Semester report
by **Pham Tran Hung**
PhD Program: Materials science
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PhD Thesis title: Lattice defects and mechanical properties of novel multicomponent materials

Introduction:

One of the most important tasks of materials science is the development of new materials with advanced functional performances. In last decades, several novel multicomponent materials have been developed with prominent properties, and one of such materials is multi-principal element alloys (MPEAs), including high-entropy alloys (HEAs), which exhibit high strength, good conductivity, as well as excellent corrosion resistance and thermal stability. Additionally, plastic properties of MPEAs can be improved by an appropriate selection of lattice defect structure. This can be realized by severe plastic deformation (SPD) or thermal treatments. In the frame of the planned project we will study the correlation between the lattice defect structure (grain boundaries, planar faults and dislocations) and the mechanical performance of MPEAs. Our main goal for all the studied materials is to recognize the influence of the type and density of lattice defects on the mechanical properties which are important from the point of view of practical applications. Additionally, we investigate the relationship between the processing conditions and the lattice defect structure of novel multicomponent materials. Moreover, the thermal stability of the defect structure and phase composition of the multicomponent materials is also studied.

Summary of research work carried out in the previous three semesters:

The specimens are provided by international partners. The materials studied are CoCrFeNi and HfNbTiZr with equal elemental ratios, and underwent a SPD process by high-pressure torsion (HPT) up to 10 HPT turns. This results in samples with different shear strains, depending on the number of HPT turns, as well as the position from the axis of applied torsion. The samples are investigated with X-ray line profile analysis (XLPA) for characterization of crystallite sizes, dislocations and planar faults. Moreover, the thermal stability of the microstructures is examined using differential scanning calorimetry (DSC) up to 1000 K. From the results of the DSC, the characteristic temperatures were selected, to which the HPT samples were annealed for further investigations. For both CoCrFeNi and HfNbTiZr, the phase analysis was carried out using X-ray diffraction (XRD). The microstructure was studied using Convolutional Multiple Whole Profile (CMWP) method. In this method, the XRD pattern is fitted by theoretical functions, providing a quantitative characterization of crystallite size distribution, dislocations and planar faults, even when there are multiple phases. Furthermore, transmission electron microscopy (TEM) was also utilized in order to obtain direct observation of the microstructures, as well as obtaining the compositions of the chemical elements. The hardness was measured using nano-indentation test. Only the samples with highest strain has been studied, which are the periphery of the disk processed by 10 HPT turns for both CoCrFeNi and HfNbTiZr. For CoCrFeNi, the characteristic temperatures in the DSC thermogram were 500, 750 and 1000 K. It was found that the sample persisted as a single fcc phase material throughout the heat treatment. For HfNbTiZr, the characteristic temperatures were 740, 890 and 1000 K. It was revealed that while the material has a single bcc phase at room temperature, the microstructure decomposes into three different phases at high temperatures. Moreover, other MPEA compositions processed by HPT were also investigated ($Fe_{40}Mn_{40}Co_{10}Cr_{10}$, $Fe_{35}Mn_{35}Co_{10}Cr_{10}Ni_{10}$, and $Co_{33}Ni_{33}Cr_{19}Mn_{15}$ processed).

In addition to my PhD topic, several other materials provided by our international partners were also studied using XLPA. Cu nano foams synthesized under various conditions and annealed to different temperatures were examined as a potential candidate for anode of lithium ion batteries. Their microstructures were also inspected using electron microscopy. Other materials that were also analyzed are series of Mg alloys (AZ80 and AZ80-SiC), Ti processed by rotational constrained bending (RCB), and CuZr and TiMo alloys processed by free bending.

Description of research work in current semester:

The evolution of microstructures and hardness during annealing of CoCrFeNi and HfNbTiZr MPEAs processed by HPT at the saturated strain were studied in the previous semester. In this semester, the continuation of previous works was conducted, and the study expands to materials at various equivalent strains. Moreover, synchrotron X-ray radiation was utilized in order to investigate the microstructure across the depth of the HPT disks.

The investigation of Cu nanofoams with more synthesis conditions and heat treatment processes was also carried out. An overview of previous and new results was published.

Conference in current semester:

1. Pham Tran Hung, Megumi Kawasaki, Jae-Kyung Han, János Lábár and Jenő Gubicza*"Thermal stability of microstructure and hardness of multi-principal element alloys by severe plastic deformation"*. The presentation was given at the Materials Research Society spring conference (2021).
2. Pham Tran Hung, Péter Jenei, Csilla Kádár, Gigap Han, Heeman Choe and Jenő Gubicza "*Influence of Pack Cementation Time and Annealing on Microstructure of Cu Nanofoams processed by Dealloying"*. The presentation was given at the Materials Research Society spring conference (2021).

Publications:

1. J. Gubicza, P. Jenei, G. Han, P.T. Hung, Y. Song, D. Park, Á. Szabó, Cs. Kádár, J-H. Kim, H. Choe, Effect of heat treatment on the microstructure and performance of Cu nanofoams processed by dealloying: an overview, Materials 14 (2021) 2691.
2. T. Krajňák, M. Janecek, P. Minárik, J. Gubicza, P.T. Hung, F. Novy, A.G. Raab, G.I. Raab, R. Asfandiyarov: Microstructure evolution in Cu – 0.5 wt% Zr alloy processed by a novel severe plastic deformation technique of rotational constrained bending, Metals 11 (2021) 63.
3. T. Krajňák, M. Janecek, P. Minárik, J. Vesely, P. Cejpek, J. Gubicza, P.T. Hung, D. Preisler, F. Novy, A.G. Raab, G.I. Raab, R. Asfandiyarov: Microstructure evolution and mechanical properties of cp-Ti processed by a novel technique of rotational constrained bending, Metall. Mater. Trans. A 52 (2021) 1665-1678.
4. P.T. Hung, M. Kawasaki, J.K. Han, J.L. Lábár, J. Gubicza: Microstructure evolution in a nanocrystalline CoCrFeNi multi-principal element alloy during annealing, Materials Characterization 171 (2021) 110807.

5. P.T. Hung, M. Kawasaki, J.K. Han, J.L. Lábár, J. Gubicza: Thermal stability of a nanocrystalline HfNbTiZr multi-principal element alloy processed by high-pressure torsion, Materials Characterization 168 (2020) 110550.
6. P. Jenei, G. Han, P.T. Hung, H. Choe, J. Gubicza: Influence of pack cementation time on the microstructure of Cu nanofoams processed by dealloying, IOP Conf. Ser.: Mater. Sci. Eng. 903 (2020) 01204.
7. P. Jenei, Cs. Kádár, G. Han, P.T. Hung, H. Choe' J. Gubicza: Annealing-Induced Changes in the Microstructure and Mechanical Response of a Cu Nanofoam Processed by Dealloying, Metals 10 (2020) 1128.
8. A.K. Chandan, P.T. Hung, K. Kishore, M. Kawasaki, J. Chakraborty, J. Gubicza: On prominent TRIP effect and non-basal slip in a TWIP high entropy alloy during high-pressure torsion processing, Materials Characterization (2021) submitted.

Studies in current semester:

Subject code	Subject name	Lecturer	Credits	Requirements	Class per week (T/P/L)	Grades
FIZ/3/015E	Carbon Nanostructures	Kürti Jenő Dr.	6	exam	2/0/0	Excellent