

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.

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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

transitions were detected at high temperature, with removal of superlattice peaks and symmetry increase. An *ab initio* periodic quantum-mechanical simulation of possible locally ordered structures was then performed, by use of the B3LYP hybrid functional and of an all-electron basis set of atomic orbitals [4]. The two compositions $\text{Li}_{0.5}\text{La}_{0.5}\text{TiO}_3$ and $\text{Li}_{0.3125}\text{La}_{0.5625}\text{TiO}_3$ were considered, with 4 to 16 formula-units of LLTO per primitive unit-cell, and with symmetry lowered to monoclinic *Pm*. Several different La-Li ordering patterns within the (001) layers of A-cages were devised. The structures were fully optimized by energy minimization, so as to localize the preferred lithium sites for each ordering scheme. Maps of the electrostatic potential were also computed in ionized Li-free model structures, in order to study the electric field acting on Li^+ ions. It was found that the anti-phase octahedral tilt is reproduced only for layers with mixed La-Li composition, and not for full La-Li ordering in different layers. Further, the positions adopted by lithium depend significantly on the locally ordered environment, so that the two sites appearing in the experimental average structure can be assigned to specific ordered configurations on the basis of the theoretical results obtained. The most populated Li site, close to the O_4 windows separating adjacent A cavities in the layer, corresponds to La-poor local configurations, and is actively involved in the ion migration process. The other one, closer to the cage centre, is related to La-rich local environments, and is a trapping location less favourable to the transport mechanism.

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MS17 P04

Structural and crystallographic characterization of compacted and induction melted Cu-Al alloys Yacine Debili, Kebkache Ismahane University Annaba, BP 12 eL-HADJAR, 23000, Annaba, Algeria
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Keyword : Cu-Al alloys ,Cu₉Al₄, Hume-Rothery phase

We have elaborated several copper based (Cu-Al) alloys with various aluminum compositions (25.2, 25.85, 26.02, 26.50, and 26.86 % at. Al) by fusion melting after cold compaction of Al and Cu powder, and we have been interested by structural and crystallographic characterization which permits us to identify the intermetallic compounds appearing during solidification as AlCu phase (monoclinic), Cu₉Al₄ phase (Sc) and Cu₃Al phase (Orthorhombic).

Cu₉Al₄ is an electronic compound belonging to Hume-Rothery phase. The $\alpha(\text{Cu})$ lattice parameter decrease in an anomalous way as deviation from Vegard's law with Al content between (25.20%at. Al and 26.86%at. Al)

MS17 P05

The microstructure of low-aqueous liquid detergents by X-ray diffraction Ruud den Adel^a, Eli Roijers^a, John

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Keywords: low-aqueous liquid detergents, microstructure, X-ray diffraction

To build up knowledge about the phase behaviour and microstructure of liquid detergents, different compositions are measured using the ternary phase diagram with axes water, solvent and surfactants percentages. In this ternary phase diagram the liquid crystalline (LC) and an isotropic area can be distinguished. The phase diagram is determined by classical light microscopy, using polarised light. The liquid crystalline phase scatters light and has an appearance in the range of milky to translucent. The isotropic phase is transparent. Of interest is the region up to 5% water.

The X-ray powder diffraction measurements are performed on the Bruker D8-Discover in a theta/theta configuration. A copper anode is used, and the K- α radiation with wavelength 0.15418 nm is selected. Long spacings are measured by performing X-ray diffraction in the transmission mode. The X-ray source and the detector are positioned in front of each other (Theta1 and Theta2 = 0 degrees). To prevent the detector being hit by the primary beam a leaden beam stopper is precisely positioned in the middle and just in front of the detector. The sample is placed in a sample holder between Mylar film.

In this ternary phase diagram the following sets of samples are described:

- Along the water axis
- Along the organic solvent axis
- 80% surfactants along the water-solvent axis
- 60% surfactants along the water-solvent axis
- 40% surfactants along the water-solvent axis
- Along the line from 100% surfactants to 50%water/50%solvent

It is found that the concentrated surfactants system shows an order of surfactant molecules in the reversed micellar L2-phase and the swelling of the surfactant mixtures is dominated by water. On increasing the water level the layer thickness increases and the disorder of the surfactant molecules decreases.

On increasing the organic solvent level the layer thickness remains constant, the disorder of the surfactant molecules increases and/or the domain sizes decreases.

The transition from the lamellar liquid crystalline into the isotropic phase is a gradual change in microstructure.

MS17 P06

Structure Prediction-versus-Determination of B-site Doped La-Sr-Mn Perovskite A. A. Ramadan^(a), M. El-Hagry^(a), A. M. Moustafa^(b), Y. A. Shoker^(a) and A. M. El-Shabiny^(b) ^(a) Phys. Dept., Helwan Univ., Helwan, Cairo, Egypt. ^(b) Phys. Dept., National Research Center, Dokki, Cairo, Egypt

Keywords: Ab-initio powder structure determination, Prediction, Perovskite structures.

Ab-initio crystal structure determination from X-ray powder diffraction data suffers from limitations and is associated with intrinsic challenges. However, in recent years there has been substantial progress in this approach. The crystal structure of Cu-doped $\text{La}_{0.7}\text{Sr}_{0.3}\text{Mn}_{1-x}\text{Cu}_x\text{O}_3$ ($x = 0.0, 0.1$ and 0.2) perovskite was predicted starting only