Distortion mode anomalies at T_{MIT} = T_N in bulk $PrNiO_3$

Y. M. Klein[1], D. J. Gawryluk[1], T. Shang[1], D. Sheptyakov[2], V. Pomjakushin[2], L. Keller[2], N. Casati[3], Ph. Lacorre[4], M. T. Fernández-Díaz[5], J. Rodríguez-Carvajal[5], and M. Medarde[1]

[1]Laboratory for Multiscale Materials Experiments, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland, [2]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland, [3]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland, [4]Institut des Molécules et Matériaux du Mans (IMMM) - UMR 6283 CNRS, Le Mans Université, Avenue Olivier Messiaen, 72085 Le Mans, France, [5]Institut Laue Langevin, 71 avenue des Martyrs, CS 20156 -38042 Grenoble CEDEX 9, France

Maximilian.Klein@psi.ch

Rare-earth nickelates ($RNiO_3$) are strongly correlated-electron materials with electronic, structural and magnetic instabilities, including a rare, spontaneous metal to insulator transition (MIT). The origin of the MIT and the correct description of the structural anomalies are source of intensive debate in the scientific community. Here we investigate the gap opening and the simultaneous charge ordering in $PrNiO_3$ in a temperature range from 1.5 K to 300 K by combining bulk transport and magnetic properties with high-resolution neutron and synchrotron X-ray powder diffraction. The structural information is analysed in terms of symmetry-adapted distortion modes, an unconventional, but illustrative formalism that reveals the existence of sharp anomalies in all mode amplitudes at the MIT[1] and the appearance of new modes below T_{MIT}. Our analysis also unravels a linear correlation between the breathing-mode amplitude, representing the charge order, and the staggered Ni magnetization below T_{MIT}, which in this nickelate coincides with the long-range antiferromagnetic ordering of the Ni magnetic moments. We also observe an intriguing anomaly at T
~60 K (~0.4×T_{MIT}), visible in some lattice parameters, mode amplitudes and the electrical resistivity. Possible origins of this anomaly will be discussed, among them the existence of a hidden symmetry in the insulating phase, which could be caused by polar distortions driven by the non-centrosymmetric magnetic order[2].

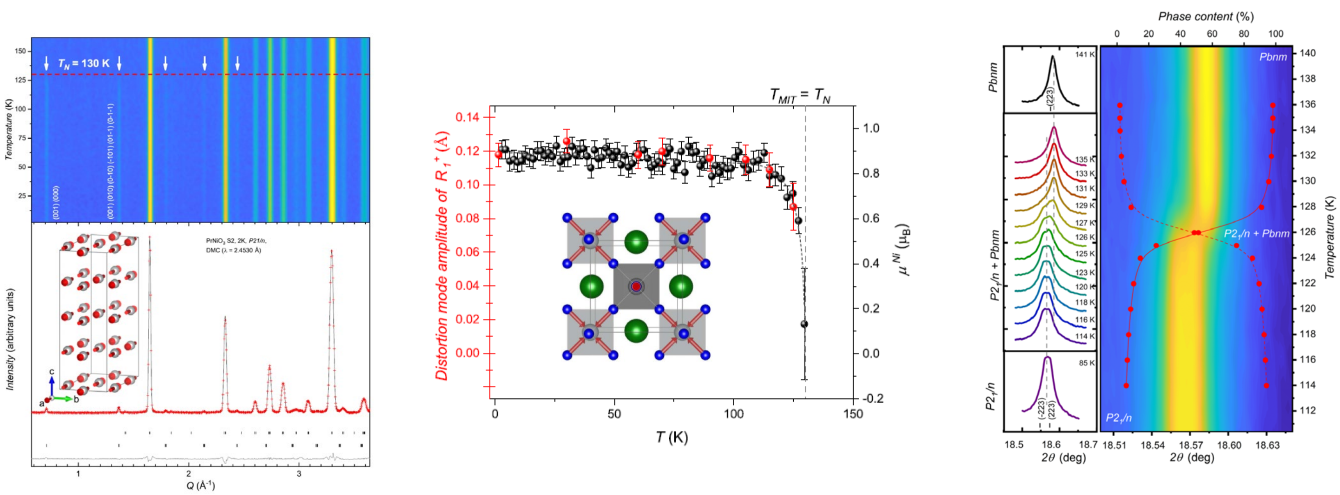

Figure 1. **Left:** 2D contour plot of the neutron powder diffraction pattern for $PrNiO_3$ across T_N. White arrows indicate the positions of magnetic reflections. **Middle:** temperature dependence of the R_1^+ breathing mode amplitude (left axis) and the staggered Ni magnetic moment (right axis). Inset: schematic representation of the R_1^+ atomic displacements. **Right:** 2D contour plot of the synchrotron x-Ray powder diffraction pattern of $PrNiO_3$ across T_{MIT} and the evolution of the Pbnm and $P2_1/n$ weight fractions. Adapted from ref. [2].

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