Anharmonicity of $Sn_2P_2S_6$ ferroelectrics

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The ferroelectrics $Sn_2P_2S_6$ (SPS) represent a wide class of low-symmetry compounds, where the strongly pronounced nonlinear phenomena have two origins: the polarizability of the anion sublattice is much higher than in oxides; the symmetry is lower (monoclinic), allowing effects which are forbidden in the high-symmetry perovskite structures. For this compound the second order phase transitions is observed which is near Lifshitz and tricritical points at the state diagram [1].

A reasonable microscopic model for the SPS ferroelectrics was developed [2] in *ab-initio* effective-Hamiltonian approach. It was found that the strong nonlinear coupling between low-energy soft optic mode and other hard modes lead to a triple-well shape of the potential-energy surface. This nonlinearity could be a reflection of the strong polarizability of Sn^{2+} cations in chalcogenide surrounding. Statistical theory for ferroelectrics based on triple-well anharmonic potential was used and model parameters were estimated [3]. It was found confirmation of the assumption that the phase transition in considered crystals is located in crossover region between order-disorder and displacive type, and very closely to tricritical point. Anisotropy of hypersound velocities of SPS crystals is investigated by Brillouin spectroscopy using different scattering geometries. The dispersion of velocity of the longitudinal sound waves was observed which can be connected with the role of acoustic phonons in soft mixed optic-acoustic modes at transition near the Lifshitz point. The linewidth of quasielastic light scattering has been measured at various temperatures. Thermodynamic and dynamic characteristics of the lattice anharmonicity are compared.

1. Yu.M. Vysochanskii, T. Janssen, R. Currat, R. Folk, J. Banys, J. Grigas, V. Samulionis. Phase transitions in phosphorous chalcogenide ferroelectrics. Vilnius University Publishing House, 2006, 453 p.
2. K.Z. Rushchanskii, Yu.M. Vysochanskii, D. Strauch. Phys. Rev. Lett., 2007, 99, 207601.
3. R.M. Yevych, Yu.M. Vysochanskii. Condensed Matter Physics, 2008, 11, 417.