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Temperature dependent oxygen disorder in Pr(2-x)Sr(x) NiO(4+δ) by high-resolution single crystal neutron diffraction on HEIDI@MLZ

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Mixed-ionic electronic conductors (MIEC) offer significant advantages over conventional cathodes especially in the intermediate temperature range for solid oxide fuel cell applications. In this context, Ruddlesden-Popper type layered oxides have taken much attention. Among them Pr2 NiO(4+δ) is a promising candidate as it offers high electronic conductivity similar to those conventional cathode materials but in addition shows a very high oxygen diffusion coefficient even at room temperature. Behind these remarkable physical properties the oxygen atoms and their disorder between interstitial and apical sites play a key role in low-moderate temperature region, allowing phonon assisted diffusion in the moderate temperature region. In a similar way to high temperature superconductors, Sr doping or hole doping may increase the electronic conductivity but significantly lowers the delocalization of oxygen atoms. Nevertheless, it offers to make a direct comparison of oxygen diffusion mechanism with the undoped sample. For these reasons, our present work focuses to analyze apical oxygen disorder in Pr(1.5)Sr(0.5)NiO(4+δ) by single crystal neutron diffraction on HEIDI@MLZ as a function of temperature. Neutrons are point scatterer and thus a perfect tool to explore disordered structures.
We will discuss the displacement amplitudes of the apical oxygen atoms as a function of Sr-doping and temperature, analyzed by classical Fourier techniques and by Maximum Entropy algorithm, in order to conclude and separate possible static and dynamic contributions

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