Shape memory alloys like NiTi (*nitinol*) show a large field of applications, i.g. as flexible glass frames, surgical instruments or as actuators in robotic systems. The shape memory effect is based on the crystallographic phase transition of monoclinic martensite to cubic austenite. In this study NiTi wire [1] were investigated by neutron diffraction using the E9 fine resolution powder diffractometer at the BERII research reactor.

The investigations showed the martensite-austenite phase transition taking place over a broad temperature range depending on the composition and thermal history of the alloy. The starting room temperature neutron diffractogram shows monoclinic phase (martensite) reported in [2]. When heated for first time a phase transition to cubic austenite [3] starts around 300°C and is finishes at 400°C. After further heating to 600°C and adjacent cooling down to room temperature a two-phase mixture was observed (martensite/austenite) showing the thermal memory effect when heated up to 70°C by forming again pure cubic austenite. Obviously the shape memory effect works independently from the phase purity and moreover works just with phase mixtures. The contribution will show all results in detail and give a brief overview into the functioning of shape memory alloy.

[1] Vendor: Memory-metalle.de. [2] Cuevas, F at al., Journal of Solid State Chemistry (2006) 179, 3295-3307. [3] Parlinski, K.; Parlinska-Wojtan, M., Physical Review, Serie 3. B – Cond. Matter (2002) 66, 064307-1-064307-8

Keywords: shape memory, phase tranition, nitinol

FA2-MS13-P13

Structural study by X-ray profile analysis and thermodynamics properties of Cu-Cr and Cu-Mo alloys processed by mechanical alloying. Claudio Aguilar[a], Paula Roja[b], Stella Ordoñez[c], Danny Guzman[d] [a]*Instituto de Materiales y Procesos Termomecánicos, Universidad Austral de Chile, Chile,* [b]*Escuela de Ingeniería Mecánica, Pontificia Universidad Católica de Valpaíso,* [c]*Departamento de Ingeniería Metalurgía, Universidad de Santiago de Chile,* [d]*Departamento de Metalurgia, Universidad de Atacama*
E-mail: ceaguilar@uach.cl

Technologically, it is interesting to pursue the development of novel high performance materials obtained using a non-equilibrium process, such as mechanical alloying (MA), Today, attention has been concentrated on synthesis of high performance materials such as intermetallics, amorphous metallic alloys and nanocrystalline materials (NCM) [1] The alloys were synthesized using Cu-5 and 8 wt.% Cr and Cu- 5 and 8 % Mo. The mixtures were placed in a stainless steel container with a 25 ml capacity and milled in a SPEX 8000D mill under an argon atmosphere between 0.5 and 50 h. The alloys were characterized by scanning and transmission electron microscopy- SEM and TEM, x-ray diffraction- XRD, Vickers microhardness- HV and differential scanning calorimetry- DSC. X-ray profile analysis was made using the modified Warren–Averbach and Williamson-Hall methods [2].

The grain size decreased as the milling time increased to values around 10 nm, the dislocation density increased until values of $1x10^{12}$ m/m^3. Stacking fault energy decreased in the Cu-Cr system until 20 mJ/m^2 and in the Cu-Cr until 10 mJ/m^2 and stacking fault probability increased to 10^{-2} and 10^{-3}, for both systems respectively. The higher HV values were measured for Cu-Mo alloys for all milling times. The typical values at 50 h of milling were around 280 HV. All alloys presented anisotropic strain, which was better interpreted applying modified Warren-Averbach and Williamson-Hall methods. These results show that anisotropic strain is caused by presence of dislocations in both systems. Due to the disappearance of peaks of Cr and Mo, decrease and increase of lattice parameter of Cu-Cr and Cu-Mo, respectively, and decrease of stacking fault energy, confirm the formation of solid solution in both systems, which are immiscible with a positive enthalpy mixing.

The extension of solid solution was modeled using a regular solution model. The increment of free energy due to the presence of crystalline defects was estimated, for the crystalline defects increasing the free energy, and free curves are moved upwards, hence the solubility limit changes. For Cu-Cr system it was that free energy increase until reach values around 8 kJ/mol and for Cu-Mo system until 10 kJ/mol when milling time increase. These values are higher than the mixing free energy of the solution determined using a regular solution model. These results confirm the formation of solid solution of both systems.

[1] Suryanarayana C., Non-Equilibrium Processing of Materials, first ed., Pergamon, New York, 1999.
[2] Ungár T., Gubicza J., Ribárik G., Borbély A., J. Appl. Cryst. 34 (2001) 298.

Keywords: X-ray diffraction and structure, Thermodynamics, Crystalline defects

FA2-MS13-P15

The crystal structure of FeAl₂. Ihor Chumak[a], Klaus W. Richter[b], Helmut Ehrenberg[a]. [a]*Institute for Complex Materials, IFW Dresden, Germany.* [b]*Department of Inorganic Chemistry/Materials Chemistry, University of Vienna, Austria.*
E-mail: i.chumak@ifw-dresden.de

The crystal structure of $FeAl_2$ was described first by Corbz and Black [1]. The authors solved the structure by use of the anomalous dispersion technique in a trigonal model with 18 atoms per unit cell: space group *P1* (№ 1), Pearson symbol *aP18*, a = 4.878(1) Å, b = 6.461(2) Å, c = 8.800(3) Å, α = 91.75(5) °, β = 73.27(5) °, γ = 96.89(3) °. Our X-ray single crystal investigations confirm the trigonal structure (a = 4.875(1) Å, b = 6.455(1) Å, c = 8.736(1) Å, α = 87.93(1) °, β = 74.40(1) °, γ = 83.06(1) °), but with one additional atom per unit cell (Pearson symbol *aP19*) and space group *P-1* (№ 2). The $FeAl_2$ structure derives from the orthorhombic YPd_2Si structure (ordered Fe_3C type, space group *Pnma* (№ 62), Pearson symbol *oP16*, a = 7.303(2) Å, b = 6.918(2) Å, c = 5.489(1) Å) [2] by including 3 additional atoms per unit cell and strong deformation. Both structures can be represented as an arrangement of the trigonal prisms, with noticeable distortions in the case of $FeAl_2$.

[1] Corby R. N., Black P.J., *Acta Cryst.,* 1973, B29, 2669. [2] Moreau J.M., le Roy J., Paccard D., *Acta Cryst.,* 1982, B38, 2446.

Keywords: X-ray structure determination, aluminium alloys, crystal chemistry of alloys.