**Section “Physico-Chemical nanomaterials science”**

**Computer simulation of nanostructure features in lead magnoniobate**

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The ferroelectric relaxor properties were discovered more than fifty years ago, are now actively used as functional matherials for the needs of electronics. Ferroelectric relaxors with a diffuse phase transition have a large temperature interval in which a phase transition occurs, in the consideration of which two cases are distinguished: - the case when the anharmonicity is small and the potential V (r) has one minimum; - the case when the strongly anharmonic potential V (r) is multiminimum, determines transitions of the order-disorder type with dynamic or static disordering of ions. It was established earlier that both cases of phase transitions can exist near the Curie point [1, 2]. In this paper we present data on the modeling of the structural features of the classical model object of this class of compounds-lead magnesium niobate (PMN) at different temperatures. An analysis of the results obtained by us suggests that with an approximation of the temperature values to the temperature Tm, ordering of the displacements of lead atoms in neighboring cells and associated antiparallel shifts of oxygen atoms can occur, which indicate possible rotation of oxygen octahedra. Such ordered displacements of atoms in PMN can be the reason for the appearance of superstructural reflexes, indicative of doubling the parameters of an elementary perovskite cell [3,4]. In favor of such a model, the temperature dependence of the peaks of super structure reflexes noted by many authors, whose nature is actively discussed, attests to the temperature dependence [3,4]. Various scenarios of the ordering process in the PMN are considered.

1 Nelmes R.I., Kuhs W.F. // Solid State Commun., 1985,v.54, p.721-723.

2. Brus F., Cowley R. // М.: MIR, 1984, 408 p. (rus)

3. Zhang Q.M., You H., Mulvihill M.L., Jang S.J.// Solid State Com., 1996, v.97, JVfo 5, p.693-698.

4 Gosula v., Tkachuk A., Chung K. and Chen H..// J.Phys. and Chem.Solids, 2000, v.61, p. 221-227.