SURFACE STATE ON FIRST-ORDER FERROELECTRICS

Abstract

In the presence of a surface the Landau-Devonshire equations of ferroelectricity must be extended to include a boundary condition. For a ferroelectric with a second-order transition in the case when the polarization $p(z)$ increases at the surface, it is well known that a surface state occurs in a range of temperature above the bulk critical temperature t_{CB}. Here we explore the corresponding effect for a first-order ferroelectric. We show that a surface state can occur, but only if the surface effect is sufficiently strong. Analytic expressions are derived and illustrated for $p(z)$, the surface value $p_S = p(0)$ and the free energy. The transition from the paraelectric state ($p=0$) to the surface state is first order, and for completeness we establish the dependence of the three critical temperatures (supercooling, thermodynamic and superheating) on a boundary-condition parameter y. In a final section, we derive and illustrate expressions for $p(z)$ in the temperature range $t<t_{CB}$.