MM 3 Symposium Modern Metallic Materials Design I

Time: Monday 10:15–12:45 Room: IFW B

MM 3.1 Mon 10:15 IFW B

Modern Metallic Materials Design — •Ze Zhang[1], Dieter Herlach[2], and Knut Urban[3] — [1]Beijing University of Technology, 100022 Beijing, P.R. China — [2]German Aerospace Center, D-51170 Köln, Germany — [3]Research Center Jülich, D-52425 Jülich, Germany

Since 2002 the Sino-German Science Center for Research Promotion Beijing, the Natural National Science Foundation of China (NNSFC) and the German Research Foundation (DFG) are supporting a priority programme on Modern Metallic Materials Design (MMMD) of Chinese and German groups. Modern materials science ranges from tailoring of structures in nanodimensions to the optimization of technical materials by the application of new physical concepts reflecting the growing atomistic insight into structure and properties of matter. The project aims on joint work in projects on metals and alloys, which are of great topicality and therefore can be considered as interesting and challenging for materials science institutions in China as well as in Germany. One group of projects concerns the solidification of metals and alloys from the melt. Another group of projects concerns metallic glasses. This field has recently seen intensive expansion after new multicomponent systems have been developed which permit to obtain bulk materials. A group of metallic alloys, which has been pioneered by Chinese scientists is quasicrystalline materials. Finally the current project addresses the new field of structurally complex alloy phases. The science of these alloys exhibiting properties between those of conventional intermetallics and those of quasicrystals. The symposium MMMD consists mainly of reports of the research done within this programme.

MM 3.2 Mon 10:30 IFW B

Complex intermetallic alloys in the Al-rich region of the ternary Al-Pd-Ni system — •Mariya Yurechko and Philipp Ebert — Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich

The phase diagram and the liquidus surface projection of the ternary Al-Pd-Ni system in the range of 50 to 100 at.% Al was determined using SEM, EDX, XRD, ICP-OES, and TEM. Isothermal sections between 750 and 1100 degrees Celsius illustrate that the binary Al-Pd intermetallic ϵ phase (known also as ξ' phase) is stable up to 15 at.% Ni. Furthermore, the binary AlPd and AlNi compounds with CsCl structure as well as the hexagonal Al_3Pd_2 and Al_3Ni_2 compounds form continuous ranges of solid solutions, labeled β and δ phases, respectively. No exclusively ternary phase was observed to be stable in the system. The results are compared with the ternary Al-Pd systems containing Mn, Fe, Co, Ru, Rh, or Re and the similarities are discussed. Finally, the growth paths of single crystals of the different phases are derived.

MM 3.3 Mon 10:45 IFW B

Atomic Structure Determination of Phason Planes in the ξ'-Al-Pd-Mn Phase — •H. Tian[1], W. Sun[2], and Z. Zhang[2] — [1]Institute of Physics and Center for Condensed Matter Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, China — [2]Institute of Microstructure and Property of Advanced Materials, Beijing University of Technology, 100 Pingle Yuan, Chao Yang District, Beijing 100022, China

The atomic structures of specific types of linear defects (phason lines) [1] and planar defects (phason planes) [2,3] in the complex metallic alloy phase ξ'-Al-Pd-Mn were determined by means of high-resolution electron microscopy (HREM) and theoretical HREM simulation. The results show that a representational atomic structural model for phason planes can be constructed by introducing a shift between two parts of the perfect crystalline structure using a translation vector of $r = \frac{1}{2}\alpha + \frac{1}{2\tau}\chi$. This typical phason plane is normally parallel to the (001) plane of the ξ'-Al-Pd-Mn phase and consists of phason lines which are arranged side-by-side with their linear direction parallel to the [010] axis. HREM simulations based on the structural model for both edge-on and inclined types of phason lines agree well with the experimental results. Taking into account the fact that the structural difference between various curved phason planes is due to the variation in the arrangement of individual phason lines, the atomic structures of the edge-on and inclined phason lines can be used to explain the various curved and broaden phason planes frequently observed in the ξ'-Al-Pd-Mn phase.

[1] H. Klein, M. Feuerbacher, P. Schall, K. Urban, Phys. Rev. Lett. 82 (1999) 3468. [2] H. Klein, M. Feuerbacher, P. Schall, K. Urban, Phys. Rev. Lett. 82 (1999) 3468. [3] H. Klein, M. Feuerbacher, K. Urban, Mat. Sci. Eng. 294 (2000) 769.

MM 3.4 Mon 11:00 IFW B

Atomic Structure Determination of structurally complex alloy Ψ Al-Pd-Mn Phase — •H. Tian[1], W. Sun[2], and Z. Zhang[2] — [1]Institute of Physics and Center for Condensed Matter Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, China — [2]Institute of Microstructure and Property of Advanced Materials, Beijing University of Technology, 100 Pingle Yuan, Chao Yang District, Beijing 100022, China

Base on the study of two-dimensional planar defects [1,2] (phason planes) in the complex metallic alloy phase ξ'-Al-Pd-Mn, the atomic structure of the-Al-Pd-Mn phase [3] was determined by means of high-resolution electron microscopy (HREM) observations and theoretical HREM simulations. The Ψ-Al-Pd-Mn phase has an orthorhombic unit cell with lattice parameters of a =23.54 Å, b =16.56 Å, and c =56.98 Å. The structure of the Ψ-Al-Pd-Mn phase can be characterized as stacking of phason planes in the ξ'-Al-Pd-Mn phase [4] along the c axis. The dimension along the c axis for the Ψ-phase is $\tau + 3$ times larger than that of the ξ'-phase. A close comparison between the experimental and simulated diffraction pattern, based on phason-plane stacking model, shows that both of the position and intensity distribution of the simulated diffraction pattern agree well with the experimental result. Furthermore, the simulated HREM image of the Ψ-Al-Pd-Mn phase based on above structure model matches also very well with the experimental results. All of the agreements indicate that the structural model of the Ψ-Al-Pd-Mn phase we proposed here is reasonable.

[1] H. Klein, M. Feuerbacher, P. Schall, K. Urban, Phys. Rev. Lett. 82 (1999) 3468. [2] H. Klein, M. Feuerbacher, K. Urban, Mat. Sci. Eng. 294 (2000) 769. [3] H. Klein, M. Feuerbacher, P. Schall, K. Urban, Phil. Mag. Lett. 80 (2000) 11. [4] H. Klein, M. Feuerbacher, Phil. Mag. 83(2003) 4103.

MM 3.5 Mon 11:45 IFW B

Single-crystal growth of complex metallic alloy phases — •Michael Feuerbacher[1], Marc Heggen[1], Carsten Thomas[1], Ze Zhang[2], and Ke Hsin Kuo[2] — [1]Institut fuer Festkoerperforschung, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany — [2]Beijing Laboratory of Electron Microscopy, 100080 Beijing, China

Complex metallic alloys represent a new field in materials science recently attracting increasing interest. The characteristic features of this class of materials are large lattice parameters, a high number of atoms per unit cell, and a local order which is determined by a cluster substructure frequently involving icosahedral atom configurations. The physical properties of these materials are widely unexplored, which is mainly due to the unavailability of high-quality sample materials. The growth of complex metallic alloys is in many cases difficult as the phases solidify incongruently, their primary solidification area in the phase diagrams are small, etc. Therefore, advanced growth methods have to be applied. We have developed single-crystal growth routes for a variety of complex metallic alloy phases employing Czochralski-, Bridgman,- and self-flux growth techniques. The spectrum of phases produced covers different structure types, different types of local order and elemental constituents and represents a solid materials basis for the experimental exploration of the physical properties of this class of materials. In the present contribution we report on the current state-of-the-art in materials production of complex metallic alloy phases.

MM 3.6 Mon 12:00 IFW B

Single-crystal growth of the complex metallic alloy β-Al-Mg. — •Marta Lipińska-Chwałek, Sergiy Balanetskyy, Carsten Thomas, and Michael Feuerbacher — Institut fuer Festkoerperforschung, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany

β-Al3Mg2 phase is a complex metallic alloy based on a giant unit cell (a=2.8 nm) containing approximately 1168 atoms. The material is very interesting also because of its low specific weight (2.2 g/cm3). Hardly any studies have been carried out on the physical properties of β-Al3Mg2. This is most probably due to the fact that until recently, high-quality single crystalline sample material was unavailable. We present the development of a single-crystal growth route for β-Al3Mg2. The phase diagram

was probed in the vicinity of the existence range of β-phase. We approached the growth employing various techniques, the most successful of which turned out to be Czochralski- and self-flux-growth. With both of them we reproducibly achieved single crystals of several cubic centimeters. While the Czochralski technique allows for the production of deliberately oriented single crystals, the self-flux technique is capable of the production of very large single grains. The size of which is only limited by the crucible volume. The material produced is now successfully used for the physical property investigations.

MM 3.7 Mon 12:15 IFW B

The complex metallic alloy phase $Al_{13}Co_4$: Plastic deformation properties and defects — •Marc Heggen[1], Dewei Deng[1,2], Michael Feuerbacher[1], Ze Zhang[2], and Ke Hsin Kuo[2] — [1]Institut fuer Festkoerperforschung, Forschungszentrum Juelich GmbH, D-52425 Juelich — [2]Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, Beijing, People's Republic of China

Plastic deformation experiments were performed on single crystals of the orthorhombic $Al_{13}Co_4$ complex metallic alloy phase in a temperature range between 600 and 800 °C. The stress-strain curves show a pronounced yield-drop effect followed by a regime of weak work hardening. Incremental experiments like stress-relaxation tests and temperature changes are conducted in order to determine thermodynamic activation parameters of the deformation process.

Microstructural investigations by means of transmission electron microscopy reveals that dislocation motion on (0 0 1) planes is the basic mechanism of plastic deformation in $Al_{13}Co_4$. Dislocation cores and attached planar defects were investigated by lattice fringe imaging and interpreted in terms of a tiling model. The planar defects are thin shear zones involving a phase transformation from the orthorhombic to a structurally closely related monoclinic phase. The dislocations cores are closely related to those of the metadislocations recently suggested by Feuerbacher and Heggen (Phil. Mag., 2005, in press) and possess the same Burgers vector of 2.9 Å.

MM 3.8 Mon 12:30 IFW B

Icoshedral connections in complex metallic alloy phases — •Ke Hsin Kuo[1], Z.B. He[1], Ze Zhang[2], Michael Feuerbacher[3], and K. Urban[3] — [1]Beijing Laboratory of Electron Microscopy, Institute of Physics, 100080 Beijing, China — [2]Beijing University of Technology, 100022 Beijing, China — [3]Institut für Festkörperforschung, Forschungszentrum Jlich GmbH, 52425 Jülich, Germany

The crystal structures of a number of complex metallic alloy (CMA) phases in Al-Cr-Si alloys have been determined by X-ray and electron crystallography. The basic structural unit in these structures is the icosahedron with the smaller and minor Cr atom at its center and the somewhat larger Al atom at its vertices. Icosahedra can be connected by mutual penetration along their fivefold axis to form icosahedral chains displaying a pseudo fivefold symmetry. Icosahedra can also be connected by face- and edge-sharing, thus forming chains displaying three- and twofold symmetry. Consequently, such CMA can form icosahedral/decagonal quasicrystals after very rapid solidification or the crystalline approximants with either cubic (point group m3), hexagonal (6/mmm), orthorhombic (mmm) or monoclinic (2/m) symmetry of these quasicrystals after slow solidification. These structural characteristics will be analyzed with the new structures under investigation.