Dvigubos histerezės kilpos $Sn_2P_2S_6$ kristaluose

Double hysteresis loops in $Sn_2P_2S_6$

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For $Sn_2P_2S_6$ (SPS) ferroelectrics the second order phase transition at T_0 ~ 337 K with mixed displacive – order/disorder character is occurred [1]. Observed evolution of the soft mode spectrum is enough complicate – several low energy optic branches linearly interact at heating and relaxational central peak growths near the phase transition temperature. By DFT methodology it was found [2] that local potential for the spontaneous polarization fluctuations in SPS ferroelectrics has three – well shape. This peculiarity is related to Sn^{2+} cations electron lone pair stereoactivity [2, 3] and to valence fluctuations P^{4+} + P^{4+} - P^{3+} + P^{5+} inside $(P_2S_6)^{4-}$ anions [4]. Microscopic origin of ferroelectric lattice instability in SPS can be described as second order Jahn-Teller effect and their thermodynamics is considered in the frame of Blume-Emery-Grffiths model. At accounting of electronic correlation, the presentation of Anderson's electron pairs flipping can be involved. At this the electronic recharging and lattice instability can be presented as pseudospin fluctuations in anharmonic potential with complicate shape. The anharmonic quantum oscillator (AQO) model is proposed [4] for description of temperature–pressure phase diagram of SPS (Fig. 1). This model we generalize by taking onto of two inequal interacting systems of oscillators and applicate for analysis of ferroelectric dynamics at temperature and pressure variation.

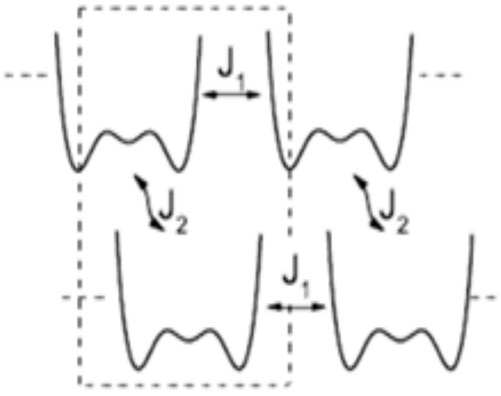

Fig. 1 The AQO model

As direct confirmation of three-well shape of the local potential in SPS, we present our observation of antiferroelectric – like double dielectric poops in this proper uniaxial ferroelectrics. Qualitively this phenomenon can be explained as repopulation of pseudospins between possible three states (-1, 0 +1) during repolarization process at external electric field influence. The calculations give us the stable and metasrable solutions which describe ferroelectric and antiferroelectric phases and corresponding types of loops depending on parameters of AQO model. The temperature – electric field diagram in the parameters of AQO model is described. Experimental condition for realization of "ferroelectric" or "antiferroelectric" loops are investigated.

Literatūra

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