Formation of metal nanoclusters in Al-based high-entropy alloys with transition elements

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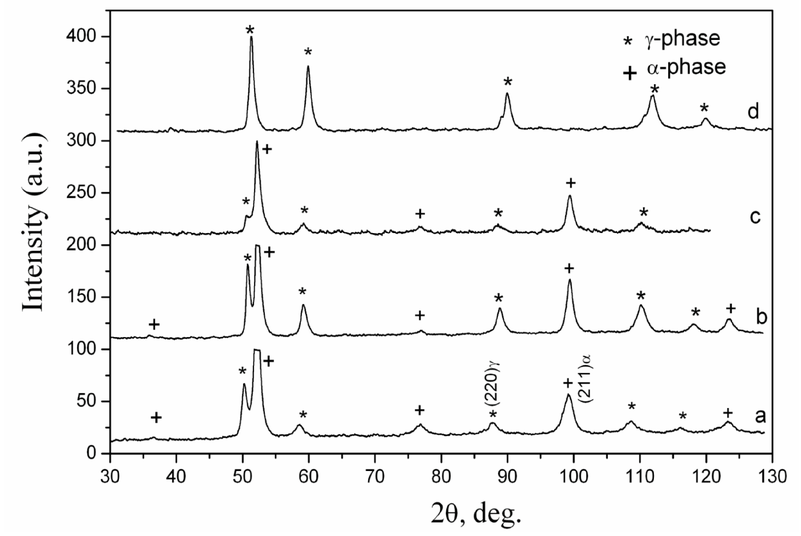
Introduction

Phase formation processes in equiatomic AlCoCuFeNiCr high entropy alloys have been studied by means of XRD method, microstructure analysis and microhardness measurements. Thermodynamic and structural criteria for predicting the phase composition of the alloys are considered. In AlCoCuFe, AlCoCuFeNi and AlCoCuFeNiCr alloys the 2-phase mixture of solid solutions on the base of the BCC and FCC lattices are formed. With a decrease in the fraction of Al -atoms, the tendency to disordering of BCC solid solution occurs. The alloys reveal a dendritic structure in which Cu-enriched FCC phase is deposited in the regions between the dendrites of the main BCC phase. Correlation of microhardness of the alloys with volume fractions of phase constituents and their thermodynamic characteristics are revealed.

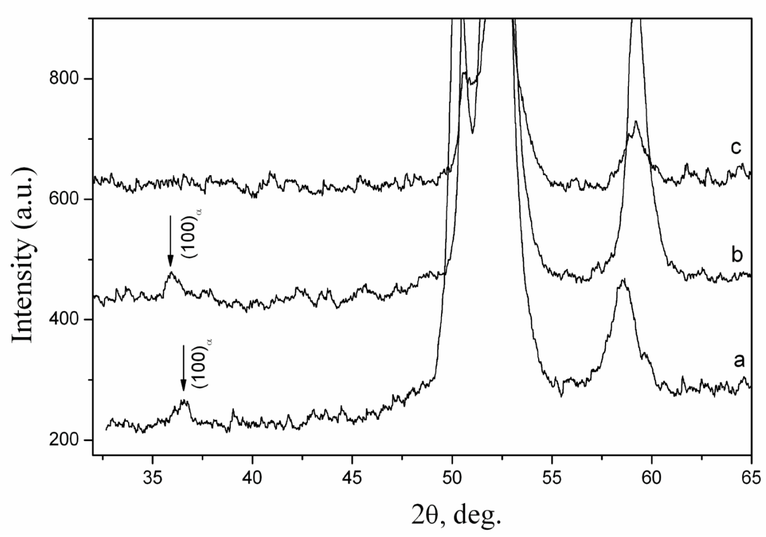
Experimental Details

- **XRD studies were carried out by means of DRON-3 diffractometer (Co-K_α –radiation, graphite monochromator, installed in diffracted beam).**
- **The structure parameters (peak positions and half-width, cell parameters of high precision, determination of subpeaks from complex diffraction maxima) have been obtained from diffraction patterns using DHN_PDS software (Włodzimierz Trzebiatowski Institute, Poland).**
- **Microstructure was investigated with help of scanning electron microscope REM-1061, attached with EDS system and giving a possibility to carry out the local chemical analysis of various phases in the alloy with resolution of 1 μm.**
- **Microhardness was measured by means of PMT-3 setup under loading 1.65 N, according to the standard method.**

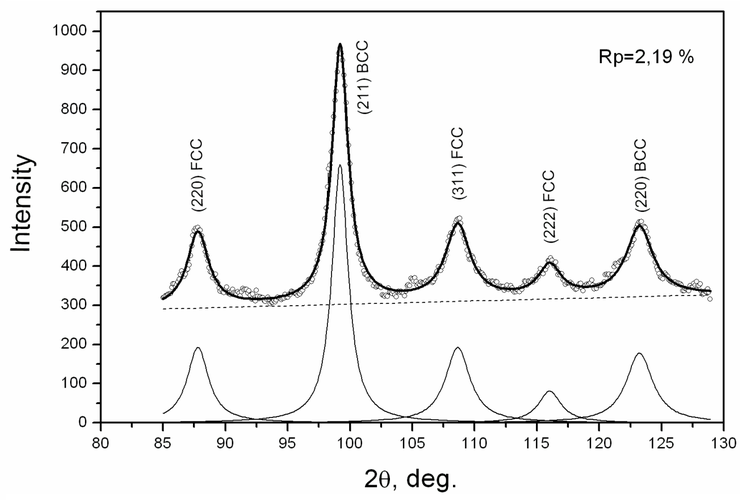
Results



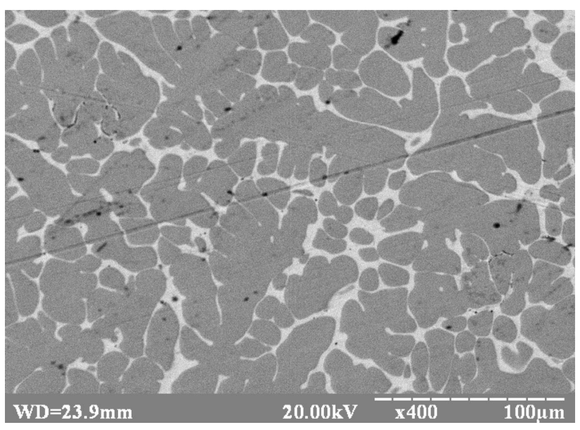
X-ray diffraction patterns of high entropy alloys. a – AlCoCuFe, b – AlCoCuFeNi, c – AlCoCuFeNiCr, d – CoCuFeNiCr



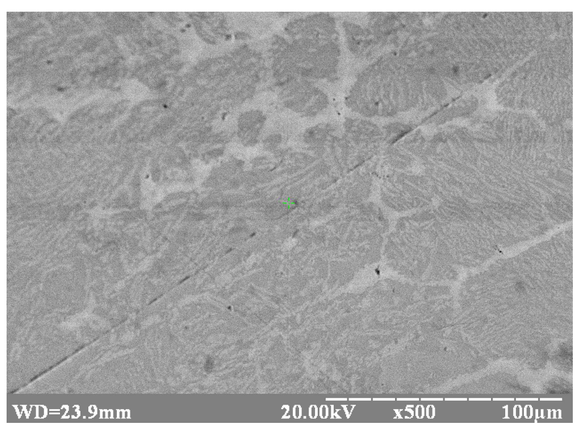
Diffraction patterns, obtained within 2θ =30 - 65° angular range: a – AlCoCuFe, b – AlCoCuFeNi, c – AlCoCuFeNiCr



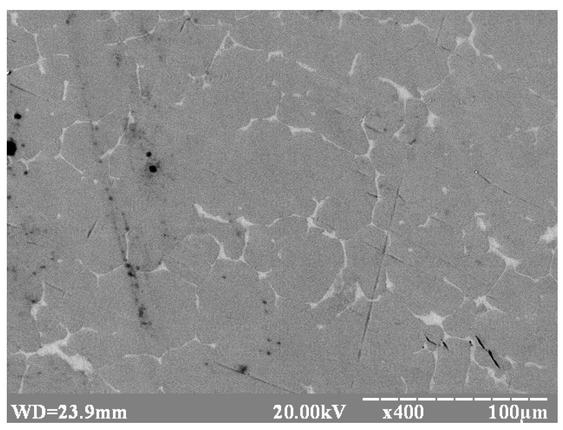
The interpretation of diffraction patterns for AlCoCuFe alloy by means of DHN_PDS software(° denotes experimental values of intensity, solid curve is a calculated scattered intensity, dash-doted curve is a background scattering, at the bottom of the figure the profiles of individual peaks are shown)



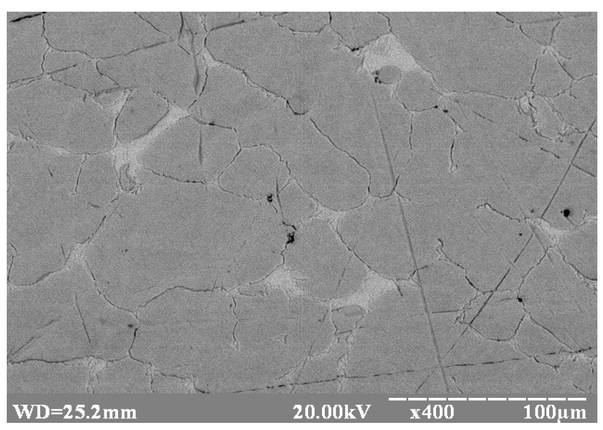
a)



b)



c)



d)

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

№	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**

Thermodynamic, structural and mechanical characteristics of HEA of nominal composition

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**

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

Conclusions

- **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 AlCoCuFeNiCr alloys has two-phase behavior and contains solid solutions with BCC (B1 or B2 structure types) FCC-lattice (A1 structure type).**
- **Addition of Al promotes the formation of the BCCphase. 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 the disordered solid solution (B2→B1).**
- **Initial BCC phase reveals the dendrite morphology and is enriched with transition elements, whereas Cu-enriched BCC solution deposits in the interdendrite space.**
- **The significant variations of microhardness versus volume fraction of phase components and its correlation with thermodynamic characteristics are revealed.**

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