MS25-P7 New approach to phasonic Debye-Waller factor.

Radoslaw Strzalka[1], Ireneusz Buganski[1], Pawel Kuczera[1], Janusz Wolny[1]

1. Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland

email: strzalka@fis.agh.edu.pl

The very serious concerns of scientists dealing with crystal structure refinement, including theoretical research, pertains to characteristic bias in calculated vs. measured diffraction intensities, observed particularly in weak reflections regime. We attribute it most distinctly to corrective factor for phasons, and give credible proofs of this in our presentation. The lack of consistent theory of phasons in quasicrystals manifests most spectacularly in a characteristic bias of fitted vs. observed diffractionintensities. In our presentation we show that the most commonly used exponential Debye-Waller factor for phasons fails in case of quasicrystals and propose a novel method of calculating the correction factor within a statistical approach. Our results obtained for model quasiperiodic systems show that phasonic perturbations can be successfully described. It is possible to include very weak reflections to a dataset during the structure refinement and fits of high quality are achievable.

By phonons we mean a rearrangement of atoms in the structure [1]. The calculations are performed for vertex decoration models based on 1D Fibonacci chain and 2D Penrose tiling. For such models, phasons can be introduced as flips of tiles violating matching rules. Such flips are easily recongnized within statistical method based ond average unit cell concept [2]. The probability distributions of atomic positions calculated against some reference lattice are sensitive to phason flips, which occur in their fragmentation as comparing to ideal shapes [3]. The level and manner of this fragmentation depends on the amount and type of flips introduced to the system. Including this in a definition of structure factor automatically solves the problem of phasons at the very basic level of calculating the diffraction pattern. Neither any multiplicative correction factor nor iterative fitting of parameters in the Gaussian's exponent is required. The only free parameter to fit would be a number of phason flips, which has a very physical grounds.

[1] de Boissieu M., Phonons, phasons and atomic dynamics in quasicrystals, Chem. Soc. Rev. 41, 6778-6786, (2012).

[2] Wolny J., The reference lattice concept and its application to the analysis of diffraction patterns, Philos. Mag. A77, 395-412, (1998).

[3] Wolny J., Buganski I., Kuczera P., Strzalka R., Pushing the limits of crystallography, submitted (2016).

Keywords: phasons, quasicrystals, correction factor

MS26 Incommensurate modulated and composite phases

Chairs: Michal Dusek, Artem Abakumov

MS26-P1 Structural complexity and O^{2-} ordering in $Pr_{2-x}Sr_xNiO_{4+\delta}$ studied by single crystal x-ray diffraction

Rajesh Dutta[1,2], Avishek Maity[1], Monica Ceretti[1], Antoine Villesuzanne[2], Werner Paulus[1]

1. Institut Charles Gerhardt, UMR 5253, CNRS-University Montpellier, 34095 Montpellier, France
2. ICMCB, UPR 9048, University Bordeaux, 33600 Pessac, France

email: rajeshatiitm@gmail.com

Ruddlesden-popper phases especially those with K_2NiF_4-type structure, are of particular interest, as they exhibit high ionic and electronic conductivity already at moderate temperatures. Among them, $Pr_2NiO_{4+\delta}$ phases have attracted much attention as promising materials, showing a rather wide range of oxygen non-stoichiometric and accommodating extra oxygen on interstitial lattice sites, suitable for membranes in next generation SOFCs. A high oxygen doping level has been shown to induce a special lattice dynamics, allowing the apical oxygen atoms to easily move to vacant interstitial sites on a shallow energy diffusion pathway [1,2].

Hole doping in Pr_2NiO_4, either by substituting Pr with Sr cations or by O^{2-} ion intercalation on interstitial lattice sites modifies the structural (ordering of O^{2-} ions) and electronic ordering in $Pr_{2-x}Sr_xNiO_{4+\delta}$. We investigated the structural evolution of the complex electronic and structural ordering as a function of x and δ by scanning the whole reciprocal space using single crystal x-ray diffraction. The average structure changes from orthorhombic $Fmmm$ (x = 0 and 0.125) to tetragonal $P4/2ncm$ (x = 0.25 and 0.5) in $Pr_{2-x}Sr_xNiO_{4+\delta}$. Due to oxygen intercalation δ up to 0.25 and long-range ordering of those O^{2-} ions, $Pr_2NiO_{4+\delta}$ forms complex superstructures with 2D-incommensurate modulation ($q_{1,2}$ = ±0.83a*+0.49b*) in the (hkn, n=integer) reciprocal plane (Fig. 1), still present in the doped crystal (x = 0.125). More complex and different modulation exists in (hkn+1/2, n=integer) plane due to ordering along c-direction which as contrary disappears in doped crystal with x = 0.125. Four twin individuals are present in the as grown $Pr_2NiO_{4+\delta}$ single crystal which also makes the incommensurate modulation more complex whereas this modulation disappear gradually and new p-type superstructure reflections appear when entering to the tetragonal phase of $Pr_{2-x}Sr_xNiO_{4+\delta}$ (x=0.25 and 0.5) with no modulated incommensurate superstructure.

Reference: