Abstract Submitted
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Local structure and orbital ordering in $YTiO_3$[1] BING LI, KEESEONG PARK, SHINICHIRO YANO, DESPINA LOUCA, University of Virginia, BIAO HU, JIANSHI ZHOU, JOHN GOODENOUGH, University of Texas at Austin — $YTiO_3$, with the strongest $GdFeO_3$-typed distortion in $RTiO_3$, is a ferromagnet below T_C of 30 K and many theoretical and experimental studies suggest it is of antiferro-orbital ordering due to magnetic superexchange. Here, the local atomic structure of $YTiO_3$ has been investigated by using elastic (inelastic) neutron scattering and the (dynamic) pair density function analysis from 5 to 350 K. Deviations are observed of the local from the average crystal symmetry and these are attributed to distortions involving the Y and O atoms. In the case of Y, the in-plane $x - y$ displacements result in an antiferrodistortive motion exerting influence on Y-O1 (apical sites of octahedral) bonds seen in the temperature dependence. At the same time, the O ion site in the basal plane of the octahedron is split to two (O2 and O3), giving rise to two unequivalent Ti-O bonds, which results consequently in different tilting of basal plane of octahedra (0.5° larger in O3), A-O covalency and about 2° larger Ti-O-Ti bond angle in O3 sites. These facts may be regarded as the structural evidences on antiferro-orbital ordering in $YTiO_3$ and suggest electron-lattice interaction may play an important role in the orbital ordering, in addition to magnetic superexchange interation.

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