FA2-MS13-P01

Diffuse Scattering in the Zn_6Sc 1/1 cubic approximant. <u>Tsunetomo Yamada</u>[a, b], Cesar Pay Gomez[c], Ryuji Tamura[b], Holger Euchner[d], Akiji Yamamoto[b], Marc de Boissieu[a]. *[a]SIMaP, Grenoble-INP, CNRS,UJF , Saint Martin d'Hères Cedex, France. [b]Department of Material & Science., Tokyo Univ. of Science, Noda, Japan. [c]National Institute for Materials Science, Tsukuba, Japan. [d]ITAP, Universitat Stuttgart, Stuttgart, Germany.*
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The low-temperature phase transition of the Zn_6Sc cubic 1/1 approximant [1] has been investigated by X-ray diffraction. It is a crystalline approximant to a recently discovered quasicrystal $Zn_{88}Sc_{12}$ [2] and has a bcc lattice composed of a Tsai-type cluster with an orientationally disordered Zn tetrahedra at the centers [3]. The phase transition undergoes below 160K and has been attributed to the orientational ordering of the Zn tetrahedra along [110] direction of high-temperature phase [1, 4]. In order to obtain an insight into the orientational ordering occurring at the phase transition, diffuse scattering has been measured. Well above the phase transition at 220K (i.e. 60 K above) we observed a broad diffuse scattering intensity which sharpen and merges into a Bragg peak as the temperature decreases and reaches the transition temperature (T_c). This signature of short-range ordering above T_c will be discussed in details and compared to refined average structures obtained between T_c and room temperature by measuring Bragg peaks.

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Keywords: Quasicrystalline approximant, Phase transition, Diffuse scattering

FA2-MS13-P02

Ir_nZn_{26-n} (n = 4,6,7): recurring γ-brass-like phases in the binary system system iridium – zinc. <u>Andreas Authmann</u>[a], Wolfgang Hornfeck[a], Ryan Henderson[a,b], Stephen Lee[b], Bernd Harbrecht[a] . *[a]Department of Chemistry, Philipps University Marburg, Germany. [b]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY, USA.*
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A recent systematic exploration of the Ir-Zn system disclosed the existence of at least 13 binaries, several of them of bewildering structural complexity.[1] Among them there are six phases resembling γ-brass-related structures: $Ir_{7+7\delta}Zn_{97-11\delta}$ ($cF403-406$)[2], $Ir_{13}Zn_{56}$ ($oC276$), $Ir_{21}Zn_{100}$ ($oC484$), and Ir_nZn_{26-n} (n = 4,6,7). The only previously known phase Ir_4Zn_{22} ($cI52$)[3] adopts the ordinary cubic γ-structure.[3] The members n = 6 and 7 with Pearson symbol *hR78* conform to two distinct rhombohedral variants of the γ-phase. The compositionally narrow phase fields of some structurally complex phases are situated between those of the recurring γ-brass-type Ir_nZn_{26-n} phases. The present contribution deals essentially with the 3 Ir_nZn_{26-n} phases. Firstly, we discuss the coloring problem[4] concerning the distribution of the constituting atoms in the structure by raising the question: Which component prefers which crystallographic site? Secondly, we present results of DFT calculations, dealing with a second question provoked by the answer of the first one: What is energetically favorable about the realized atomic decorations in Ir_nZn_{26-n}? We show that the calculated heats of formation of the derived structures fulfill - opposed to structures with various devised atomic decorations – thermodynamic stability criteria. Furthermore and most pronounced for Ir_7Zn_{19}, we find that the Fermi level of the electronic structures is positioned in or close to a pseudo-gap as expected for γ-phases stabilized by the Hume-Rothery mechanism. We conclude with deriving thermodynamic quantities of the Ir_nZn_{26-n} phases from isopiestic measurements at various Zn pressures. The experimental and calculated quantities are critically compared.

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Keywords: brass-like phases, complex metal alloys, isopiestic measurement, heat of formation

FA2-MS13-P03

X-ray studies of martensitic transformation in the Fe-Ni alloys rapid quenched from melt. <u>Ruslan M. Delidon</u>, Vitaliy Y. Danilchenko. *Institute for Metal Physics National Academy of Sciences of Ukraine, Kyiv, Ukraine.*
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Structure-phase state and characteristics of martensitic transformations in alloy (Fe – 31 wt. % Ni) ribbon quenched from melt were investigated by x-ray, optical microscopy and magnetometric methods. X-ray investigated shown the significant texture of austenite. Significantly different volume part of martensitic phase in the local areas of thin ribbons of alloys is associated with the distribution of initial austenitic grains in size. This distribution is determined by the difference in the rate of crystallization of an alloy in the local areas.

Keywords: Fe-Ni alloy, martensitic tranformation, phase hardening, hardening from melt, texture, dimensional effect

FA2-MS13-P04

Crystal structure of the $Li_{18}Cu_{15}Al_7$ intermetallic compound. <u>Grygoriy Dmytriv</u>[a], Volodymyr Pavlyuk[a], Ivan Tarasiuk[a], Helmut Ehrenberg[b], Igor Chumak[b], Hermann Pauly[c]. *[a]Department of Inorganic Chemistry, Ivan Franko Lviv National University, Ukraine. [b]Institute for Complex Materials, IFW Dresden, Germany. [c]Materials Science, Technical University Darmstadt, Germany.*
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The $Li_{18}Cu_{15}Al_7$ intermetallic compound was synthesized from the pure elements in a sealed tantalum crucible. The reaction between the metals was carried out in an induction furnace at 1100ºC. The crystal structure of this compound was investigated *via* X-ray single crystal method (BRUKER Kappa

APEXII single crystal diffractometer, MoKα radiation) and has been solved by direct methods and refined using the SHELX-97 program package [1]: *Fmmm*, $a=4.9484(7)$, $b=8.4367(7)$, $c=29.171(1)$ Å, $R_W=0.0549$, 312 unique reflections, 45 variables. The final atomic parameters for the $Li_{18}Cu_{15}Al_7$ compound are summarized in the following table.

Atom	*Wyck*	*x/a*	*y/b*	*z/c*	Occupation
Cu1	8e	1/4	1/4	0	1
Cu2	16j	1/4	1/4	0.66754(6)	1
Cu3	4a	0	0	0	1
M4	8i	0	0	0.6801(2)	0.39(4) Cu + 0.61(4) Li
Al5	8i	0	0	0.6337(3)	1
Al6	8i	0	0	0.5397(3)	0.73(7)
Li7	16m	0	0.670(3)	0.5873(9)	1
Li8	8i	0	0	0.772(1)	1
Li9	8f	1/4	1/4	1/4	1

Crystal structure of this compound is a derivative from the $CuAl_2$ binary compound. Forming of the $Li_{18}Cu_{15}Al_7$ compound can be formally presented as additional lithium layers into $CuAl_2$ with an expansion of the *c* parameter from 6.480 Å to 29.171 Å. Another peculiarity of the crystal structure of this compound is the formation of hexagonal columns which are filled by lithium atoms. Similar columns with lithium atoms in the crystal structures were established for $Li_{12}Cu_{16+x}Al_{26-x}$ and $Li_8Cu_{12+x}Al_{6-x}$ compounds [2,3].

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Keywords: lithium, intermetallic compound, crystal structure

FA2-MS13-P05

Fe-Ni-C alloy crystalline structure of tempered martensite. Viktor Iakovlev, Vitaliy Danilchenko. *G.V. Kurdyumov Institute for Metal Physics, Kyiv, Ukraine.* E-mail: zvik83@mail.ru

High-carbon crystalline structure of iron-nickel martensitic alloy after direct γ-α- and reverse α-γ- transition was studied using X-ray diffraction in single crystal specimens. The test material was Fe – 9,7 wt.%Ni – 1,54 wt.% austenite alloy. The direct transition occurred when cooling at liquid nitrogen and the reverse transition occurred when heating in salt bath at 700°C. The instability interval of retained austenite was partially overlapped by an interval of the reverse martensitic transition. This led to initiating the direct α-γ transition. The X-ray investigations were realized on single crystal specimens in rotating chamber RKV-86 with cobalt emission.

On three-phase dissolution stage during low-temperature tempering (100-200⁰C) two α-solid solutions (α₁- and χ- phases) with reduced content of carbon (1,2 % and 0,25% accordingly) were formed. Occurrence of reflections after tempering of χ- martensite testified about first stage decomposition ending at 300⁰C. On the second one-phase dissolution stage further martensite depletion led to decreasing

of χ-phase lattice tetragonality up to 1 at 300⁰C. Heating up to 700⁰C has resulted in reverse α-γ- martensitic transition. Orientation of the martensitic lattices with respect to initial austenite lattice was equal.

Considering the position of martensitic reflections on the diffraction pattern of the single crystal specimens we can arrive at a conclusion that the orientation of martensitic lattices was similar to the initial austenite lattice. This means that α-α₁- and α₁-χ- transitions are associated only with the redistribution of carbon atoms and are not connected with the crystallographic restructuring of the metal lattice atoms.

Keywords: martensitic transformation, X-ray diffraction, single crystals

FA2-MS13-P06

Cd-rich Cadmides of the System Na/K/Cd. Viktoria Mihajlov, Caroline Röhr. *Institut für Anorganische und Analytische Chemie, University of Freiburg, Germany.* E-Mail: viktoria@goethite.chemie.uni-freiburg.de

Binary alkali metal (A^I) zinkides [1] and cadmides are only known in the A^I-poor region of the respective phase diagrams. The structure of the sodium cadmide Na_2Cd_{11}, which was known from early film experiments[2] (Mg_2Zn_{11} type, cubic, $Pm3$, $a = 958.75(9)$ pm, $Z = 3$; $R1 = 0.042$) was confirmed and refined using single crystal data. The new ternary phase KNa_xCd_{11-x} ($x = 0.87/0.53$), tetragonal, $I4_1/amd$, $a = 1222.98(6)/1215.17(12)$ pm, $c = 766.05(4)/769.05(7)$ pm, $Z = 4$, $R1 = 0.021/0.024$) forms the $BaCd_{11}$ structure type, which was previously unknown for alkali metal compounds. The Ba site of the basic structure type is occupied by K, whereas one Cd site is statistically occupied by Na and Cd. In the structure, the atoms of the two pure Cd positions form channels running along the tetragonal *c* axis, in which the K and Na/Cd atoms alternate. A similar structural motif is found in the second border compound K_3Cd_{16}, formerly described as $K_{0.37}Cd_2$ [4]. In the Cd channels the K atoms are no longer disordered: A detailed inspection of the diffraction images revealed satellite reflections indicating an almost commensurately modulated superstructure. In the new structural model with a quadrupled *c* axis (tetragonal, $P4/nnc$, $a = 915.2(6)$, $c = 1159.0(4)$ pm, $Z = 2$) the formerly singular K position splits into two, resulting in three potassium cations per channel. Both the significant structural factors (strongly changing radius of the A^I-cations) and the electronic criteria, which can be assessed from the pseudo band gap calculated using FP-LAPW-DFT methods, are discussed. A structural map that takes the radius ratios $r_M{:}r_A$ and the v.e.c. into account nicely separates the different structure types of Zn/Cd-rich A^I/A^{II} metallides.

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Keywords: alkali metals, cadmides, electronic structure