

identification) and EXAFS (to find the local environment for Cr, Fe and Ni) [1,2,3,4]. The combination of powder diffraction and EXAFS makes it possible to find the preferences for Cr, Fe and Ni, respectively, which is crucial for the understanding of these materials.

Expanded austenite does not represent a thermodynamically stable state and will decompose into nitrides or carbides provided that time and/or temperature allow diffusion of the substitutional elements, viz. Cr. This meta-stable state is established due to a strong affinity between nitrogen – and to a lesser extent carbon atoms – and chromium, which explains that large quantities of interstitials (N and C) can be dissolved. We will present the results from the as prepared nitrogen and carbon expanded austenites as well as from nitrides and carbides formed during controlled decomposition.

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Keywords: expanded austenite, carbides, nitrides, EXAFS, powder diffraction

MS74.P26

Acta Cryst. (2011) **A67**, C680

Crystal structure and non-linear properties of $\text{LaEr}(\text{MoO}_4)_3$

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Sm-Ho molybdates show the usual β' - $\text{Gd}_2(\text{MoO}_4)_3$ ferroelectric-ferroelastic structure [1]. In particular $\text{Gd}_2(\text{MoO}_4)_3$ has attracted attention since it has shown to be an efficient frequency doubling medium for laser diode pumping [2]. Also, it is of great interest for the synthesis of crystallized glasses consisting of this type of ferroelectric materials [3]. Recently a new interesting compound of this family: $\text{LaEr}(\text{MoO}_4)_3$ has been investigated by the processes of energy transfer NIR to visible (upconversion) [4]. $\text{LaEr}(\text{MoO}_4)_3$ has been prepared by the conventional solid-state synthesis, and X-ray powder diffraction has been collected using a PANalytical X'Pert Pro diffractometer at room temperature. $\text{LaEr}(\text{MoO}_4)_3$ features a distorted β' - $\text{Gd}_2(\text{MoO}_4)_3$ structure under normal conditions. In this work we have applied a new alternative way of treating distorted structures using a symmetry modes analysis [5] which gives us an input file to perform with FullProf [6] the Rietveld refinement of the amplitudes of such modes, instead of the atomic positions. This new procedure will let us discuss the distorted ferroelectric-ferroelastic structure in comparison with other member of this family of materials [7]. The distorted structure has thus been decomposed in three adapted symmetry-adapted modes from the paraelectric phase. Furthermore we have performed a theoretical analysis of these modes. Also of interest is the high luminescent efficiency under the IR excitation that $\text{La}_2(\text{MoO}_4)_3$ phosphors co-doped with Er^{3+} - Yb^{3+} feature [8]. We have thus analyzed the factors affecting the up-conversion fluorescent intensity by comparing different concentrations of Er^{3+} in matrices of $\text{La}_x\text{Er}_{2-x}(\text{MoO}_4)_3$ with different crystal structures: 1) β' - $\text{Gd}_2(\text{MoO}_4)_3$ structure-

type and 2) modulate scheelites. A two-photon excitation mechanism was proposed to explain the observed experimental results. Change of Er^{3+} symmetry, phase structure and/or concentration enhanced the upconversion emissions.

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Keywords: rare-earth molybdate, ferroic, non-linear matrix

MS74.P27

Acta Cryst. (2011) **A67**, C680

Characterization of MOFs by single crystal and powder X-Ray diffraction

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Metal Organic Framework (MOF) structures are well known for their many interesting applications, such as gas storage and separation, chemical sensing and catalysis [1]. The same structural properties that allow for such excellent chemical properties [2] cause difficulty in characterization by crystallographic methods. Owing to the highly porous nature of MOFs, crystalline samples tend to lose solvent rapidly, degrading the quality of diffraction. Additionally, a high degree of disorder over long ranges frustrates single crystal structure determination efforts. In order to characterize MOF samples, our lab has investigated the complementary techniques of single crystal and powder diffraction. Series of MOF complexes with similar framework structures but subtle chemical substitutions have been studied by single crystal X-ray diffraction and compared to powder X-ray diffraction patterns obtained using a single-crystal X-ray diffractometer equipped with a $\text{CuK}\alpha$ microsource. Powder samples have been run in capillaries with and without solution, and in nylon cryoloops in order to determine the most advantageous scenarios for data collection. Powder XRD patterns are then compared to single-crystal datasets (both observed and calculated intensities) to judge not only the composition of the bulk, but the diffraction produced (and often subsequently removed) by disordered solvents.

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Keywords: metal-organic, framework, PXRD