Pressure Dependence of the Soft Mode Close to the Ferroelectric-Paraelectric Transition in $PbTiO_3$

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Pressure dependence of the Raman frequency of the A_1(1TO) soft mode is calculated using the observed volume data from the literature by means of the mode Grüneisen parameter for the tetragonal-cubic phase transition in $PbTiO_3$. From the calculated Raman frequencies of the soft mode studied as the order parameter, the damping constant is calculated as a function of pressure using the pseudospin-phonon coupled model and the energy fluctuation model by fitting to the observed Raman linewidths of this soft mode. On that basis, the reciprocal relaxation time for this soft mode is evaluated at various pressures close to the ferroelectric (tetragonal)-paraelectric (cubic) transition in $PbTiO_3$. Within the pressure region (0-12 GPa) corresponding to the temperature interval of the tetragonal-cubic transition in $PbTiO_3$, values of the activation energy are deduced from the calculated damping constant for the soft mode A_1(1TO) in this ferroelectric material ($PbTiO_3$) using both models (pseudospin-phonon coupled model and the energy fluctuation model)

Our results show that both models studied here, are satisfactory to explain the observed behavior of $PbTiO_3$, in particular, the observed Raman frequencies and the linewidths of the A_1(1TO) soft mode. Our prediction of the inverse relaxation time for this mode as a function of pressure and our values of the activation energy can be compared with those obtained experimentally when the observed data are available in the literature for $PbTiO_3$.