**JAN DŁUGOSZ UNIVERSITY IN CZĘSTOCHOWA**
**THE FACULTY OF MATHEMATICS AND NATURAL SCIENCES**

**Pavlo Lyutyy**

# Thermodynamical properties and crystal structure investigation of the selected ternary compounds in the 3d transiton metall {Cr, Fe, Co, Cu, Ni} – Ga - Si ternary systems

## Abstract

In the present dissertation I investigate the influence chemical composition as well as replacement (exchange) the III-valent by IV-valent atoms into electronic structure and physical properties of the some synthesized binary and ternary compounds.

For a more complete understanding of the phenomena occurring in synthesized materials we performed magnetic measurements of synthesized by author $Fe_6Ga_{6-x}Si_{1+x}$ ($x$ = 0.05(2)), $NiGa_{0.84}Ge_{0.16}$, $NiGa_{0.82}Si_{0.18}$ and $NiAl_{0.46}Si_{0.54}$ ternary compound in wide temperature spectrum. We discovered the sequences of reversible phase transitions in the firstly synthesized compounds. The investigations of thermodynamics properties were done by means of DSC measurements and additionally conformed by structural as well as magnetic experiments.

Based on performed in the frame of this thesis structural measurements (both single crystal and powder X-ray diffraction methods) and metallographic analyses of the synthesized alloys, the isothermal section of phase diagrams of

the {Cr, Fe, Co, Cu}–Ga–Si system at 870 K in whole concentrations range were constructed firstly. I showed that no ternary compound exist at the temperature of the investigation in {Cr, Co, Cu}–Ga–Si system. The formation of the extensive solid solution of substitution type, based on binary $Cr_3Si$, CoSi, CoGa, $Ni_2Si$ were established and precisely determined by means of Rietveld refinement and metallographic analysis.

Crystal structure of the nine ternary: $\mathbf{Mn_8Ga_{5-x}Si_x}$ ($x$ = 0.265) – $P$-43$m$ space group, $a$ = 9.2128(4) Å; $\mathbf{Fe_6Ga_{6-x}Si_{1+x}}$ ($x$ = 0.05(2)) – $R$-3$m$ space group, $a$ = 12.4174(2) Å, $c$ = 7.7368(2) Å, own structure type; $\mathbf{NiGa_{0.82}Si_{0.18}}$ – $P2_13$ space group, $a$ = 4.61976(4) Å; $\mathbf{NiGa_{0.84}Ge_{0.16}}$ – $P2_13$ space group $a$ = 4.6393(2) Å; $\mathbf{NiAl_{0.46}Si_{0.54}}$ – $P2_13$ space group, $a$ = 4.55434(3) Å; $\mathbf{Ni_{1.745}Ga_{0.65}Si_{0.35}}$ – $P6_3/mmc$ space group, $a$ = 3.9563(2) Å, $c$ = 4.9658(3) Å; $\mathbf{Ni_{5-x}Ga_{x+y}Sn_{5-y}}$ – $Cmcm$ space group, $a$ = 4.09234(5) Å, $b$ = 12.3917(2) Å, $c$ = 11.4064(2) Å; $\mathbf{ZrGa_{0.925}Si_{0.075}}$ – $Cmcm$ space group, $a$ = 3.8956(4) Å, $b$ = 10.179(1) Å, $c$ = 3.8187(4) Å; $\mathbf{Pd_{12}Ga_3Si_4}$ – $P6_3/m$ space group, $a$ = 9.3523(5) Å, $c$ = 3.6019(3) Å and one $\mathbf{Cu_{0.826(8)}Si_{0.174(8)}}$ binary compound which crystallizes in $P4_132$ space group, $a$ = 6.21986(2) Å **were determined firstly**. The $Fe_{33}Ga_5Si_{62}$ (λ) ternary compound was synthesized. However crystal structure determination was unsuccessful only supposition that structure is relative to $FeSi_2$ was made.