

FA2-MS13-P01

Diffuse Scattering in the Zn₆Sc 1/1 cubic approximant. Tsunetomo Yamada^{a,b}, Cesar Pay Gomez^c, Ryuji Tamurab, 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 Zn₆Sc cubic 1/1 approximant [1] has been investigated by X-ray diffraction. It is a crystalline approximant to a recently discovered quasicrystal Zn₈₈Sc₁₂ [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 iridium – zinc. Andreas Authmann^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: Ir₇₊₇₈Zn₉₇₋₁₁₈ (*cF403-406*)^[2], Ir₁₃Zn₅₆ (*oC276*), Ir₂₁Zn₁₀₀ (*oC484*), and Ir_nZn_{26-n} (n = 4,6,7). The only previously known phase Ir₄Zn₂₂ (*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 Ir₇Zn₁₉, 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. Ruslan M. Delidon, 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 transformation, phase hardening, hardening from melt, texture, dimensional effect

FA2-MS13-P04

Crystal structure of the Li₁₈Cu₁₅Al₇ intermetallic compound. Grygoriy Dmytriv^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 Li₁₈Cu₁₅Al₇ 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 1100°C. The crystal structure of this compound was investigated via X-ray single crystal method (BRUKER Kappa