Poster Sessions

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Multiferroics have engendered increasing interest because of their many potential applications for micro- or nano-electronic devices, magnetic storage elements and interesting fundamental physics. The term "multiferroic" means coexistence of ferroelectric and magnetic ordering in a single phase or multiphase material. However, the two ordering parameters are mutually exclusive because ferroelectricity and magnetism require different filling states of the d-shells of transition metal ions. Empty d- shells mainly exist in ferroelectricity, while partially filled d-shells are required in magnetism. Therefore multiferroics are rare.

It exists several different microscopic mechanisms which may cause multiferroic behaviour. One of the most interesting is when a spontaneous polarization exists in a spiral or cycloidal magnetic structure. Accordingly, one strategy to find new multiferroic materials is to look for magnetic systems with that kind of magnetic structures.

The complex metal oxides $\rm Mn_3 TeO_6$ and $\rm Co_3 TeO_6$ have been prepared both as single crystals by chemical transport reaction and as polycrystalline powders by a solid state reaction route. The crystal structure and magnetic properties have been investigated using a combination of x-ray and neutron powder diffraction, electron microscopy, calorimetric and magnetic measurements. It has been shown that at room temperature $\rm Mn_3 TeO_6$ adopts a trigonal structure, space group R-3 (a= 8.8679(1)Å, c= 10.6727(2)Å) and $\rm Co_3 TeO_6$ the monoclinic spacegroup C 2/c (a=14.7830(2)A, b=8.8395(1)A, c=10.3426(2)A).

A long-range magnetically ordered state has been identified through variable temperature neutron diffraction and magnetic susceptibility measurements. The magnetic structure for the two compounds is very different. Mn₃TeO₆ has an incommensurate helix structure while Co₃TeO₆ shows a complicated but commensurate spin structure.

Keywords: neutron, ferroic, magnetism

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Thermal decomposition of ternary layered hydroxides

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Hydrotalcite are natural clays or synthetic defined as layered double hydroxides (LDH). These compounds exhibit various structural and chemical properties, besides having a high thermal stability, making them of great technological importance in obtaining new catalysts [1], [2].

Hydrotalcites samples containing Co, Mg and Al were subjected to increasing temperature in the range of 250-950 °C and measurements made X-ray diffraction in situ at Brazilian Synchrotron Light Laboratory (LNLS). The major changes occur between 250 and 400 °C, where the reflections of MgO begin to appear in X-ray diffraction (XRD) pattern. The XRD pattern reveals that the Mg-Al-Co hydrotalcite structure at 250 °C is not fully decomposed. It can be seen in relation to peaks in similar positions of the sample at room temperature, although only slightly wider and overlapped peak are observed. At temperatures above 400 °C the sample is completely decomposed and shows the disappearance of reflections at angles less than 30° indicating that the

structure of hydrotalcite collapsed during the calcination. In this stage occurs the formation of corresponding mixed oxides, a spinel mixture (MgAl₂O₄, Co₂MgO₄, Al₂MgO₄), and overlapping peaks of oxides as Co₃O₄. Between 400 and 600 °C, small variations are observed.

Calcination temperatures above 400 °C, occurs the Co^{2+} to Co^{3+} oxidizes forming phases Co_3O_4 , Co_2AlO_4 and $CoAl_2O_4$. All these compounds have cubic symmetry Fd-3m and it is not possible to distinguish one type of spinel phase from each other. At temperatures higher than 950 °C apparently is no longer observed any kind of modification.

A study was conducted to verify the regeneration capacity of the layered structure of hydroxides triple by simple exposure of the calcined material into the atmosphere where there is the presence of carbon dioxide and moisture. This material was characterized by X-ray diffraction. For this study, the calcined products performed at 800 °C and at 950 °C were calcined for one hour at each temperature. The samples were left in an inert atmosphere of nitrogen until the measurement of XRD was performed. Upon completion of the measurement, the samples were exposed to the atmospheric environment for 1 week and again performed the XRD measurements. It could prove the existence of two crystalline phases after calcination, attributed to a magnesium oxide and another characterized as spinel. The second phase is thermodynamically more stable and contributes to the broadening of diffraction peaks of the sample. The product of calcination showed a low-quality crystal, although there was a slight increase in the crystallinity of the material after exposure to the atmospheric. After exposure of the samples the air for one week there was no change in the diffraction pattern, indicating that calcination above 800 °C do not regenerate the layered structure of hydrotalcite therefore did not have the memory effect.

[1] E.L. Crepaldi, J. B. Valim, *Química Nova*, **1998**, *26*, 300-311. [2] R.E. Johnsen, F. Krumeich, P. Norby, *Journal of Applied Crystallography*, **2010**, *43*, 3, 434-447.

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The reordering transition in layer disordered solids: Rare earth-transition metal intermetallic.

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Planar faults are very frequently crystal defects. The quantification of this kind of defects has been the focus of attention since decades due to the fact that many alloys and compounds can be described as layer structures. The disruption of the periodicity in the stacking order leads to measurable effects in the profiles of the maxima of the diffraction pattern of a crystal. In this work, planar faulting is quantitatively studied beyond the model of independing faulting events [1], [2], [3] showing the strength of direct methods to extract defects information from the diffraction patterns [4], [5], [6]. The correlation length can be extracted from the diffraction data without need to assume the random faulting model by directly fitting the diffraction data. It is showed that the analysis of the decaying term of the probability correlation function, does not only allow quantifying the loss of memory in the system through the correlation length but also, the strength of interaction between faults. The behavior of the decaying terms turns