Transverse Field Effect in GPI Ferroelectrics: Microscopic Consideration

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Glycinium phosphite (GPI) crystal belongs to the family of ferroelectrics with hydrogen bonds. It is usually supposed that the phase transition to the ferroelectric phase at T=225K is connected with ordering of protons on bonds. The corresponding model was proposed in [1]. An important feature of GPI, that was revealed experimentally [2], consists in possibility of reorientation of the local dipole moments (formed by protons and the adjacent glycine groups) by the external electric field E_z perpendicular to the ferroelectric axis OY. It manifests in the proportional to E_z^2 decrease of T_c and in the increasing with E_z anomalies of transverse permittivity ε_{zz}. The latter effect was explained in [2] assuming the smearing of phase transition in the presence of field E_z.

Starting from the model [1] we extend in this work the investigation of field effects in GPI. The approach is supplemented by allowance for piezoelectric coupling of the proton subsystem with the lattice strain. Calculations of thermodynamic, dielectric and elastic characteristics are performed in the frames of the two-particle cluster approximation. At the proper choice of the model parameters the satisfactory quantitative description of the wide set of the available experimental data has been obtained.

A separate attention is paid to the E_z influence on the permittivity ε_{zz} and polarization P_z. It is shown that the quite good description of the measured in [2] temperature dependence of ε_{zz} can be achieved, when the presence of the small longitudinal component E_y (of the order of ~0.05E_z) is supposed (fig.1). Such a component could appear due to incomplete reorientational relaxation of the glycine groups; one can not exclude, also, the possibility of some deflection of the applied transverse field from the OZ-axis during experiment. We have calculated also the $P_y(T)$ and $P_z(T)$ dependences at various values of E_z. The plots for $P_z(T)$ presented in fig.2 confirm the parabolic lowering of T_c under influence of E_z.

Our consideration shows, that along with the reordering of protons, the remarkable role in the field effects in GPI can be served by the glycine groups.

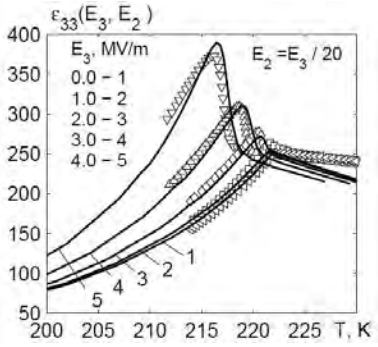

Figure 1. The temperature dependence of dielectric permittivity ε_{zz} at different values of field E_z and at field E_y=0.05E_z. Symbols are experimental data taken from [2].

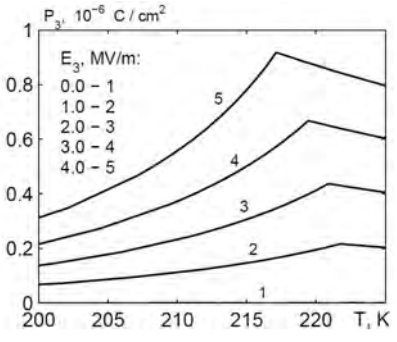

Figure 2. The temperature dependences of the P_z component of polarization of GPI crystal.

[1] I.V. Stasyuk, O.V. Velychko, *Ferroelectrics* **300** (2004) 121.
[2] I. Stasyuk, Z. Czapla, S. Dacko, O. Velychko, *J. Phys.: Condens Matter* **16** (2004) 1963.