MICROSCOPIC MECHANISM OF STRUCTURAL PHASE TRANSITION, ELASTIC AND LATTICE ANOMALIES IN $La_{2/3}Ba_{1/3}MnO_3$ PEROVSKITE

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Temperature dependences of elastic and magnetic properties of polycrystalline perovskite manganite $La_{2/3}Ba_{1/3}MnO_3$ have been studied by ultrasonic and SQUID magnetometer techniques previously. Minimum of the temperature dependent sound velocity *v(T)* and corresponding maximum of the decrement $\delta(T)$ have been found in the vicinity of the structural phase transition $R\bar{3}c \leftrightarrow Imma$ at $T_s \sim 200$ K temperature. Giant alteration of *v* and δ indicates a structural phase transition of the soft mode type. Hysteretic temperature behavior of ultrasound properties is evident of the 1st order phase transformation. A negative value of the linear thermal expansion coefficient along one of the crystallographic axis has been found in the *Imma* phase near T_s.

Microscopic mechanism explaining of the previouslyfound anomalies are proposed. The unit cell construction of $La_{2/3}Ba_{1/3}MnO_3$ is typical for perovskites and is similar to the classical perovskite compound $BaTiO_3$, which exhibits a set of the 1st order structural phase transitions and have a cubic paraphase. The displacement of the central atom reduces symmetry of the crystal lattice and elongates corresponding crystal axis, becomes tetragonal, orthorhombic, or rhombohedral. Almost free movement of the central ion should lead to a highly symmetric (cubic) perovskite structure near the temperature T_s of the structural phase transition. Therefore, the crystal lattice parameters should be close to each other near T_s. A negative value of the linear thermal expansion coefficient along one of the crystallographic axis can be explained by this mechanism. Expansion of the free-energy density in powers of the order parameter components for the first order phase transition was analyzed. The system is described by two interacting order parameters (namely, displacement and elastic deformation), a polarization is possible. In the phase transition, the interaction term makes a significant contribution to the free energy and can change the relative height of the potential minima. It may change the relative depth of the potential wells for and cause displacement of the atoms with an ultrasound frequency. This mechanism gives a microscopic picture of the absorption and the appearance of the soft mode in the spectrum of the lattice vibrations. Therefore the attenuation and the velocity behavior are connected with the dynamics of the order parameter. Therefore, the crystal lattice parameters should be close to each other near T_s. Temperature So, we can expect the anomalous temperature dependent behavior of dielectric constant.