Dielectric, piezoelectric, elastic, dynamic, and thermal properties of KH_2PO_4 type ferroelectric compounds

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Within the framework of the modified proton ordering model for KH_2PO_4 family crystals that takes into account linear over strains ε_6 and ε_4 contributions to the proton subsystem energy and neglects tunneling, we use a four-particle cluster approximation to calculate the corresponding thermodynamic potentials of the system. Using appropriate equations of state, we find spontaneous polarization, longitudinal and transverse dielectric permittivities of mechanically free and clamped crystals, piezoelectric characteristics related to shear strains ε_6 and ε_4, elastic constants c_{66} and c_{44}, and specific heat of the crystals.

Dynamic characteristics of the crystals are explored within a stochastic Glauber approach for the proton subsystem with taking into account dynamics of piezoelectric strains ε_6 and ε_4 via Newtonian equations of motion. Ultrasound velocity and attenuation, longitudinal and transverse dynamic permittivities of mechanically free and clamped crystals of the KH_2PO_4 family crystals are found.

A thorough numerical analysis of the calculated characteristics is performed for the MD_2XO_4 (M = K, Rb, ND_4; X = P, As) compounds. The quantities for partially deuterated crystals are calculated in the mean crystal approximation. The obtained sets of the model parameters allow a proper description of available experimental data for these ferroelectrics. Phenomena of crystal clamping by a high-frequency field and piezoelectric resonance are described. Peculiarities of the ultrasound attenuation in these crystals are described. A presence of a cut-off frequency in the frequency curves of attenuation is predicted. It is shown that taking into account piezoelectric coupling hardly affects the calculated spontaneous polarization or specific heat, but gives rise to differences in dielectric permittivities of mechanically free and clamped crystals and increases the relaxation dispersion frequency.