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 $Li_{0.5}La_{0.5}TiO_3$ and $Li_{0.3125}La_{0.5625}\square_{0.125}TiO_3$ 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, Kebbache 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), Cu_9Al_4 phase (Sc) and Cu_3Al phase (Orthorhombic).
Cu_9Al_4 is an electronic compound belonging to Hume-Rothery phase.The α(Cu) lattice parameter decrease in an anomalous way as deviation from vegard's low 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 van de Pas [a] [a]*Unilever Research R&D, Vlaardingen, The Netherlands.* E-mail: ruud-den.adel@unilever.com

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 transparant. 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- alpha 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:
a.) Along the water axis
b.) Along the organic solvent axis
c.) 80% surfactants along the water-solvent axis
d.) 60% surfactants along the water-solvent axis
e.) 40% surfactants along the water-solvent axis
f.) 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-Determenation 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*

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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 interinsic challenges. However, in recent years there has been substantial progress in this approach. The crystal structure of Cu-doped $La_{0.7}Sr_{0.3}Mn_{1-x}Cu_xO_3$ (x = 0.0, 0.1 and 0.2) peroveskite was predicted starting only