MS37-O5 Diffraction Studies on Displacive Transitions in Copper Based Shape Memory Alloys. Osman Adiguzel, *Firat University, Department of Physics, 23169 Elazig-Turkey*,
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Shape memory effect is an unusually property exhibited by certain alloy systems, and shape memory behaviour is evaluated on the basis of structural changes on unit cell level. Sshape memory effect is based on a displacive transition, martensitic transformation, which causes to the changes in internal crystalline structure of materials. Copper based alloys exhibit this property in metastable β-phase region. These alloys transform martensitically from the high symmetry ordered structures to the low symmetry layered structures on cooling from high temperatures.

Martensitic transformations occur in a few steps with the cooperative movement of atoms less than interatomic distances by means of lattice invariant shears on a {110}-type plane of austenite matrix which is basal plane of martensite. Product phase in this transition has the unusual layered structures which consist of an array of close-packed planes with complicated stacking sequences called as 3R, 9R or 18R martensites depending on the stacking sequences on {110}-type planes of parent phase.

X-ray diffraction and electron diffraction studies were carried out on two copper based ternary alloys, CuZnAl and CuAlMn, at room temperature. Transformation temperatures of both alloys are over the room temperature, and both alloys are fully martensitic at room temperature. X-ray powder diffractograms and electron diffraction patterns exhibit super lattice reflection. An x-ray powder diiffractogram taken from Cu-11%Al-6%Mn (in weight) alloy sample is shown in Figure 1. These studies reveal that both alloys have unusual layered structure in martensitic condition.

X-ray powder diffraction profiles have been taken several times after post-quench heat treatments. These profiles reveal that peak locations and intensities of some diffracted planes change with ageing, and one can say that these changes lead to the rearrangement of atoms in crystal lattice of the materias. The {110} - type planes of parent phase turn into hexagon with martensitic transition, and atom sizes have important effect.

The basal plane becomes ideal hexagon in the disordered case taking the atom sizes approximately equal, and deviations occur from the hexagonal arrangement in the ordered case. Different between the interplane distances of some plane pairs providing a special relation between miller indices changes with ageing, and this change leads to disordering in martensite. The knowledge of deviation allows us to obtain information on the ordering degree of material crystal in the martensitic state.

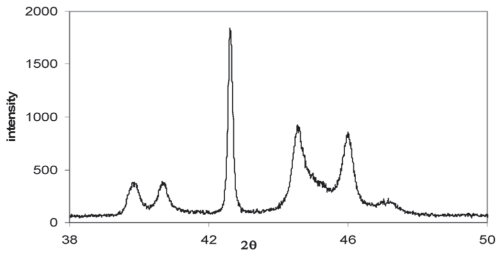

Figure 1. An x-ray powder diiffractogram taken from Cu-Al-Mn alloy sample.

Keywords: Shape memory effect, martensite, layered structures, atom sizes.

MS38-O1 Different approaches to solving&refining inorganic structures from electron diffraction. Joke Hadermann,[a] Senne Van Rompaey,[a] Artem M. Abakumov,[a]
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Knowledge of the structure of materials is important to be able to control their properties. There are different situations where the precise determination of the structure using the commonly applied techniques of X-ray and/or neutron powder diffraction (XRD/NPD) can encounter problems. Examples are when the material has the form of nanoparticles, if defects occur which cause broadening of the peaks, if modulations occur of which the reflections are not clearly distinguishable from the noise. In such cases precession electron diffraction (PED) is a useful alternative for the structure determination and refinement. Also, when compared to other transmission electron microscopy techniques, PED, and electron diffraction in general, has specific advantages: several classes of interesting emerging materials are unstable under the intense beam needed for TEM imaging (for instance, Li based battery materials, hydrogen storage materials, etc.). However, electron diffraction patterns can be taken at a very low incoming electron dose, reducing the risk of destroying the material. In this lecture, first, the structure solution and refinement from PED data of several powder materials will be demonstrated. The materials exemplify different combinations of heavy/light scatterers and different stabilities towards electron beam irradiation. Among the examples used are complex perovskite based materials with ordered anion and cation patterns [1], Ruddlesden-Popper structures with intergrowths of perovskite slabs of different thickness, incommensurately modulated materials, light hydrides and lithium based battery materials [2] that are sensitive to the electron beam and of which the positions of the light elements (Li, H,...) are hard to reliably determine. It will be shown that in each of these cases the structure could be succesfully solved and refined when being resourceful enough pertaining the methods that are used. Therefore, these examples will be used to point out several methods of structure solution and refinement that are helpful to treat PED data and greatly expand the range of materials PED can be useful for. The methods include a global optimisation with Monte Carlo simulations, the rigid body approach, difference Fourier maps, phase analysis from ring patterns and symmetry mode analysis.

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Keywords: precession; structure refinement; transmission electron microscopy