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Determination of the dominant factor affecting the change of the phase transition point in thin ferroelectric films

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Size effects in nanoscale ferroelectrics lead to a significant change in their properties compared with bulk ferroelectric materials. The manifestation of the size effect consists of both in a change of the value of the dielectric constant and in the displacement of the phase transition point.

The purpose of the work is to determine the factor that has the greatest influence on the phase transition in thin ferroelectric films. In this work, the Ising model is used to describe the ferroelectric phase transition. The calculations were carried out by the Monte Carlo method. The solution of the task consists of 4 stages:

(1) Investigation of the influence of boundary conditions on the phase transition point. The plotted temperature dependences of the heat capacity of a ferroelectric film under various boundary conditions show a shift of the phase transition point, but this effect is significant only for films with a thickness of about 2-3 unit cells. However, experimental techniques allowed to detect the size effects for ferroelectric film with a thickness of 10 unit cells [1].

(2) Investigation of the influence of the correlation effects on the phase transition point in thin ferroelectric films. At this stage, it was taken into account that the distance between the dipoles will change depending on the temperature. A shift in the phase transition point was also observed. However at this stage the critical size was not detected.

(3) Investigation of the influence of the depolarizing field on the phase transition point. The inclusion of a depolarizing field leads to a decrease in the Curie point. Similar results for ferroelectric composites with spherical ferroelectric inclusions were obtained in work [2]. Taking into account this factor has been shown that the polarization in sufficiently thin films is not observed even at low temperatures. This is explained by the fact that its thickness is less than two values of the thicknesses of the "dead" layer. The double thickness of the "dead" layer is considered as the critical size of ferroelectric films, which disappear its ferroelectric properties.

(4) In conclusion, the study of the influence of all factors on the shift of the Curie point was conducted.

As a result of modeling, it was shown that the dominant factor that has the greatest influence on the phase transition in thin ferroelectric films is the depolarizing field.

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