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Charge Density Wave Order in Doped Praseodymium Nickelate studied by Resonant Soft X-ray Scattering

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The solid oxide fuel cells (SOFCs) have attracted considerable attention due to their high energy conversion efficiency and lower production of pollutants. However, high temperature is needed creating issues related with compatibility, thermal expansion and stability.
Therefore, oxide materials with high oxygen ion conductivity are of particular interest especially in their applications as oxygen membranes and electrolytes in SOFCs. In particular, perovskite type oxides, A(2)BO(4) (Ruddlesen-Popper phase have shown interesting ionic and electronic transport properties and the possibility to tune the properties by doping (oxygen intercalation at room temperature).
The compounds in the K(2)NiF(4) family are the lanthanide oxides with the general formula of Ln(2)MO(4) (where Ln = La, Pr, Nd and M = Cu, Ni, Co). Their properties vary drastically on doping, which can be huge, modifying (anisotropic) oxygen mobility, the charge ordering and the valence of the transition metal, by changing the oxygen stoichiometry and the temperature.
Indeed, in K(2)NiF(4) family, structural changes are a function of charge transfer.
The chosen material to be investigated is Pr(2)NiO(4+delta), because at low temperature, besides the antiferromagnetism, long-range ordered superstructures can arise, generating an electronic correlation that only oxygen intercalation can induce. These superstructures are known as magnetic and charge-stripe phases, static or dynamic, i.e. local AFM regions with anti-phase boundaries.
Such phases are visible as incommensurate peaks by analysing the material with high-brilliance X-ray sources, like synchrotron. However, their interpretation is challenging and their origin can be often confused, due to their low intensity but also due to imperfections of the material, such as NiO segregation or Pr(6)O(11) hydrolization.
For this reason, large single crystals of $Pr(2)NiO(4+delta) will be prepared in order to achieve clear satellite peaks related to commensurate/incommensurate reflections.
Such very defined diagrams provided the motivation for this work.
This work will focus on the energy of the incommensurate peaks in order to identify from which physical phenomenon they are originated. Therefore, an energetic distribution of peaks will be performed, by exploiting Resonant Soft X-Ray Scattering (RSXS), an energy-dispersive analysis technique. The possible explanations are related to the charge or orbital ordering arising from Ni or O ions, whose transition energies are separated only by few eV.
The aim of this work is to give a better understanding of the structural and electronic properties of Ruddlesen-Popper phase perovskite oxide Pr(2}NiO(4+delta) with several delta values, as well as the lattice dynamics and the valence distribution of nickel ions.

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