong candidate for nano/microelectronics component with ultra-high energy storage density with low electric field [1]. One of the key strategies to achieve such high energy storage density is by creating a secondary phase nanostructure around the morphotropic phase boundary.

Here we show detailed characterisation of (Bi, Na)TiO3 (BNBT) thin films grown on SrTiO3 single crystal substrate. The nanostructures in the thin films as well as their electronic structures and composition variations were characterised using 4D STEM. Due to the presence of Na, it has been found that the BNBT structure can change under the electron beam, causing by the migration of Na. The ultra-fast ARINA detector allows acquisition of 4D STEM data with only few pA current, and short dwell time to avoid the electron beam damage to the BNBT film. Moreover, electron energy loss spectroscopy (EELS) was acquired using the K3 detector, to probe the composition and the electronic structure across the nanostructured domains.

We found that there is Bi segregation forming strips of half unit cell wide Bi2O3 layers. Such composition is confirmed by the atomic resolution EELS maps, showing no presence of Ti within the Bi2O3 bright strips. The effect of the Bi2O3 layers is to laterally displace the lattice above the defect by half a unit cell, resulting a morphotropic anti-phase domain boundary. In addition, the Bi2O3 segregation layer gives about 22% longer c-axis for the 3 unit cell around the defect. Such large expansion of c-axis is attributed to the presence of the super-tetragonal phase (super-T) [2-3]. The electronic structures of Ti and O sites adjacent to the Bi2O3, measured using EELS Ti L edge and O K edge, is consistent with the lattice distortions. Density functional theory calculations were carried out to probe that the origin of the super-T structure is likely due to the oxygen vacancies around the Bi2O3 strips.

Such complex nanostructures with multiple structure phases con-existent forming nanodomains is found to be the key for the ultra-high performance of such ferroelectric thin films.

Graphic:



Keywords:

4D-STEM, EELS, ferroelectric

Reference:

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