Graphical Synopsis

Special Issue: Complex Intermetallics – Structures and Properties
Guest Editor: Julia Dshemuchadse

Preface

Ken Miyazaki, Vincent J. Yannello and Daniel C. Fredrickson

Electron-counting in intermetallics made easy: the 18-n rule and isogonal bonds across the Os–Al system

DOI 10.1515/zkri-2017-2044
Z. Kristallogr. 2017; 232(7–9): 487–496

Synopsis: We illustrate how structural progressions across the four binary phases of the Os–Al system can be simply understood using the 18-n bonding scheme. Throughout this work, we emphasize how the 18-n scheme can be applied from structural inspection alone, with theoretical calculations confirming or refining these conclusions.

Tatiana G. Akhmetshina and Vladislav A. Blatov

Topological methods for complex intermetallics

DOI 10.1515/zkri-2016-2027

Synopsis: We show how the topological methods realized in the so-called nanocluster approach can be applied to elucidating extremely complex intermetallic compounds.

Koichi Kitahara and Kaoru Kimura

Local cluster networks and the number of valence states in aluminium–transition metal face-centred icosahedral quasicrystals

DOI 10.1515/zkri-2016-2035

Synopsis: Local cluster networks in aluminium–transition metal face-centred icosahedral quasicrystals were analysed on the basis of a six-dimensional model, and the relations between the cluster networks and the number of the valence states were discussed.
Michael Schwarz, Marco Wendorff and Caroline Röhr

**Complex cubic metallides** $AM_{6}$ $(A=Ca, Sr; M=Zn, Cd, Hg)$. Synthesis, crystal chemistry and chemical bonding

DOI 10.1515/zkri-2016-2029
Z. Kristallogr. 2017; 232(7–9): 515–541

**Synopsis:** The complex cubic structure of CaZn$_{1.31}$Hg$_{3.69}$: Four different space-tiling [Hg$_{24}$] cuboctahedra, filled with Zn/Hg cubes (C), tetrahedra stars (TS) and double tetrahedra stars (DTS).

Bodo Böhme, Kaya Wei, Matej Bobnar, Yurii Prots, Ulrich Burkhardt, Michael Baitinger, George S. Nolas and Yuri Grin

**A type-II clathrate with a Li-Ge framework**

DOI 10.1515/zkri-2017-2046
Z. Kristallogr. 2017; 232(7–9): 543–556

**Synopsis:** Na$_{16}$Cs$_{8}$Li$_{x}$Ge$_{136-x}$ $(x \approx 2.8$, space group $Fd3m$) is the first intermetallic type-II clathrate with a lithium-substituted framework. The [LiGe$_4$]$^{3-}$ entities formed in the framework are rationalized by the Zintl concept as formal overall three-electron acceptors compensating part of the excessive electrons delivered by the alkali metal atoms in the polyhedral cages.

Frank Tambornino and Constantin Hoch

**The simplest representative of a complex series: the Hg-rich amalgam Yb$_{11}$Hg$_{54}$**

DOI 10.1515/zkri-2016-2036

**Synopsis:** The crystal structure of Yb$_{11}$Hg$_{54}$ is a new member of a growing series of amalgam structures which can be described as hettotypes of the Gd$_{14}$Ag$_{51}$ structure type. All members show individual disorder phenomena, introducing different degrees of complexity. Yb$_{11}$Hg$_{54}$ is the only representative of this family crystallising in a fully ordered structure.
Stefan Seidel, Ute Ch. Rodewald and Rainer Pöttgen

**YRh₂Ga – a new intergrowth variant of MgNi₂ and CeCo₃B₂ related slabs**

DOI 10.1515/zkri-2016-2016
Z. Kristallogr. 2017; 232(7–9): 567–571

**Synopsis:** YRh₂Ga is a new $n=1$ member of the $\text{RE}_{2+n}T_{3+3n}X_{1+2n}$ structure series (Parthé intergrowth variants).

Fabian Eustermann, Rolf-Dieter Hoffmann and Oliver Janka

**Superstructure formation in PrNi₂Al₃ and ErPd₂Al₃**

DOI 10.1515/zkri-2016-2023
Z. Kristallogr. 2017; 232(7–9): 573–581

**Synopsis:** PrNi₂Al₃ and ErPd₂Al₃ were found to crystallize in an i7-superstructure of the ternary ordered CaCu₅ type structure. Two crystallographic independent rare-earth sites are found of which one (1b) is shifted by $z=1/2$, causing a distortion in the structure along with a recoloring of the $T$ and Al atoms in the network.

Katherine A. Benavides, Gregory T. McCandless and Julia Y. Chan

**The single crystal structure determination of Ln₆MnSb₁₅ (Ln=La, Ce), Ln₆Mn₁₋ₓZnxSb₁₅ (x~0.5), and Ln₆ZnSb₁₅ (Ln=La – Pr)**

DOI 10.1515/zkri-2016-2025
Z. Kristallogr. 2017; 232(7–9): 583–591

**Synopsis:** Single crystal analysis of Ln₆MnSb₁₅ (Ln=La, Ce), Ln₆Mn₁₋ₓZnxSb₁₅ (x~0.5), and Ln₆ZnSb₁₅ (Ln=La – Pr) reveal a highly disordered structural variant of the La₆MnSb₁₅ structure type.
**Synopsis:** A view of the octamer unit composed of \((\text{Cd/Mn})\text{Sb}_4\) shared tetrahedra linked through a Sb–Sb bond, along with the Sr/Eu substituted cations of the title compound, \(\text{Sr}_{21-x}\text{Eu}_x\text{Cd}_{4-y}\text{Mn}_y\text{Sb}_{18}\) \((x \sim 8, y \sim 1)\). Pink shading indicates the tetrahedral with the largest % of Mn.

**Synopsis:** Reinvestigation of \(\gamma\)-region of Mn–Al phase diagram revealed that the \(\gamma\text{-Mn}_{5-x}\text{Al}_{8+x}\) phases adopt a rhombohedrally distorted \(\text{Cr}_5\text{Al}_8\) type structure. Single crystals of the \(\gamma\)-phase \(\text{Mn}_{5-x}\text{Al}_{8+x}\) were successfully grown using a Sn-flux. Tight-binding electronic structure calculations (LMTO-ASA with LSDA) showed that the calculated Fermi level for \(\gamma\)-“Mn\text{Al}_8\” falls within a pseudogap of the density of states.

**Synopsis:** A \(\gamma\)-brass-related Hume-Rothery phase \(\text{RhCd}_{9+\delta}\) \((-1.18 \leq \delta \leq 0.29)\) has been uncovered in the Rh–Cd binary system and the average structure has been characterized by single crystal X-ray diffraction experiment. The average structure of the phase is isostructural to \(\text{Rh}_{7-x}\text{Mg}_{44+x}\). The structure has been described by the “cluster concept”.

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Elizabeth L. Kunz Wille, Joya A. Cooley, James C. Fettinger, Nasrin Kazem and Susan M. Kauzlarich

A new solid solution compound with the \(\text{Sr}_2\text{Mn}_4\text{Sb}_{18}\) structure type: \(\text{Sr}_{13}\text{Eu}_8\text{Cd}_3\text{Mn}_1\text{Sb}_{18}\)

DOI 10.1515/zkri-2016-2034
Z. Kristallogr. 2017; 232(7–9): 593–599

Srinivasa Thimmaiah, Zachary Tener, Tej N. Lamichhane, Paul C. Canfield and Gordon J. Miller

Crystal structure, homogeneity range and electronic structure of rhombohedral \(\gamma\text{-Mn}_5\text{Al}_8\)

DOI 10.1515/zkri-2017-0003

Partha Pratim Jana

\(\text{RhCd}_{9+\delta}\) \((-1.18 \leq \delta \leq 0.29)\) a \(\gamma\)-brass related cubic giant cell structure

DOI 10.1515/zkri-2017-2045
Z. Kristallogr. 2017; 232(7–9): 611–617
Dante G. Quirinale, Andreas Kreyssig, Scott Saunders, Daniel Messina, Warren E. Straszheim, Paul C. Canfield, Matthew J. Kramer and Alan I. Goldman

**The solidification of Al–Pd–Mn studied by high-energy X-ray diffraction from electrostatically levitated samples**

DOI 10.1515/zkri-2016-2037
Z. Kristallogr. 2017; 232(7–9): 619–627

**Synopsis:** High-energy x-ray investigations of the solidification products in Al–Pd–Mn close to the ideal composition for the icosahedral phase show that the primary solidification product from the melt is $i$-Al–Pd–Mn and a significant remaining liquid component. The solidification pathway is consistent with the liquidus projection and pseudo-binary cut through the ternary phase diagram.

Julian Ledieu, Émilie Gaudry, Vincent Fournée, J. A. Smerdon and Renee D. Diehl

**Fullerene adsorption on intermetallic compounds of increasing structural complexity**

DOI 10.1515/zkri-2016-2028
Z. Kristallogr. 2017; 232(7–9): 629–645

**Synopsis:** Fullerene adsorption on complex intermetallic surfaces: structures and properties.

Magdalena Wencka, Stanislav Vrtnik, Primož Koželj, Zvonko Jagličić, Peter Gille and Janez Dolinšek

**Anisotropic electrical, thermal and magnetic properties of Al$_{13}$Ru$_4$ decagonal quasicrystalline approximant**

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**Synopsis:** The anisotropic electrical and thermal transport coefficients, the magnetization and the specific heat of the Al$_{13}$Ru$_4$ monoclinic approximant to the decagonal quasicrystal are presented, in comparison to the isostructural Al$_{13}$Fe$_4$.

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