東京大学大学院工学系研究科 総合研究機構
第16回「次世代電子顕微鏡法」講演会
2023年12月14日 14:00 – 15:30 ハイブリッド開催

Ferroelectricity by phonon-decoupled oxygen tetrahedra in brownmillerite oxides

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Ferroelectricity is an intriguing phenomenon essential for non-volatile memory device applications with the advantages of high operation speed and low power consumption, which store information by spontaneous electric polarization. An innate property of ferroelectricity is that the spontaneous polarization can be switched under the application of an electric field. Singly-oriented polarization is electrostatically unstable because of the uncompensated charge at the surface, and a domain is formed to minimize the free energy. The domain size or pattern of conventional ferroelectrics is mostly determined by mechanical boundary conditions, such as interfacial strain and electrical boundary conditions. In this regard, there have been lots of efforts to reduce the ferroelectric domains; *i.e.*, an ultrafine ferroelectric domain structure with an approximate width of 10 nm has been reported in conventional perovskites, $Pb(Zr,Ti)O_3$ thin films, and the critical size of ferroelectric domains in a $BaTiO_3$ nanocrystal is limited to approximately 5–10 nm scale.

Ferroelectric HfO_2 has been considered as an appropriate candidate owing to its ultimately fine domains and half-unit cell width.[1] The orthorhombic phase of HfO_2 can be switched to zero-width domain walls contrary to the case in $PbTiO_3$ having diffused domain walls. Freestanding membrane $CsBiNb_2O_7$ has also been known to have unit cell wide ferroelectric domains;[2] however, there is insufficient understanding of the application of these materials to actual devices. In this talk, I do introduce a controllable unit cell-scale domain in the brownmillerite oxides.[3] The first-principles phonon calculations show that the phonon modes related with oxygen-octahedra are fully decoupled from those with oxygen-tetrahedra, and the strongly localized oxygen-tetrahedral phonons enable site-selective control of the unit cell-wide domain. By combining atomic-scale imaging and in situ transmission electron microscopy, we visualized unit cell-wide ferroelectricity separated by electrically neutral unit cell-wide walls and its switchable characteristics. Our findings provide inspiration for designing high-density memory devices at the quantum limit.

[1] H.-J. Lee, M. Lee, K. Lee et al., Science **369** 1343-1347 (2020).
[2] Y. Guo, B. Goodge, L. Zhang et al., Phys. Rev. Mater. **5** 044403 (2021).
[3] Jinhyuck Jang, Yeongrok Jin, Heung-Sik Park et al., doi.org/10.21203/rs.3.rs-3343923/v1.

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