

**s3.m11.p11** **Topological order parameter in the magnetically modulated crystals.** Pawel Gusin, Jerzy Warczewski, University of Silesia, Institute of Physics, ul. Uniwersytecka 4, PL-40007 Katowice, Poland. E-mail: warcz@us.edu.pl

**Keywords: Magnetically modulated structures; Order parameter; Topological invariant**

Any magnetic ordering presents a modulation of a crystal structure. This modulation consists in that in the crystal containing magnetic ions there appears a periodic spatial distribution of the magnetic moments. It turns out that one can relate all the magnetic orderings to a certain order parameter which has properties of a topological invariant. Moreover, different special values of such an order parameter correspond to different types of the magnetic ordering. In the present paper all the magnetic orderings are considered as deformations of either ferromagnetic or antiferromagnetic ordering. Several examples of different types of the magnetic ordering are discussed using this approach.

A general hypothesis has been put forward that particular condensed matter systems (not only magnetic) can be distinguished by different values of certain topological invariants.

**s3.m11.p12** **Modulated phases in the LiCdVO<sub>4</sub>-LiCd<sub>4</sub>(VO<sub>4</sub>)<sub>3</sub> system. Relationships with the olivine-type structure.** Zúñiga F. J.<sup>a</sup> Ben Yahia A., Gaudin E.<sup>b</sup>, Darriet J.<sup>b</sup>, Schönleber A.<sup>a</sup> and Perez-Mato J. M.<sup>a</sup>, <sup>a</sup>Departamento de Física de la Materia Condensada, Facultad de Ciencias, Universidad del País Vasco, Apdo 644, 48080 Bilbao, Spain. <sup>b</sup> Institut de Chimie de la Matière Condensée de Bordeaux (I.C.M.C.B-CNRS) U.P.R. 9048., 87, Av Dr. Schweitzer, 33608 Pessac Cedex, France. Email: wmpzulaj@lg.eh.es

**Keywords: Modulated; Incommensurate; Batteries**

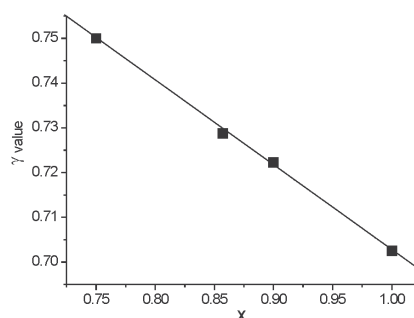
Olivine-type compounds are the subject of great interest as candidate materials for lithium-ion batteries since the discovery of insertion-deinsertion properties of lithium in LiFePO<sub>4</sub>[1]. The ideal formula unit of olivine-type compounds is AA'BO<sub>4</sub>. The structure can be described in terms of hexagonal stacking of closed packed O<sub>4</sub> layers with A, A' cations and B cations in two octahedral sites and one tetrahedral site, respectively.

A solid solution (1-x)LiCdVO<sub>4</sub> - xLi<sub>1/3</sub>Cd<sub>1/3</sub> 1/3CdVO<sub>4</sub> has been observed for 0 ≤ x ≤ 1. Two domains of the solid solution have been distinguished. The first one for 0 ≤ x ≤ 0.6 corresponds to the LiCdVO<sub>4</sub> sub-structure of the Na<sub>2</sub>CrO<sub>4</sub>-type [2]. For 0.7 ≤ x ≤ 1 satellites peaks are observed which correspond to a modulated structure.

LiCdVO<sub>4</sub> and LiCd<sub>4</sub>(VO<sub>4</sub>)<sub>3</sub> [3] are isostructural to Na<sub>2</sub>CrO<sub>4</sub> but in the case of the last compound some extra peaks have been observed in the diffraction pattern. LiCdVO<sub>4</sub> (x=0) crystallizes in Cmc<sub>2</sub>m space group with a=5.911, b = 8.975 and c=6.513 Å. In the structure the cadmium atoms occupy the octahedral site, lithium and vanadium atoms are in tetrahedral sites. The structures in the domain 0.7 ≤ x ≤ 1 have been solved for x= 3/6, 6/7 and 1. All these phases are modulated with an one-dimensional incommensurate **q**-vector **q** = γc\* and γ values of 0.75, 0.733 and 0.703 respectively. The superspace group is X<sub>m</sub>cm(10γ) where X stand for (1/2, 1/2, 0, 1/2) centring. A linear relation between the **q**-vector and the composition x has been evidenced (see figure).

According to the general formula Li<sub>1-2x/3</sub>Cd<sub>x/3</sub> 1/3CdVO<sub>4</sub> of the solid solution, the structures shows a different distribution of Li/Cd/ on the tetrahedral A-type position. The main result is a strong occupation modulation of lithium and cadmium in one tetrahedral site, which can be described by a crenel function. This occupancy modulation is associated to appears together with a displacive modulations.

These two types of modulation induce the incommensurability of the structure.



- [1] Pahdi, A. K., Nanjundaswamy K., S., and Goodenough, J. B. (1997) *J. Electrochem. Soc.*, **144**, 1188.
- [2] Niggli A., (1954). *Acta Cryst.*, **7**, 776.
- [3] Ben Amara, M., PhD thesis, (1979), Université de Bordeaux 1.