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Antiferromagnetic and structural phase transitions in tetragonal-like BiFeO₃ H.M. CHRISTEN, G.J. MACDOUGALL, W. SIEMONS, Oak Ridge National Laboratory, J.H. NAM, Korea Institute of Ceramic Engineering and Technology, J.L. ZARESTKY, M.D. BIEGALSKI, S. LIANG, E.R. DAGOTTO, S.E. NAGLER, Oak Ridge National Laboratory — The recent observation that strain stabilizes a tetragonal-like (“T-like”) polymorph of BiFeO₃ has illustrated how epitaxial constraints can fundamentally alter the properties of this multiferroic material. We performed detailed temperature-dependent neutron and x-ray scattering experiments on epitaxial BiFeO₃ films on different substrates (SrTiO₃, LaAlO₃, YAlO₃) to study the nature of the monoclinic crystal structure and of the antiferromagnetic (AFM) order. In agreement with Monte Carlo simulations for a classical Heisenberg model, we observe a much lower Néel temperature in the T-like morph ($T_N \simeq 325\text{K}$) than in less-strained (“R-like”) films ($T_N \simeq 645\text{K}$), and additionally a low-temperature coexistence of C-type and G-type AFM. Independent of the antiferromagnetic transition, at $T \simeq 375\text{K}$ we also observe a structural phase transition from one type of monoclinic distortion to a different one. In combination, these measurements shed light on the complexity of the phase diagram of BFO, and provide routes to explore how the material’s properties can be tuned by external parameters. Research supported by the U.S. DOE, BES, MSED (H.M.C., W.S., S.L., E.D., H.M.C) and SUFD (M.D.B., G.J.M, J.L.Z, S.E.N.).

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