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Phase diagram of $Ba_{0.5}Sr_{0.5}TiO_3$ thin films KRISTOPHER E. ANDERSEN, Northern Arizona University, C. STEPHEN HELLBERG, Naval Research Laboratory — $Ba_{0.5}Sr_{0.5}TiO_3$ (BST) thin films are a promising material for tunable microwave applications, which require large, tunable dielectric constants and low loss. By controlling the (i) substrate and (ii) oxygen partial pressure, it is possible to tune the tetragonal strain of these films. For example, in-plane strains between -0.48% (highly compressive) and +0.30% (highly tensile) have been reported for BST thin films grown on MgO(001) using rf magnetron sputtering. The ability to control the strain makes it possible to optimize the dielectric properties of the film for microwave (and other) applications; however, the strain-temperature phase diagram has not been systematically explored to-date. In this talk, the phase diagram of BST is studied using first-principles calculations, focusing initially on the $T = 0$ phases. Results for displasive as well as coupled ferroelectric/antiferroelectric phases (recently discussed by Zhang, Cagin, and Goddard in connection to $BaTiO_3$) will be presented.

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