Distortion mode anomalies at $T_{MIT} = T_N$ in bulk PrNiO$_3$

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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 $T \sim 60$ K ($\sim 0.4 \times T_{MIT}$), 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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