MS46-P4 **Effect of Cr-doping on structural, magnetic and electrical transport properties of $La_{0.67}Ba_{0.33}Mn_{1-x}Cr_xO_3$ ($0 \leq x \leq 0,1$) perovskites manganites.** Marwène Oumezzine,[ab] Octavio Peña,[b] Sami Kallel[a], Thierry Guizouarn[b], Mohamed Oumezzine[a] *[a] Laboratoire de Physico-chimie des Matériaux, Département de Physique, Faculté des Sciences de Monastir,Université de Monastir, 5019, Tunisia. [b]Institut des Sciences Chimiques de Rennes, UMR 6226, Université de Rennes 1, 35042 Rennes cedex, France.*
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We report the synthesis of polycrystalline samples with nominal compositions $La_{0.67}Ba_{0.33}Mn_{1-x}Cr_xO_3$ ($0 \leq x \leq 0,1$) via the solid state reaction route and our study of their structural, magnetic and electrical transport properties with the variation of doping concentration of Cr. Rietveld analysis of fitted and observed XRD patterns exhibited the single-phase nature phase of all the studied materials, which crystallize in R-3C space group when . Energy Dispersive X-ray Analysis (EDAX) confirms the expected stoichiometry of all samples. Successive substitution of Cr at Mn site in $La_{0.67}Ba_{0.33}Mn_{1-x}Cr_xO_3$ manganites makes both the Curie temperature T_c and the magnetization M to diminish, which is ascribed to the reduction of the DE interaction by Cr doping. Nevertheless, Cr doping makes the saturation magnetization at 5K to decrease, which indicates that the Cr^{3+} moments tend to be antiparallel to the Mn^{3+} moments at low temperature. The Cr-doped manganites exhibit a large variation in resistivity values. The increase of Cr doping leads to an increase of the electrical resistivity. Below 10 at.% of Cr^{3+}, the electrical resistivity shows a metallic behaviour, which is well fitted by the relation $\rho = \rho 0+ \rho 2T_2+ \rho 4.5T_{4.5}$, indicating the importance of the grain/domain boundary, the electron-electron scattering effects and, to a lesser extent, the electron (magnon,phonon) scattering effects in the mechanism of conduction.

Keywords: Rietveld structure analysis; electrical properties; magnetic properties

MS46-P5 **Recognizing the better solutions in powder charge runs** Dubravka Šišak, Lynne B. McCusker, Christian Baerlocher, *Laboratory for Crystallography, ETH Zurich, Switzerland*
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To what extent does the success of the powder charge flipping algorithm [1,2] implemented in the program *Superflip* [3,4] depend upon the input parameters used? In order to answer this question, two cases were studied: one inorganic (ZrPOF-Q1 [5]) and one organic (D-ribose, [6]). This proved to be a fairly straightforward exercise for the zirconium phosphate, but for D-ribose, the algorithmfailscompletely in default mode. However, by optimizing the input parameters andgenerating starting phases from an approximate structure, some fully interpretable maps could be produced. Unfortunately, it proved to be difficult to identify these10 maps within the full set of 200 solutions generated bySuperflip. Therefore better criteria for ranking the solutions had to be found. Several approaches have been explored in an attempt to address this problem: (a) combining the various figures of merit produced by *Superflip*, (b) performing a cluster analysis of the solutions, and (c) calculating the entropy of the solutions.While the $R_{SF}$and R_{symm}values produced by *Superflip* could be used to identify very bad solutions, they did not appear to distinguish between the mediocre and good solutions. Reasoning that good solutions should be more similar and less random than incomplete solutions, two clustering procedures were tested. One was based on a comparison of the electron density (already implemented in *Superflip*), and the other on a comparison of phase sets [7]. In both cases, the cluster with the highest similarity was found to contain partial or near-complete solutions, but did not include the best ones.The figures of merit used in the maximum entropy method program MICE [8] to evaluate phase sets offered a third alternative. In this case, the phase sets are classified by their entropy (and other) values. Preliminary tests showed no obvious correlation between the entropy and the quality of the solution. However, the lowest entropy value criterion appears to be powerful enough to filter out at least one fully interpretable solution from the complete solution set.This evaluation scheme involvesseveralsteps. *Superflip* solutions are input as *n* lists of reflections with their corresponding amplitudes and phases. From each list, *N* percent of the weak reflections are discarded to speed up the calculation.Then a small (random) subset of the remaining reflections are excluded and those remaining define a basis set. The entropy of the system is then maximized and the maximum entropy (ME) map calculated. Fourier analysis of this map should reproduce both the phases and the amplitudes from the basis set and predict those in the excluded set. The agreement between the ME prediction and the amplitudes and phases in the *Superflip* solution defines the quality of the *Superflip*phase set. This is expressed as the entropy or as the log-likelihood gain (LLG). By taking the average of the lowest entropy maps and using that map to generate starting phases for another *Superflip* run,solution sets containing only fully interpretable solutions were produced in all of the cases. Tests are still in progress, but the entropy approach appears to be a most promising one.

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