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ADIABATIC POTENTIAL ENERGY SURFACE OF THE JAHN-TELLER COMPLEXES IN $SrF_2:Cr^{2+}$ CRYSTAL

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In SrF_2 crystal doped with Cr^{2+} ions, attenuation of all the normal ultrasonic modes with the wave vector k < 110 > were investigated at 52-162 MHz in the temperature region of 4-180 K. The observed peaks of relaxation origin were interpreted as manifestation of the Jahn-Teller effect.

Temperature dependence of attenuation of ultrasonic normal modes, one longitudinal and two transverse ones polarized along [001] and [1,1',0] axes and propagationg along the [110] crystallographic axis in strontium fluorite crystal doped with chromium ions with the dopant concentration $1.6 \cdot 10^{19}$ cm^{-3} is described in the framework of a phenomenological approach, whereas the contribution of the sub-system of the Jahn-Teller complexes is presented by the microscopic theory. Analysis of experimental data, obtained at the frequency of 52-162 MHz in the temperature range of 4 – 180 K, and calculation of isothermal contribution indicated $T \otimes (e+t2)$ Jahn-Teller effect problems with important impact of quadratic term in the vibronic Hamiltonian. The value of activation energy was derived from the temperature dependence of relaxation time with account of three mechanisms of relaxation: thermal activation $1/\tau_a = v_0 \cdot \exp(-V_0/K_BT)$, tunnelling through the potential energy barrier $1/\tau_a \propto T$, and two-phonon mechanism similar to Raman scattering $1/\tau_R \propto T^3$. The extrema points of adiabatic potential energy surface: six orthorhombic global minima, three tetragonal and four trigonal saddle points were calculated in 5-dimensional space of symmetrized coordinates (two tetragonal Q_θ, Q_ε and three trigonal ones Q_ζ, Q_η, Q_ξ).