Volume Collapse at the Jahn-Teller Transition in $LaMnO_3$

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We have investigated the Jahn-Teller (JT) transition accompanied by the orbital order-disorder transition in $LaMnO_3$ by high temperature X-ray powder diffraction with synchrotron radiation and also neutron powder diffraction. The unit cell volume of $LaMnO_3$ decreases with increasing temperature in a narrow temperature range below T_{JT} = 750 K, and then undergoes a volume collapse at T_{JT}. We interpret this effect as due to the more efficient packing of the MnO_6 octahedra in the orbitally disordered or orbital liquid state. The orbital melting phenomenon can be qualitatively compared with the melting of ice. By constructing a model Hamiltonian involving the pseudospin of Mn^{3+} e_g states, the staggered JT distortion and the volume strain coordinate, we show that the anharmonic coupling between these primary and the secondary order parameters leads to the the first-order J-T phase transition associated with a comparatively large reduction of the unit cell volume. We explain the temperature dependence of the JT distortions and volume strain and discuss the volume change as a function of the anharmonic coupling constant. A continuous change to a second-order transition as a function of the model parameters is obtained. This behaviour has been observed experimentally by us on doping $LaMnO_3$ with Ba.

Keywords: neutron diffraction, x-ray diffraction, Jahn-Teller phase transition