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Origin and Dynamics of Morphotropic Phase Boundary in Multiferroic Films JINXING ZHANG, ROBERT ZECHES, GUANG SHENG, JAN SEIDEL, PU YU, QING HE, CHANHO YANG, YINGHAO CHU, LONGQING CHEN, RAMAMOORTHY RAMESH — Materials with morphotropic phase boundary (MPB) compositions attract people's interests because of their huge electromechanical response. The ambiguity of crystal structure, phases and physics behind presents a challenge to interpret the origin of abnormally high piezoelectric coefficient. Recently, epitaxial strain can be used to stabilize the MPB in $BiFeO_3$. [1] However, to better understand the origin of MPB in multiferroic perovskite, it is essential to probe into the strain/polarization coupling mechanism. In this abstract, origin and dynamics of the phase transition in $BiFeO_3$ near MPB have been investigated by exploring the ferroelectric domains. Careful analysis of domain configurations across the phase boundary reveals the rotation of ferroelectric vectors from phase to phase, a new strain/polarization coupling state in nature. The phase transition dynamics are assisted by the re-orientation of ferroelectric polarizations. Phase-field simulation further proves the origin of this MPB is the strain-driven rotation and re-orientation of ferroelectric vectors. This investigation provides new insight into the study of high electromechanical response in MPB-like crystal and helps engineer other lead free-ferroelectrics. Reference: 1. R. J. Zeches, et al., Science 326, 977 (2009).

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