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Strained $BiFeO_3$ Films: Rhombohedral-Orthorhombic and Rhombohedral-Tetragonal Phase Transitions. Part I: Phase-Field Simulations[1] GUANG SHENG, JINGXIAN ZHANG, ZI-KUI LIU, LONG-QING CHEN, Department of Materials Science and Engineering, The Pennsylvania State University, YULAN LI, Pacific Northwest National Laboratory, THE PENNSYLVANIA STATE UNIVERSITY TEAM, PACIFIC NORTHWEST NATIONAL LABORATORY COLLABORATION — In this study, the strain-temperature phase stability diagrams of (001) $BiFeO_3$ thin film were constructed using both thermodynamic analysis and phase-field simulations. The predicted diagram reveals a tetragonal to distorted rhombohedral phase boundary around 4.3% compressive strain and rhombohedral to orthorhombic boundary at around 2% tensile strain, both at room temperature. The predicted transition temperatures for rhombohedral-orthorhombic and rhombohedral-tetragonal transitions are in reasonable agreement with experimental observations. We will also discuss domain structure evolutions of $BiFeO_3$ thin films during the above two transitions from phase-field simulations.

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