

MS17 P01**Premartensitic and martensitic transitions and crystallography in copper based shape memory alloys**Osman Adiguzel, *Firat University, Department of Physics 23169, Elazig/Turkey*. E-mail : oadiguzel@firat.edu.tr**Keywords: shape-memory effect, martensitic transition, layered structures**

Copper-based beta-phase alloys constitute a class of materials which exhibit shape memory effect within a certain range of composition. This effect in beta-phases of ternary alloys based on noble metal copper is evaluated by the structural changes in microscopic scale with a displacive transformation called martensitic transition which is first-order transformation, due to the metastable character and change their internal crystalline structures with changing temperature.

Beta phases of copper based alloys have the disordered bcc structure, (β)-phase, at high temperatures and undergo two types of ordered reactions called premartensitic transitions with cooling. The first transition is a first-nearest neighbour (nn) ordering reaction and results in a B2-type superlattice. However, bcc to DO₃ transition induces the next-nearest neighbour (nnn) ordering reaction.

The martensitic transition occurs from the B2(CsCl) or DO₃(Fe₃Al) type ordered structures to the layered structures on further cooling.

Martensitic transformations in these alloys occur in a few steps. In this kind of transformation, internal stress is effective and one of the steps is $\{110\} \rightarrow \{110\}$ type shear mode occurring on close-packed planes of matrix phase called basal plane of martensite.

Product martensite phase has the long period layered structures which consist of an array of close-packed planes with complicated stacking sequences called as 3R, 9R or 18R structures depending on the stacking sequences. It is determined that the basal plane of 9R (or 18R) martensites originates from one of the $\{110\}$ -planes of the parent, and a homogenous shear occurs on this plane in two opposite directions during the transformation.

Also, the basal plane is subjected to the hexagonal distortion with martensite formation on which atom sizes have important effect. In case the atoms occupying the lattice sites have the same size, the hexagon becomes regular hexagon otherwise

Otherwise deviations occur from the hexagonal arrangement. The knowledge of the associated distortion allows us to obtain information on the ordering degree in the martensite.

In the present contribution, x-ray diffraction and transmission electron microscopy (TEM) studies were carried out on two copper based ternary alloys aged for long term, nearly 20 years.

MS17 P02**New phase in the Na-Y-Mn-O system** Benabbas, A., Bounar, N., Bouremmad, F. and Rida, K. *L.I.M.E. Laboratory. University of Jijel. Algeria***Keywords: manganese compounds; powder diffraction; order-disorder.**

Manganese oxide and derived compounds have been of great interest since Wollan and Koehler's pioneering work on the magnetic order [1, 2]. Such materials exhibiting

particularly perovskite or ordered rock-salt structures have shown a great variety of physical properties and found applications in several fields such as cathodes in solid oxide fuel cells, catalysts, rechargeable batteries... The discovery one decade ago, of colossal magnetoresistance effects in the mixed valent manganites with the perovskite structure [3] has renewed interest for these compounds. Our investigation of the Na-Y-Mn-O system has allowed a new phase to be isolated. Its synthesis was carried out by solid state reaction and its structure was studied by X-ray powder diffraction. The crystal parameters were obtained by TREOR [4]. The structure has been resolved and refined by the Rietveld method [5] using RIETICA software [6]. The reflection's intensities were extracted from whole pattern decomposition according to Le Bail method. A part of atomic positions have been deduced from the Patterson function and the remaining positions by successive Fourier difference series. The crystal structure of this phase has common features with CsCl structure, it can be considered as a deficient supercell of the latter. The cationic order-disorder is considered. The coordination polyhedron and the mixed valence of manganese are important details of this structure.

[1] E. O. Wollan and W. C. Koehler, *Phys. Rev.* 100, 545 (1955).[2] W. C. Koehler and E.O. Wollan, *J. Phys. Chem. Solids* 2, 100 (1957).[3] R. von Helmolt, J. Wecker, B. Holzapfel, L. Schultz, and K. Samwer, *Phys. Rev. Lett.* 71, 2331 (1993).[4] P. -E Werner, L. Eriksson and M. Westdahl, *J. Appl. Cryst.* 18, 367 (1985).[5] H. M. Rietveld, *J. Appl. Cryst.* 2, 65 (1969).

[6] B. A. Hunter, "Rietica: A Visual Rietveld Program" in "Commission on Powder Diffraction Newsletter" Vol. 20, p. 21 (1998).

MS17 P03**Powder Neutron Diffraction and Ab Initio study of superionic LLTO perovskites** M. Catti, M. Sommariva, *Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, Italy*. E-mail: catti@mater.unimib.it**Keywords: superionic conductivity, powder neutron diffraction, ab-initio calculations**

LLTO ($\text{Li}_x\text{La}_{2/3-x/3}\text{TiO}_3$) is one of the materials with the highest lithium ion electrical conductivity (about $10^{-3} \text{ S cm}^{-1}$ for $x=0.3$) at room temperature, of interest as solid electrolyte or cathode in lithium batteries [1-3]. Structural studies of the $x=0.3$ term were performed by TOF neutron powder diffraction (ISIS Facility, R.A.L., UK, HRPD instrument) on samples with different thermal history, i.e. naturally cooled from 1300 °C and quenched into liquid N₂. Tetragonal perovskite superstructures with $\sim\sqrt{2}a_p \times \sqrt{2}a_p \times 2a_p$ unit-cells ($a_p \sim 3.87 \text{ \AA}$ for cubic perovskite; $Z=4$) were demonstrated, on the basis of a detailed analysis of superlattice Bragg peaks. By Rietveld refinements in the $P4/nbm$ (unquenched) and $I4/mcm$ (quenched sample) space groups, the main findings were: anti-phase octahedral tilting a^0a^0c , partial La-Li ordering in two independent (001) layers for the unquenched sample, and lithium atoms located in two distinct disordered sites with fourfold oxygen coordination within the A-type dodecahedral cage of ABO₃ perovskite. The short Li-Li' distances account for the high ionic mobility and suggest a mainly (001) two-dimensional mechanism of ion hopping among Li sites. Further, a number of phase