MM 9 Symposium Complex Metallic Alloys II

Zeit: Freitag 15:15–16:30 Raum: TU H1058

MM 9.1 Fr 15:15 TU H1058

Prinzipien der Strukturbildung in kondensierter komplexer Materie — •P. Häussler, J. Barzola-Quiquia, W. Rauchhaupt, M. Stiehler und D. Hauschild — TU Chemnitz, Institut für Physik, 09107 Chemnitz

In ungeordneten Systemen zeigt sich immer deutlicher, dass räumlich begrenzte, sphärisch-periodische Anordnungen der Atome um jedes Aufatom existieren (Spiegelsphären statt Spiegelebenen wie im Kristall). Diese sphärisch-periodische Ordnung (SPO) bildet sich durch eine sich selbst organisierende Optimierung einer Resonanz zwischen den Valenzelektronen als Ganzem und der sich bildenden statischen Struktur. SPO ist somit das Ergebnis eines globalen Ordnungsmechanismus, der die lokale Quantenchemie ergänzt. Es wurde dabei registriert, dass SPO sowohl bei flüssigen und amorphen metallischen Systemen, aber auch Halbleitern, Isolatoren, Quasikristallen, 1/2Heusler-Legierungen und ionisch gebundenen Systemen auftritt. Verschiedentlich treten Winkelkorrelationen als weiteres resonanz-induziertes Ordnungsphänomen auf. Ob ein System elektrisch leitend ist, hängt von der Stärke der Resonanzen ab, da sich, korreliert mit diesen, eine Energielücke an der Fermikante bildet (Peierls-artig).

Es werden im Vortrag die bis heute bekannten verschiedenen Szenarien der Optimierung der Resonanzen vorgestellt. Da flüssige und amorphe Systeme die Prekursoren für Kristalle sind, sind die beschriebenen Mechanismen von grundsätzlicher Bedeutung.

MM 9.2 Fr 15:30 TU H1058

The atomic pair distribution function (PDF) as a nano-scale structure probe for CMA — •Stefan Brühne[1], Eckhard Uhrig[1], Michael Feuerbacher[2], and Wolf Assmus[1] — [1]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Robert-Mayer-Str. 2-4, D-60054 Frankfurt am Main — [2]Institut für Mikrostrukturforschung, Forschungszentrum Jülich GmbH, D-52425 Jülich

The local atomic structure of any condensed matter is accessible via the atomic pair distribution function (PDF) from powder diffraction. We recently succeeded in unraveling the local structure of some icosahedral Mg-Zn-RE (RE = Y and Ho) alloys from in-house X-ray experiments in a sphere of 5.4 nm. Synchrotron data yield better resolved PDFs though they result in the same structural units of $\sim$1.5 nm in diameter. The method also applies well to the investigation of inherent disorder of Complex Metallic Alloys (CMA). The local structures of the Mg-Zn binaries $MgZn_2$ (hP12) and Mg_4Zn_7 (mC110) are discussed: The different length scales of the local structures *vs.* large translations become directly visible. The PDF of β-Al_3Mg_2 (cF1832-664, $a \approx 2.8$ nm), one of the most complex CMA in terms of unit cell dimension and atomic disorder, is examined. PDF will serve as a probe for monitoring the local atomic structure in the course of tailoring CMA structures w.r.t. their physical and mechanical properties.

MM 9.3 Fr 15:45 TU H1058

Investigation of Ti-Base Alloys with Positron Annihilation Techniques — •Falko Baier[1], Wolfgang Sprengel[2], and Mariana Calin[3] — [1]Physical Metallurgy, TU Darmstadt, Petersenstr. 23, 64287 Darmstadt — [2]ITAP, Stuttgart University, Pfaffenwaldring 57, 70550 Stuttgart — [3]Materials Science and Engineering, University Bucharest, Romania

The research and development of Ti-based alloys for biomedical applications is focused on the development of low rigidity beta-phase Ti alloys composed of non-toxic elements with good mechanical properties and workability. A major drawback of these alloys is their poor workability. In order to overcome these limitations lots of work has been spent in order to find new Ti-alloys by varying the compositions or modifying the existing ones for the improvement of the formability. We present measurements of the positron lifetime and coincident Doppler broadening of the positron-electron annihilation photon line in as-cast and deformed Ti-base alloys in order to show the advantages of this non-destructive method for the field of engineering applications, because the sensitivity of positrons to defects in plastically deformed metals has been well-known since the 1960s. The addition of the element-sensitive Doppler broadening technique gives access to the chemical nature of the dislocation environment.

MM 9.4 Fr 16:00 TU H1058

Structures and Properties of the Refractory Silicides Ti_5Si_3 and $TiSi_2$ — •Georg Frommeyer and Rainer Rosenkranz — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The refractory titanium silicides Ti_5Si_3 and $TiSi_2$ with complex hexagonal $D8_8$ and orthorhombic C54 lattice structures exhibit some superior physical and mechanical properties, such as high lattice energies and melting temperatures; high hardness, elastic stiffness and flow stresses; low densities and excellent creep and oxidation resistance. In addition titanium silicides possess appropriate electrical and thermal conductivity, and good compatibility to silicon and titanium substrates. Therefore, these silicides are also suitable for electronic interconnections, diffusion barriers and graded bioactive glass coatings The complex lattice structures and a large constribution of covalent bonding to the total binding energies of these compounds predestine these less common quasi intermetallics to be considered for high-temperature applications in the aviation and space industry.

MM 9.5 Fr 16:15 TU H1058

Surfaces of Al-rich complex metallic alloys — •Vincent Fournée[1], Amy Ross[2], Tom Lograsso[2], Jack Barrow[2], Masahiko Shimoda[3], An-Pang Tsai[3], and Patricia Thiel[2] — [1]LSG2M, CNRS-UMR7584, Ecole des Mines, Parc de Saurupt, 54042 Nancy, France — [2]Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA — [3]NIMS, 1-2-1 Sengen, Tsukuba-shi, Ibaraki 305-0047 Japan

Understanding the structure and physical behaviour of complex metallic alloy surfaces is of key importance. Up to now, most studies have been focused on the surface structure of Al-rich quasiperiodic alloys. It is found that the surface is formed at dense Al-rich layers of the bulk structure, with no reconstruction. This result is rather surprising as even for simpler systems like periodic bimetallic alloys, surface truncation of the bulk structure can give rise to atomic and chemical rearrangements, including surface relaxation, modification of the bulk periodicity (reconstruction) or the chemical composition (surface segregation). Here, we have investigated the surface structure of some related periodic alloy phases, namely the xsi-AlPdMn approximant, which is an orthorhombic crystal with a large unit cell. The surface perpendicular to its pseudo ten-fold axis was investigated by STM, LEED and XPD. The surface structure can also be interpreted as bulk-terminated, corresponding to dense Al-rich layers of the bulk structure. Similarities and differences between the quasicrystal and its periodic approximant will be outlined.