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Experimental evidence of stress-induced R-M_A-M_C-T phase transition in $BiFeO_3$ films HANS CHRISTEN, JOONG-HEE NAM, CHARLEE BENNETT, HYUN-SIK KIM, MICHAEL BIEGALSKI, Oak Ridge National Laboratory — Recent reports on epitaxial $BiFeO_3$ films show that the crystal structure changes from nearly rhombohedral ("R-like") to nearly tetragonal ("T-like") at strains exceeding ≈-4.5%, with the "T-like" structure being characterized by a highly-enhanced c/a ratio. While both the "R-like" and the "T-like" phases are monoclinic, our detailed x-ray diffraction results reveal a symmetry change from M_A and M_C type, respectively. Therefore, the ferroelectric polarization is confined to different (pseudocubic) planes in the two phases. By applying additional strain or by modifying the unit cell volume of the film by substituting Ba for Bi, the monoclinic distortion in the "T-like" M_C phase is reduced, i.e. the system approaches a true tetragonal symmetry. Therefore, in going from bulk to highly-strained films, a phase sequence of rhombohedral(R)-to-monoclinic("R-like" M_A)-to-monoclinic("T-like" M_C)-to-tetragonal(T) is observed. This sequence is otherwise seen only near morphotropic phase boundaries in lead-based solid-solution perovskites (i.e. near a compositionally induced phase instability), where it can be controlled by electric field, temperature, or composition. Our results now show that this evolution can occur in a lead-free, stoichiometric material and can be induced by stress alone.

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