Dipole ordering and strain effects in the deformable Blume–Emery–Griffiths model

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Ferroelectrics belonging to the $Sn_2P_2S_6$ family (with the possible partial substitutions Sn $\rightarrow$ Pb and S $\rightarrow$ Se) are known for their sensibility to a hydrostatic pressure. The *ab initio* calculations showed that ionic groups P_2S_6 exist in three configurations (determined by their shape and distribution of electronic charge), which in the paraelectric phase are described by a symmetrical three-well potential in the configurational space. In the absence of external influence, the $Sn_2P_2S_6$ crystal exhibits the second order phase transition to the ferroelectric phase due to a dipole ordering of these structure elements. At the increase of pressure the temperature of the second order phase transition decreases, a tricritical point is achieved, and, finally, the ferroelectric state is suppressed.

For such a crystal we proposed a modified version of the BEG model taking into account the microscopic mechanism of the external pressure influence on thermodynamics and phase transitions in lattices with a three-well local lattice potential. We assume that the influence of pressure is not a direct one but it is mediated by the crystal lattice strain. Namely, the crystal deformation leads to the change of internal field and displacements of atoms surrounding the structure elements (ionic groups); configurations of the latter are determined by the mentioned above local potential. Our modification of the BEG model supplementarily considers the shift of local energy levels (due to restructuring of local anharmonic potentials) under the influence of deformation caused by a uniform pressure or tension. Such an approach allows to describe the deformational effects accompanying the phase transitions to the state with a dipole ordering (the ferroelectric phase).

Based on this model, the pressure dependences of the $u = \Delta V/V$ volume deformation are calculated for the $Sn_2P_2S_6$ crystal. The presence of anomalies of $u(p)$ function in the regions of ferroelectric phase transitions of the first and second order as well as the tricritical point is established; the behaviour of the volume compressibility is investigated. Metastability phenomena related to a possible hysteresis are also analysed. Obtained results are compared the experimental data.