XXII International Seminar on Physics and Chemistry of Solids (eISPCS'20)
June 17-19, Lviv, Ukraine

STRUCTURAL AND MICROSTRUCTURE OF Al-BASED HIGH-ENTROPY ALLOYS WITH TRANSITION ELEMENTS

M. Dufanets, Yu. Plevachuk, V. Sklyarchuk

Ivan Franko National University of Lviv, Department of Metal Physics,
Kyryla i Mefodiya St. 8, 79005 Lviv, Ukraine

- CONVENTIONAL alloys are mainly based on one principal element with different kinds of alloying elements added to improve their properties
- any multi-component alloy consisting of 5 or more principal elements, which have a concentration between 5 and 35 at. pct, belongs to the HEA family
- these alloys have significantly higher mixing entropies, which lead to the formation of liquid or random solid solution states
- Due to the unique multi-principal element composition, HEAs possess extraordinary properties:

- **high strength/hardness,**
- **outstanding wear resistance,**
- **exceptional high-temperature strength,**
- **good structural stability,**
- **good corrosion and oxidation resistance.**

Phase formation processes in equiatomic AlCoCuFeNiCr high entropy alloys have been studied by means of XRD, microstructure analysis and microhardness measurements.

Experimental Details

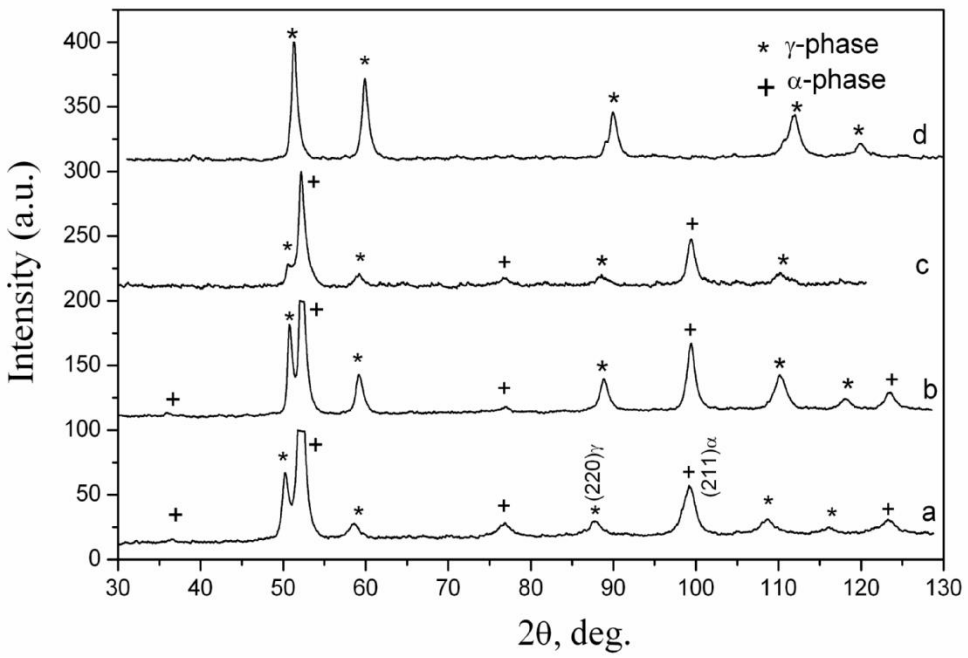
Samples of HEA under investigation with concentration, corresponding to AlCoCuFe (**1**), AlCoCuFeNi (**2**), AlCoCuFeNiCr (**3**) and CoCuFeNiCr (**4**) stoichiometry and mass of 25 g have been obtained by arc melting method in argon atmosphere.

XRD studies have been carried out by means of DRON-3 diffractometer (Co-K_α –radiation, graphite monochromator, installed in diffracted beam).

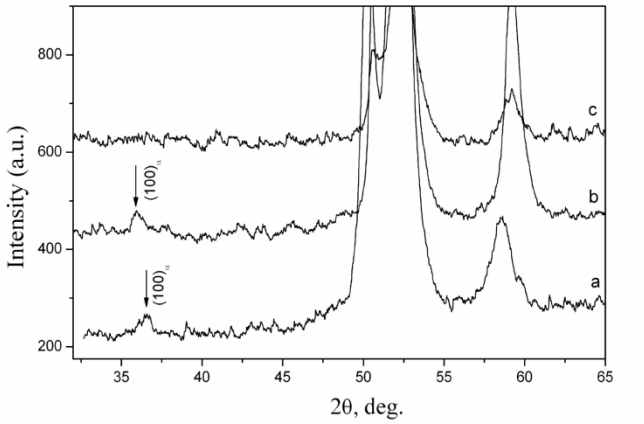
Table 1 Structural – phase and chemical composition of HEA

№	Alloy	Chemical composition, at.%						Phase	a, Å	ε, %
		Al	Ni	Co	Cu	Fe	Cr			
1	**AlCoCuFe**	**10.6**	**-**	**5.6**	**78.9**	**4.9**	**-**	**FCC**	**3.6525**	**0.20**
		20.0	**-**	**34.3**	**13.8**	**31.9**	**-**	**BCC**	**2.8790**	**0.24**
2	**AlCoCuFeNi**	**9.2**	**19.9**	**18.2**	**36.5**	**16.2**	**-**	**FCC**	**3.6195**	**0.12**
		13.5	**22.8**	**23.9**	**17.6**	**22.2**	**-**	**BCC**	**2.8739**	**0.07**
3	**AlCoCuFeNiCr**	**10.0**	**13.3**	**5.4**	**62.9**	**5.0**	**3.4**	**FCC**	**3.6232**	**0.20**
		12.4	**19.4**	**19.1**	**19.6**	**17.4**	**12.0**	**BCC**	**2.8741**	**0.02**
4	**CoCuFeNiCr**	**-**	**11.0**	**3.3**	**78.7**	**3.8**	**3.1**	**FCC (γ_1)**	**3.6085**	**-**
		-	**21.0**	**23.9**	**9.7**	**22.0**	**23.4**	**FCC (γ_2)**	**3.5824**	**0.04**

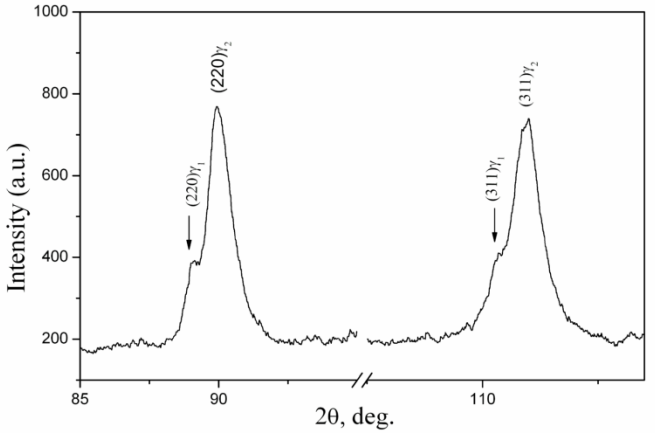
Results



X-ray diffraction patterns of high entropy alloys. a – AlCoCuFe, b – AlCoCuFeNi, c – AlCoCuFeNiCr, d – CoCuFeNiCr

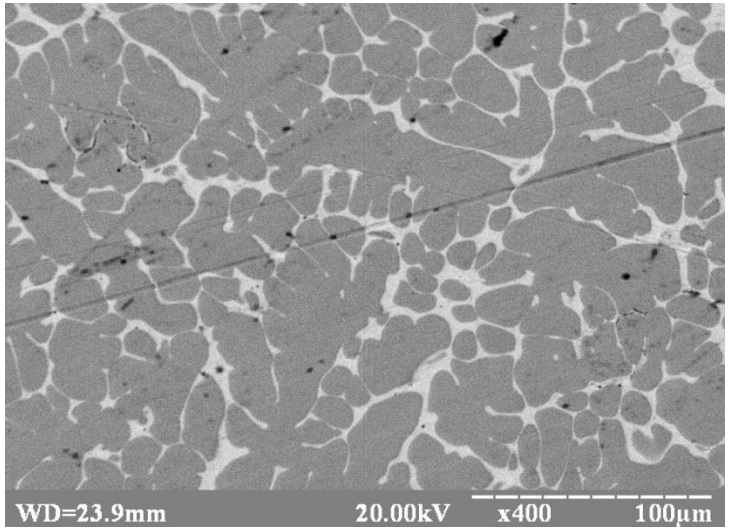


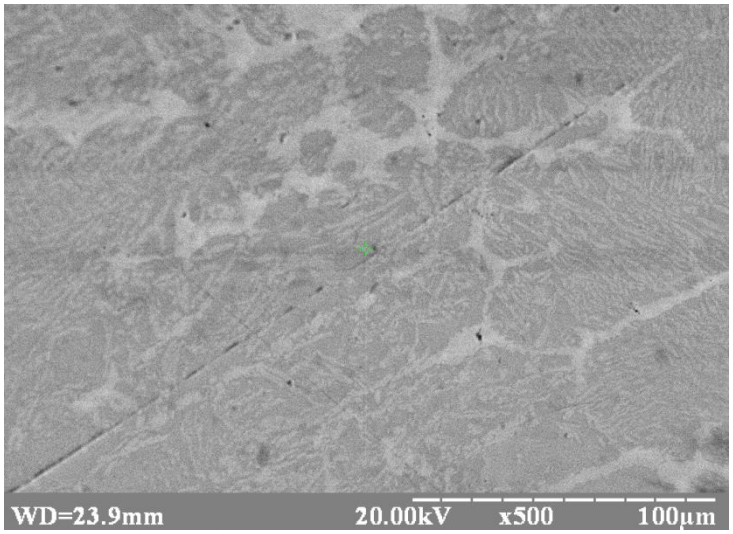
Diffraction patterns fragment alloys: a – AlCoCuFe, b – AlCoCuFeNi, c – AlCoCuFeNiCr

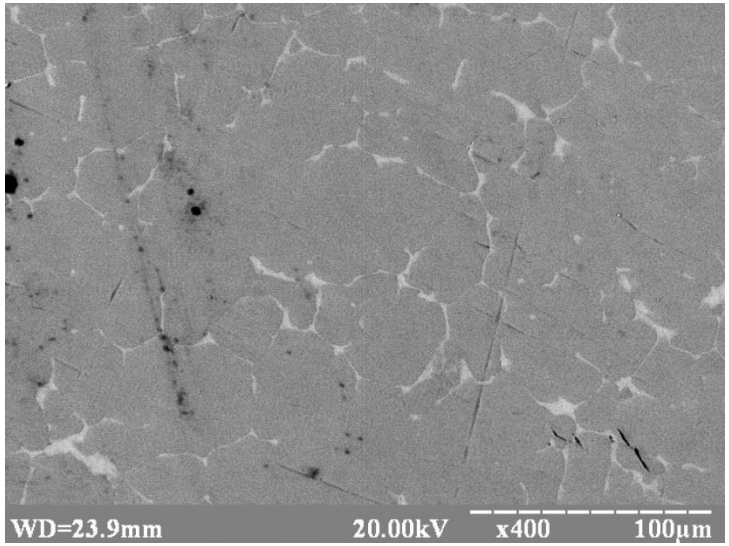


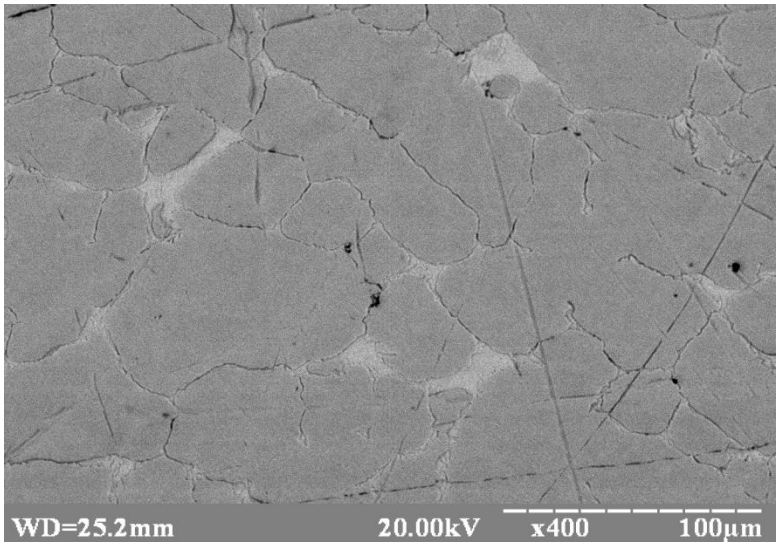
Diffraction pattern fragment alloy CoCuFeNiCr

Results









Microscopic image of high entropy alloys. a – AlCoCuFe, b – AlCoCuFeNi, c – AlCoCuFeNiCr, d – CoCuFeNiCr.

Results

Table 2 Thermodynamic, structural and mechanical characteristics of HEA of nominal composition

№	Alloy	ΔS, J/ K·mol	ΔH, kJ/mol	T_L, .K	Ω	δ, %	H_μ, GPa
1	AlCoCuFe	11.52	-3.25	1466	5.2	5.59	**5.45**
2	AlCoCuFeNi	13.34	-5.28	1518	3.8	5.44	**4.56**
3	AlCoCuFeNiCr	14.86	-5.62	1631	4.3	5.02	**5.93**
4	**CoCuFeNiCr**	**13.34**	**+1.92**	**1767**	**12.3**	**1.12**	**2.74**

Table 3 The enthalpy of mixing of binary alloys ΔH_{AB} (kJ/mol)

Element	Al	Co	Cu	Fe	Ni	Cr
Al		-19	-1	-11	-22	**-10**
Co			+6	-2	0	**-4**
Cu				+13	+4	**+12**
Fe					-2	**-1**
Ni						**-7**

Results

Table 4 Thermodynamic and structural characteristics of the phase constituent HEA

№	Alloy	Phase, type	ΔH, kJ/mol	Ω	T_L, K	δ, %	X, %
1	AlCoCuFe	BCC (B2)	-5.14	3.33	1557	5.13	**77.1**
		FCC (A1)	+2.04	4.04	1354	3.65	**22.9**
2	AlCoCuFeNi	BCC (B2)	-3.51	5.94	1579	4.76	**66.1**
		FCC (A1)	+1.77	10.92	1537	3.97	**33.9**
3	AlCoCuFeNiCr	BCC (B1)	-5.46	4.59	1695	4.53	**82.9**
		FCC (A1)	+1.72	8.42	1434	3.78	**17.1**
4	**CoCuFeNiCr**	$FCC_{\gamma 1}$ (A1)	-0.70	33.9	1825	1.03	**71.4**
		$FCC_{\gamma 2}$ (A1)	**+3.80**	**2.46**	**1450**	**0.86**	**28.6**

Conclusions

1. In correspondence to thermodynamic and structural criteria and based on X-ray phase and microstructure analysis it is shown that a structure of the equiatomic high entropy Al-Co-Cu-Fe-Ni-Cr alloys has two-phase behavior and contains solid solutions with BCC (B1 or B2 structure types) FCC-lattice (A1 structure type).

2. Addition of Al promotes the formation of BCC-phase. Besides, in alloys with higher content of Al the ordering and appearing of superstructure of B2 type is observed. Decreasing of the Al content leads to transition to disordered solid solution (B2→B1).

3. Initial BCC-phase reveals the dendrite morphology and is enriched with transition elements, whereas Cu-enriched BCC-solution deposits in the interdendrite space.

4. The significant variations of microhardness versus volume fraction of phase components and its correlation with thermodynamic characteristics are revealed.