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Local orthorhombic distortion and enhanced susceptibility in $LaNiO_3$ paramagnet BING LI, SHINICHIRO YANO, DESPINA LOUCA, University of Virginia, LUKE MARSHALL, JIAN-SHI ZHOU, JOHN GOODENOUGH, University of Texas at Austin, MIKHAIL FEYGENSON, JORG NEUEFEIND, Oak Ridge National Laboratory — The perovskite $LaNiO_3$ is metallic, and unlike other systems in this class of materials, it remains paramagnetic where only an enhancement in the magnetic susceptibility (χ) is observed below 200 K. Other rare earth nickelates are antiferromagnetic with an enhancement of χ in paramagnetic metallic state. Using neutron powder diffraction and the pair density function analysis, it is observed that the temperature dependence of the local atomic structure cannot be reproduced assuming the average crystal symmetry which is rhombohedral with the $R\bar{3}c$ space group. With rising temperature, octahedral distortions involving displacements of oxygen set in, and the symmetry is reduced to $Pbnm$. In this symmetry, the equivalent O site in the $R\bar{3}c$ splits into two and can account for all the features observed in the local lattice. The structural changes occur gradually, between 100 and 200 K. The local Ni-O-Ni bond angles are reduced from 164.5 to 163.5 ° during this transition. Such reduction of Ni-O-Ni bond angles may facilitate antiferromagnetic coupling and responsible for the temperature dependence of χ observed in $LaNiO_3$ below 200 K.

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