Particle size and surface effects on critical thickness for ferroelectricity of BaTiO$_3$ by first-principles calculation


A silicon dioxide (SiO$_2$) film is used as a gate insulator in metal-oxide-semiconductor (MOS) devices. The electrical thickness of such an insulator must decrease with the channel length of a MOS field-effect transistor in miniaturization to maintain high performance of the devices. Since recent researches of tunneling phenomena have shown that leakage current through thin SiO$_2$ films become unacceptably large, ferroelectric films with a perovskite crystal structure have attracted attention for use in a gate capacitor. It has been reported that the Curie temperature of a thin ferroelectric film may be different from that of a bulk ferroelectric material and ferroelectricity may disappear at a certain nanoscale size of the material. The present authors reported that the critical thickness on ferroelectricity of BaTiO$_3$ particles depended on the particle size. In this paper, we report computational results of critical thickness and surface effects on the ferro-to-paraelectric transition of nanoscale rectangular BaTiO$_3$ particles with various sizes.