Atomic-Scale Polarization Switch in Wurtzite Ferroelectrics

V.S. Calderon, J. Hayden, S.M. Baksa, W. Tzou, S. Trolier-McKinstry, I. Dabo, J.P. Maria, E.C. Dickey

Ferroelectric wurtzites have the potential to revolutionize modern microelectronics because they are easily integrated with multiple mainstream semiconductor platforms. However, the electric fields required to reverse their polarization direction and unlock electronic and optical functions need substantial reduction for operational compatibility with complementary metal-oxide semiconductor (CMOS) electronics. To understand this process, we observed and quantified real-time polarization switching of a representative ferroelectric wurtzite (Al0.94B0.06N) at the atomic scale with scanning transmission electron microscopy. The analysis revealed a polarization reversal model in which puckered aluminum/boron nitride rings in the wurtzite basal planes gradually flatten and adopt a transient nonpolar geometry. Independent first-principles simulations reveal the details and energetics of the reversal process through an antipolar phase. This model and local mechanistic understanding are a critical initial step for property engineering efforts in this emerging material class.