Synthesis and Characterization of Intermetallic Compounds $(Ba,Ca)(V,Nb)_xSi_y$, $BaNi_{16-x}T_xSi_{12}$ (T = V,Nb), $(Ta,Nb,V)_4Ni_{14.7}Ge_{3.3}$

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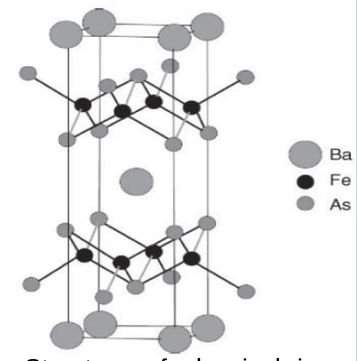
Introduction

The research on novel phases with new superconducting properties and higher critical border is very emerging area in solid state science. Ternary phases combining alkali earth metal, transition metal and adamantogen are of particular interest taking into account, that their binary compounds are well examined structures, following Hume-Rotery and Zintl crystallization tendencies.[1][2][3] Transition metals V, Nb and Ta are considered to be good candidates to build the structures with polyanionic layers following the superconducting principle of iron pnictides, which are structured as trilayers.[4] It is supposed that comparable layered 2D polyanionic structures with V, Nb and Ta could be achieved. Tertiary systems Ba-Nb-Si, Ba-V-Si, Ca-V-Si, Ba-V-Ge, Ca-V-Ge, V-Ni-Ge, Nb-Ni-Ge, Ta-Ni-Ge varying the ratios of the metals were investigated. The examination of last three systems in 4:14.7:3.3 composition was inspired due accidental discovery of $Ta_8Ni_{29.4}Ge_{6.6}$ compound during the synthesis of $CaNi_5Ge_3$[5] in the Ta-container. In addition, it was interesting to investigate the existence of isostructural compounds in the systems with Nb and V instead of Ta. Furthermore, possible formation of solid solutions of substitution based on $BaNi_{16}Si_{12}$[5], was studied exploring $BaNi_{16-x}V_xSi_{12}$ and $BaNi_{16-x}Nb_xSi_{12}$ with x = 6 structures. According X-Ray diffractometry measurements the novel $(Ta/Nb)_8Ni_{29.4}Ge_{6.6}$ and V_2Ni_3Ge structures are formed via high-temperature ceramic synthesis. However, the combination of alkali earth metal, transition metal and adamantogen does not give any evidence of new phases.

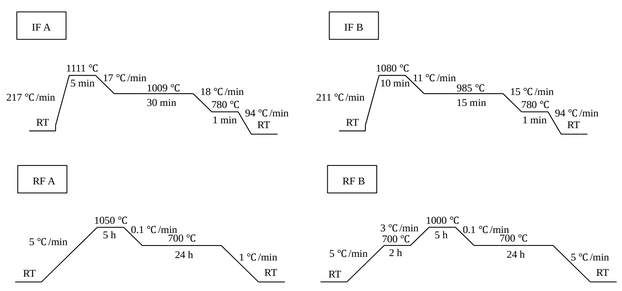


Structure of classical iron pnictide $BaFe_2As_2$. Iron arsenide (iron pnictogen) layers are typical for this structure.[6]

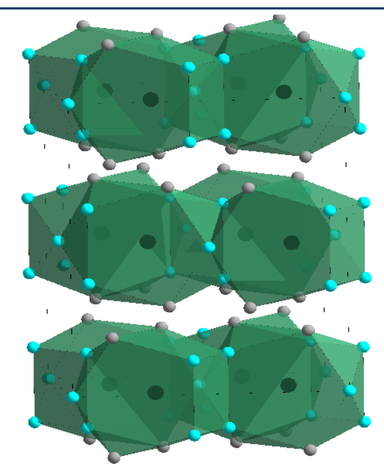
Investigated systems

System	Furnace	Obtained phases
1Ba:2Nb:3Si	AMF	$BaSi_2$, Ba_3Si_4, Nb_5Si_3
1Ba:2V:3Si	AMF	$BaSi_2$, Ba_3Si_4
1Ba:2V:3Si	AMF	$BaSi_2$
1Ba:4V:5Si	AMF	$BaSi_2$, Ba_3Si_4
1Ba:4V:5Si	IF A	Ba_3Si_4,V_5Si_3
2Ba:4V:5Si	IF A	Ba_3Si_4, V_5Si_3
1Ba:1V:3Si	IF A	$BaSi_2$, Ba_3Si_4, V_5Si_3
1Ba:10Ni:6V:12Si	AMF	$BaNi_{16}Si_{12}$, $VNi_{1.2}Si_{0.8}$
1Ba:10Ni:6Nb:12Si	AMF	$NbSi_2$, $Nb_{0.19}Ni_{0.81}$, NbNiSi
1Ca:1V:3Si	IF A	CaSi, V_5Si_3
2Ca:4V:5Si	IF A	CaSi, V_5Si_3
4Ta:14.7Ni:3.3Ge	IF A	$Ta_8Ni_{29.4}Ge_{6.6}$
4Ta:14.7Ni:3.3Ge	IF B	$Ta_8Ni_{29.4}Ge_{6.6}$
4Ta:14.7Ni:3.3Ge	RF A	$Ta_8Ni_{29.4}Ge_{6.6}$
4Nb:14.7Ni:3.3Ge	IF A	$Nb_8Ni_{29.4}Ge_{6.6}$
4Nb:14.7Ni:3.3Ge	IF B	$Nb_8Ni_{29.4}Ge_{6.6}$
4Nb:14.7Ni:3.3Ge	RF A	$Nb_{0.08}Ni_{0.92}$, $Ni_{3.2}Ge_{0.8}$, unknown phase
4V:14.7Ni:3.3Ge	IF A	-
4V:14.7Ni:3.3Ge	IF B	V_2Ni_3Ge
4V:14.7Ni:3.3Ge	RF A	$V_{0.3}Ni_{0.5}Ge_{0.2}$, VNi_3, $Ni_{3.2}Ge_{0.8}$, unknown phase
1Ba:1V:3Ge	RF B	$BaGe_2$, Ba_6Ge_{25}, V_5Ge_3
2Ba:4V:5Ge	RF B	$BaGe_2$, V_5Ge_3
1Ca:1V:3Ge	RF B	$CaGe_2$
2Ca:4V:5Ge	RF B	$CaGe_2$

Temperature programs, structure of new compound

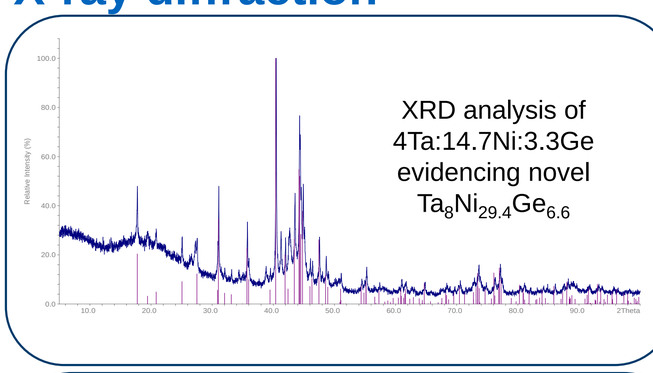


Temperature programs for induction and resistance furnaces.

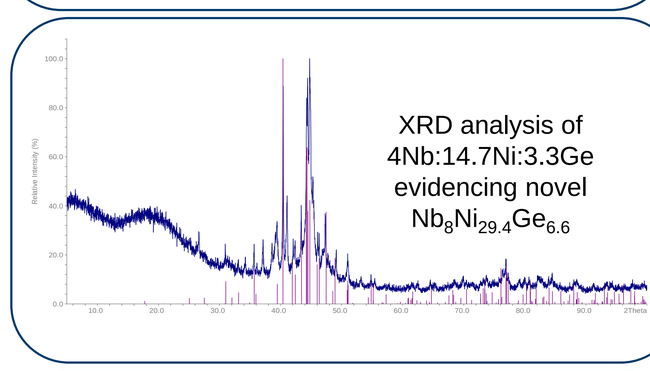


Crystal structure of $(Ta/Nb)_8Ni_{29.4}Ge_{6.6}$ showing Ta/Nb atoms in black, Ni atoms in emerald-green and Ge atoms in grey.

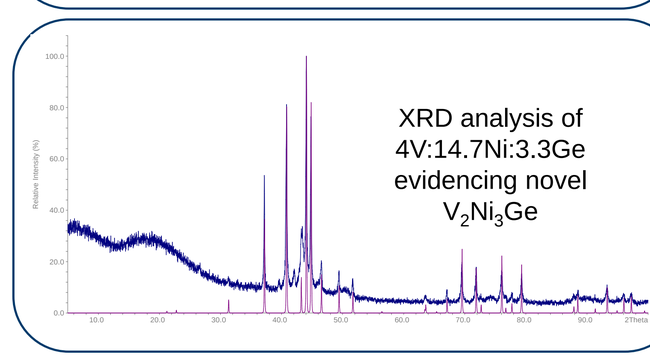
X-ray diffraction



XRD analysis of 4Ta:14.7Ni:3.3Ge evidencing novel $Ta_8Ni_{29.4}Ge_{6.6}$



XRD analysis of 4Nb:14.7Ni:3.3Ge evidencing novel $Nb_8Ni_{29.4}Ge_{6.6}$



XRD analysis of 4V:14.7Ni:3.3Ge evidencing novel V_2Ni_3Ge

Calculated theoretical patterns are showed in purple, experimental – in blue.

Conclusion

Overall no binding tendency was observed for alkali earth metal and transition metal. The absolute success was achieved in resulting ternary $Ta_8Ni_{29.4}Ge_{6.6}$ phase in high purity. The synthesis conditions did not show any influence on the stability of this compound. However, in case of Nb, prolonging the annealing time presumably resulted in tendency to decomposition into binary phases. New phase V_2Ni_3Ge was identified conducting the experiment in induction furnace. This novel compound is suggested to have $MgZn_2$-type structure and is analogous to Mn_2Co_3Ge compound. This phase should be further examined conducting Rietveld refinement or single crystal analysis. More compositions should be further examined to complete the overview of binding tendencies between alkali earth metals, transition metals and adamantogens.

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