Supplementary Information for “High pO₂ Floating Zone Single Crystal Growth of the Perovskite Nickelate PrNiO₃”

Hong Zheng ¹*, Junjie Zhang ², Bixia Wang ¹, Daniel Phelan ¹, Matthew J. Krogstad ¹, Yang Ren ³, William Adam Phelan ⁴, Omar Chmaissem ⁵, Bisham Poudel ⁵ and John F. Mitchell ¹

¹ Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA; Zheng@anl.gov (H.Z.); bixia.wang@anl.gov (B.X.W.); krogstad@anl.gov (M.J.K.); mitchell@anl.gov (J.F.M.)
² Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA; zhangj4@ornl.gov
³ Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA; yren@anl.gov
⁴ Platform for the Accelerated Realization, Analysis and Discovery of Interface Materials (PARADIM), Department of chemistry, The Johns Hopkins University, Baltimore, MD 21218, USA; wphelan2@jhu.edu
⁵ Department of Physics, Northern Illinois University, Dekalb, IL 60115, USA
* Correspondence: zheng@anl.gov

In the main text, we considered the single crystal X-ray diffraction patterns (Figure 5) in pseudocubic symmetry. In doing so, we considered twinned orthorhombic (space group Pbnm) and monoclinic (P2₁/n) structures. When twinned, there are six matrix transformations that relate these two space groups to the pseudocubic axes:

\[
M = \begin{bmatrix}
-\frac{1}{2} & 0 & \frac{1}{2} \\
\frac{1}{2} & 0 & \frac{1}{2} \\
0 & 1 & 0
\end{bmatrix},
\begin{bmatrix}
\frac{1}{2} & 0 & \frac{1}{2} \\
0 & 1 & 0 \\
\frac{1}{2} & 0 & \frac{1}{2}
\end{bmatrix},
\begin{bmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
\frac{1}{2} & 0 & \frac{1}{2}
\end{bmatrix},
\begin{bmatrix}
0 & 0 & \frac{1}{2} \\
0 & \frac{1}{2} & 0 \\
\frac{1}{2} & 0 & \frac{1}{2}
\end{bmatrix},
\begin{bmatrix}
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
0 & 0 & 0
\end{bmatrix},
\begin{bmatrix}
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
0 & 0 & 0
\end{bmatrix}
\]

such that \((a, b, c)_{pc} = (a, b, c)_{m,n} M\). The Miller indices transform by the same matrices such that \((h, k, l)_{pc} = (h, k, l)_{m,n} M\). The following reflection conditions exist for the Miller indices in the Pbnm space group: for \(0kl\), \(k=2n\) (where \(n\) is an integer); for \(h0l\), \(h+l=2n\); for \(h00\), \(l=2n\); for \(0k0\), \(k=2n\); for \(00l\), \(l=2n\). For the P2₁/n space group, the \(0kl\) condition is deleted, and all other conditions remain. When calculating the positions of systematic absences that are marked in Figure 5 of the main text, we transformed all allowed reflections for the Pbnm and P2₁/n space groups to the pseudocubic coordinates using the above matrices.