Particle size and surface effects on critical thickness for ferroelectricity of $BaTiO_3$ by first-principles calculation

K. Ishizumi, H. Kawanishi, R. Nakao, I. Takahashi, H. Terauchi, K. Miura and Y. Hayafuji

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_2films 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.