Critical thickness for ferroelectricity of $BaTiO_3$ by first-principles calculations

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Abstract:

The critical thickness for ferroelectricity of a $BaTiO_3$ film was determined by the first-principles discrete variational-X α molecular orbital method and population analysis. Under the assumption that most ferroelectric perovskite oxides are predominantly ionic, a series of model clusters were developed for a $BaTiO_3$ particle consisting of a $Ba_8Ti_7O_6$ cluster constructed on the basis of the crystal structure of $BaTiO_3$ phase and point charges surrounding the $Ba_8Ti_7O_6$ cluster. The size of the model cluster was exactly defined by the size of a three-dimensional point-charge array. By comparing the dependence of the net charge of Ba, Ti, and O ions and of the overlap population between Ti 3*d* and O 2*p* orbitals on particle thickness in tetragonal and cubic $BaTiO_3$ particles, the critical thickness for ferroelectricity was calculated to be about 12 nm for a $BaTiO_3$ particle with a basal area of 20×20 nm.