FA2-MS13-T01

Phase Stability, Disorder Phenomena and Modeling of Complex Metallic Alloy Phases Guido Kreiner[a], Rico Berthold[a], Marek Mihalkovic[b]. [a]*Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany.* [b]*Slovakian Academy of Sciences, Bratislava, Slovakia.*
E-mail: kreiner@cpfs.mpg.de

Although Complex Metallic Alloy phases (CMAs) are known since the beginning of the last century, they have long been considered as rare and special cases of intermetallic compounds. Recent phase diagram studies using state of the art techniques have shown that CMAs occur frequently not only in multinary but also in binary systems. Hence it is important to understand how these structures of tremendous complexity are stabilized. Because phase diagram studies are tedious, expensive and time consuming, special attention has been paid during the last two decades primarily to Al and Mg based systems promising the design of advanced light metal intermetallics. The aim of this contribution is to present examples of recent studies of Mg-based phase diagrams containing large numbers of complex metallic alloy phases. The following topics will be addressed in more detail: i) The art of phase diagram determination, i.e., advanced preparation and characterisation techniques for complex phase diagrams; ii) How do we describe large unit cell structures with thousands of atoms? iii) Disorder phenomena and their role in structure stabilisation—enthalpy versus entropy; iv) What can we learn from calculations combined with data mining techniques and/or experimental data?
We gratefully acknowledge the support of the European Network of Excellence Complex Metallic Alloys, Contract No. NMP3-CT-2005-500140.

Keywords: Phase stability, alloy phases, magnesium compounds

FA2-MS13-T02

Atomic Structures of Quasicrystals and related Complex Metallic Alloys. Cesar Pay Gómez[a]. [a]*Department of Materials Chemistry, Ångström Lab, Uppsala University, Sweden.*
E-mail: cesar.paygomez@mkem.uu.se

In this work we will give a comprehensive review of different order/disorder phenomena in quasicrystals (QCs), approximants (APs) and other related complex metallic alloys (CMAs). Special attention will be given to positional and chemical order/disorder, but short-range order and superstructure formation will also be discussed. Different approximant structures will be compared to each other and to related QCs, and we will further introduce the concepts of chemical twinning and intergrowth as mechanisms for the formation and structure descriptions of these phases.[1, 2] The talk will mainly focus on structures related to the i-$YbCd_{5.7}$ QC,[3] and the expansion of concepts and structure descriptions developed throughout the process of analyzing this binary parent phase to other types of QCs and APs.

[1] Pay Gómez C., Lidin S., *Solid State Sci.* 2002, *4*, 901. [2] Pay Gómez C., Ohhashi S., Yamamoto A., Tsai A. P. *Inorg. Chem.* 2008, 47, 8258. [3] Takakura H., Pay Gómez C., Yamamoto A., de Boissieu M., Tsai A. P. *Nature Materials*. 2007, 6, 58.

Keywords: quasicrystals, alloys, structural disorder alloys

FA2-MS13-T03

Understanding the structures of complex cubic intermetallic phases. Julia Dshemuchadse, Daniel Y. Jung, Walter Steurer. *Laboratory of Crystallography, ETH Zurich, Switzerland.*
E-mail: julia.dshemuchadse@mat.ethz.ch

In the past decades, a large number of structurally highly complex intermetallic phases was found and described by crystallographers. A systematization of this class of structures has not yet been achieved and should be attempted in order to derive basic principles of structure building in intermetallic phases. Therefore we examined the structures of intermetallic compounds with huge unit cells, starting with a large group of cubic face-centered unit cells containing approximately 400 atoms. The studied structures crystallize in space group symmetries $F\bar{4}3m$ and $Fd\bar{3}m$.
The geometrical building principles of an aristotype of more than 30 structures are discussed by means of two different methods, *i. e.* the cluster approach and the modular approach. The former describes the structure as a packing of polyhedral clusters, which may consist of several cluster shells. The choice of clusters can be considered as justified when leading to a description of the structure, which is as simple as possible. This mostly involves a high degree of transferability of a model to a different structure type, as well as highly symmetric polyhedra. By those means, the degree of complexity of a structural model may be reduced and underlying packing principles made intelligible. The modular approach constitutes crystal structures by structure modules, which are part of other structure types as well.
We start our investigations with structures described by the highest-symmetric lattice and thus described in cubic face-centered space groups. The chosen class of structures stands out in the multitude of intermetallics due to its quantity: only a small number of singular structures were found to exhibit bigger unit cells and it is a large enough group of structures to additionally substantiate the significance of a detailed study. All structures consist solely of pure metals, but nevertheless show a high diversity in their chemical composition. We discuss stabilizing forces in the investigated structures: thorough geometrical analysis and symmetry considerations are complemented by first-principles studies of the examined structures. Consequently, we hope to clarify the influences of packing principles and crystal-chemical driving forces on the building scheme of intermetallic structures.

Keywords: intermetallic phases, cluster structures, ab-initio calculations

FA2-MS13-T04

Studies of domains and defects in ternary FeCo alloys by neutrons and positrons. Ralph Gilles[a], Michael Hofmann[a], Yan Gao[b], Frank Johnson[b], Debashis Mukherji[c], Christoph Hugenschmidt[a], Philip Pikart[a]. [a]*Technische Universität München, Forschungsneutronenquelle Heinz Maier-Leibnitz*