# MM 38: Structural materials

Time: Wednesday 10:15–11:45 Location: IFW B

MM 38.1 Wed 10:15 IFW B

**Relation between thermodynamic stability and stacking fault energies in Mg alloys: An ab-initio study** — •Zongrui Pei[1,2], Li-Fang Zhu[1], Martin Friák[1], Stefanie Sandlöbes[1], Stefan Zaefferer[1], Bob Svendsen[1,2,3], Dierk Raabe[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Germany — [3]Faculty of Georesources and Materials Engineering, RWTH Aachen University, Germany

Pure magnesium and most commercial wrought magnesium alloys exhibit a low room temperature ductility which can be significantly increased by the addition of Y or rare earth (RE) elements (Acta Mater. 59 (2011) 429). Understanding the mechanisms causing this ductility enhancement on an atomistic and electronic-structure level would provide a systematic approach to identify alternative favorable solutes. Therefore, in order to obtain a deeper insight into the mechanisms active in the Mg-Y and Mg-RE alloys, an ab-initio study of the compositional dependence of intrinsic stacking fault (ISF) energies have been performed. Employing density functional theory (DFT) calculations, the ISF energies have been determined within the Axial Next-Nearest-Neighbour Ising (ANNNI) model. An in-depth analysis of the theoretical data shows reduced ISF energies as a direct consequence of the dramatically reduced thermodynamic stability of hexagonal Mg-Y solid solutions when the Y concentration approaches its solubility limit in Mg (Acta Mater. 60 (2012) 3011).

MM 38.2 Wed 10:30 IFW B

**The effect of extreme uniaxial and biaxial loading conditions in transition-metal disilicides: an ab initio study** — Dominik Legut[1], •Martin Friák[2,3,4], Mojmír Šob[4,3,5], and Jörg Neugebauer[2] — [1]Nanotechnology Centre & IT4Innovations, VSB-Technical University of Ostrava, Ostrava, Czech Republic — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [3]Institute of Physics of Materials, AS CR, v.v.i. Brno, Czech Republic — [4]Central European Institute of Technology (CEITEC MU), Masaryk University, Brno, Czech Republic — [5]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Transition-metal disilicides constitute a promising basis for a new generation of high-temperature structural materials that can significantly improve the thermal efficiency of energy conversion systems and advanced engines. Although they have been studied quite intensively, the complexity of their mechanical behavior is still not completely understood. Employing first-principles (ab initio) calculations of electronic structure, we investigate the effect of uniaxial loading for disilicides with hexagonal C40 structure, namely for $NbSi_2$, $CrSi_2$, $VSi_2$ and $TaSi_2$, and compare their behavior with previously studied $C11_b$ structure disilicides. Further, the C40 structure disilicides are subjected to biaxial loading and the values of strains are extended up to their extreme levels, beyond materials stability limits represented here by the values of theoretical tensile strength. We find a direct correspondence between the electronic structure characteristics and the onset of strength instability.

MM 38.3 Wed 10:45 IFW B

**High Strength Light-Metal composites** — •Juliane Scharnweber[1], Jan Romberg[2], Andy Eschke[1], Carl-Georg Oertel[1], Tom Marr[2], Jens Freudenberger[2], Ludwig Schultz[2], Ilya Okulov[2], Uta Kühn[2], Jürgen Eckert[2], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, D-01171 Dresden, Germany

Ti/Al laminated sheets were produced by accumulative roll bonding (ARB) at ambient temperature. Intermediate annealing was found to be suitable to overcome the issue of layer-crossing shear band formation usually observed for comparable metal combinations. This treatment resulted in composite sheets of technically relevant size with layer stability down to thicknesses of about 2 *m. The microstructure and local texture was characterized by scanning electron microscopy combined with electron backscatter diffraction, while the global texture was measured by neutron diffraction. Strength and ductility were measured in tension. The evolution of microstructure, texture and strength is described and discussed with regard to number of ARB cycles and annealing temperature. Additionally, the formation of intermetallic phases at the interfaces is addressed.

MM 38.4 Wed 11:00 IFW B

**Delta' precipitation in Al-Cu-Li alloys** — •Pascal Neibecker[1], Haider Ferdinand[1], and Al-Kassab Tala'at[2] — [1]University of Augsburg, Augsburg, Germany — [2]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Due to their high strength, high Young's modulus and low density, Al-Cu-Li alloys are of special interest in aerospace applications. The process mainly responsible for the excellent mechanical properties of these alloys is precipitation hardening. Understanding the microstructure evolution upon artificial aging of Al-Cu-Li alloys and the corresponding underlying mechanisms is thus of great importance. In mechanically untreated binary Al-Li and ternary Al-Cu-Li alloys with a high Li content, the major hardening phase is the metastable delta' (Al3Li) phase which already partly develops during natural aging of the alloy. The formation mechanism leading to delta' precipitation thereby was controversially discussed in the last decades.

This work investigates the kinetics of the delta' evolution in an Al- 1.7 at. % Cu- 5.6 at. % Li model alloy upon artificial aging at 160 °C with Differential Scanning Calorimetry and Atom Probe Tomography. Here, the volume fraction and size evolution of the delta' phase is determined and additionally, by using the Pearson coefficient, quantitative statements about Li and Cu ordering in the alloy are made. The findings give insights into the formation mechanism of the delta' phase in Al-Cu-Li alloys.

MM 38.5 Wed 11:15 IFW B

**High-temperature interactions of liquid aluminum with titanium diboride ceramic** — •Lixia Xi[1], Rafal Nowak[2], Ivan Kaban[1,3], Bartlomiej Korpala[2], Grzegorz Bruzda[2], Natalia Sobczak[2], Norbert Mattern[1], and Jürgen Eckert[1,3] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 270116, 01171 Dresden, Germany — [2]Foundry Research Institute, Center for High-Temperature Studies, Zakopianska Str. 73, 30-418 Cracow, Poland — [3]TU Dresden, Institute of Materials Science, 01062 Dresden, Germany

Temperature-dependent interactions in the liquid Al/TiB2 ceramic system has been investigated by the sessile drop technique in the temperature range from 700 to 1400 C. The microstructure of the Al/TiB2 interfaces in the solidified couples after sessile drop tests has been characterized by scanning electron microscopy, coupled with an energy-dispersive X-ray spectroscopy and X-ray diffraction. Up to about 800 C, pure Al exhibits rather poor wetting and a weak reactivity with TiB2 ceramic; only few titanium aluminide particles were found to be formed at the interface. Starting from 800 C, the wetting improves either with time or upon further heating. Above 1000 C liquid Al completely spreads over the ceramic and penetrates along the TiB2 grain boundaries or into the pores. Al3Ti and Al2O3 were found to precipitate at the interface.

MM 38.6 Wed 11:30 IFW B

**Structural analysis of dissimilar Al-Ti FSW joints** — •Roland Marstatt[1], Markus Krutzlinger[2], Maximilian Gnedel[1], Ferdinand Haider[1], and Michael F. Zaeh[2] — [1]Lehrstuhl fuer Experimentalphysik I, Universitaet Augsburg, Augsburg, Germany — [2]Institut fuer Werkzeugmaschinen und Betriebswissenschaften (iwb), Technische Universitaet Muenchen, Garching, Germany

Friction Stir Welding (FSW) is a suitable technology to join dissimilar materials. In contrast to fusion welding processes the material does not exceed the solidus temperature during FSW. As a consequence high quality joints can be produced with a minimum of deleterious intermetallic phases. Due to the process conditions, FSW seems to be a good choice to form dissimilar joints as e.g. between aluminium and titanium alloys. However, a comprehensive description of the effective joining mechanisms of friction stir welded dissimilar material joints - formation of metallic bonds vs. interlocking mechanisms - is still a subject of research.
In this study first results of the analysis of the effects on the structure of the weld seam caused by stirring material flow are presented. FSW-joints of aluminium and titanium alloys in lap joint configuration have

been investigated under varying process conditions. The results seem to show a transport of Ti into Al, which leads to considerable solid solution hardening close to the weld seam. But until now, no indication for the formation of brittle intermetallic phases has been found. Furthermore, the thermal stability of the joint with possible formation of intermetallic phases and subsequent embrittlement was studied.