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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.*
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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?

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Keywords: Phase stability, alloy phases, magnesium compounds

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Atomic Structures of Quasicrystals and related Complex Metallic Alloys. Cesar Pay Gómez[a]. [a]*Department of Materials Chemistry, Ångström Lab, Uppsala University, Sweden.*
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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

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Understanding the structures of complex cubic intermetallic phases. Julia Dshemuchadse, Daniel Y. Jung, Walter Steurer. *Laboratory of Crystallography, ETH Zurich, Switzerland.*
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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

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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*

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The recent years have seen a reawakened interest in FeCo alloys due to the increased demands of modern electrical power generation and distribution equipment. For industrial application the challenge involves increasing the tensile strength and ductility of FeCo alloys while maintaining an acceptable balance of magnetic properties (brittleness).

The effects of alloying FeCo with Pt, Pd, etc. have been investigated by neutron diffraction as part of this work. In the composition range of about 30% Co, ternary FeCo alloys undergo a continuous order-disorder phase transformation in the temperature range of 615±30°C [1]. Whereas the T_c temperature is independent of the thermal history, the microstructure of ordered domains is sensitively dependent on thermal history and on the kinetics of the order/disorder transition.

Neutron diffraction is the adapted method to study the order process due to the favourable different scattering length density of Fe and Co. It allows easy distinction between the two elements in a common structure in comparison to X-rays.

Measurements on the alloy system were performed at the neutron facility Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II). The high temperature measurements to follow the order-disorder phase transition were performed on the diffractometer STRESS-SPEC equipped with a 2-dimensional area detector covering around 15° in 2θ diffraction angle. This allowed following in situ the evolution of a superlattice reflection and a fundamental Bragg reflection in the temperature region T = 25–700°C. The samples were mounted in a high temperature vacuum furnace with aluminium windows to avoid air scattering and oxidation of the sample. The furnace was installed on the sample table of StressSpec, just after the collimator and close to the detector.

Samples of FeCo with different ternary elements were heat treated and cooled down together in a furnace, and in addition samples of the same composition were cooled down with different cooling rates.

Samples with the same cooling rates prepared in thin disc shape of 1 mm thickness were used for defect measurements at the positron facility NEPOMUC (FRM II) which delivers 9×10^8 positrons /sec at 1 keV beam energy. The beam energy was set up to 24 keV in order to study the bulk defect concentration in dependence on cooling rate and composition of the alloy.

[1] Gilles R., Hofmann M., Gao Y., Johnson F., Iorio L., Larsen M., Liang F., Hoelzel M., Barbier B., *Metallurgical and Materials Transactions A, 2009, 41A, 1144-1150.*

Keywords: neutron diffraction, order-disorder transitions, domain structure

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Effect of atomic order in ferromagnetic shape memory alloys studied by neutron diffraction.

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The contrast provided by neutron radiation for elements with similar atomic number and the possibility of using bulk samples, in which the properties induced by thermal treatments remain unchanged (which is not the case in powder samples) makes of single crystal neutron diffraction a valuable tool in fields like Ferromagnetic Shape Memory Alloys (FSMA).

FSMA have awakened a great interest in recent years for practical application in sensors and actuators due to the achievement of huge magnetic-field-induced strains (MFIS). The MFIS effect is associated with the rearrangement, under an applied magnetic field, of the crystallographic domains (twin variants) formed as a result of a thermoelastic Martensitic Transformation (MT) taking place from a high symmetry high temperature phase (austenite) to a lower symmetry low temperature phase (martensite).Up to now, the highest MFIS has been observed in Ni-Mn-Ga alloys close to the stoichiometric composition Ni_2MnGa (regarded as the prototypical FSMA system). The modification of the atomic ordering highly affects both the MT and the magnetic properties of the Ni-Mn-Ga alloy and one of the easiest ways of modifying the atomic order in a controlled manner is performing thermal treatments.

The correlation between the L21 atomic order degree and the MT and Curie temperatures on both polycrystalline and single-crystalline alloys subjected to different thermal treatments has been studied by single-crystal and powder neutron diffraction together with calorimetric and magnetic measurements. It is found that both transformation temperatures show exactly the same linear dependence on the degree of L_{21} atomic order, pointing out a high influence of magnetism on the structural transformation. Furthermore, the calculated correlation between transformation temperatures and atomic order allowed us to quantitatively determine the effect of atomic order on the relative stability between the structural phases. [1]

[1] Sánchez-Alarcos, V., Pérez-Landazábal, J.I., Recarte V., Gómez-Polo, C., Rodríguez-Velamazán, J.A., Chernenko, V.A., *J. Phys.: Condens. Matter,* 2010, 22, 166001.

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