MM 3: Microstructures and Phase Transformations: Metals & Alloys

Time: Monday 10:15–12:45 Location: H45

MM 3.1 Mon 10:15 H45

Analysis of the precipitates in rapidly quenched Al-Cu alloys obtained in a magnetic pulse weld and through a melt spinning process — •David Stein, Maximilian Gnedel, and Ferdinand Haider — Universität Augsburg, Institut für Physik, Universitätsstraße 1, 86159 Augsburg, Germany

Magnetic pulse welding (MPW) is a collision welding technique, where a flyer is accelerated towards a target using induced magnetic fields. This technique enables the welding of dissimilar metals. The microstructure of the interface is well described in the literature and typically displays a wave like structure. In the eye and wake of these waves an area of intermetallic phases can be found, depending on the materials and welding parameters. In this case an Al 1050 flyer and Cu DHP target were used. The structure of the interface has given strong indications of melting. Atomic resolution HAADF STEM was performed on this part and GP I and GP II Zones and disc shaped Θ' phases were found in the same area. The latter typically only form after longer heat treatments at elevated temperature. Albeit the theoretically predicted shape of Θ' Phases is disc shaped with very large diameter to thickness ratio, in the case studied here, they are much more compact and have a far smaller diameter to thickness ratio. The current working hypothesis is, that in the MPW process rapid solidification of the melt occurs, which leads to a high density of excess vacancies in the crystal structure, allowing for higher atom mobility. In an ongoing study we follow the precipitation process in rapidly quenched Al-Cu alloys obtained through a melt spinning process.

MM 3.2 Mon 10:30 H45

Crystal nucleation in undercooled Cu-Ge melts — •Manoel W. da Silva Pinto, Martin Peterlechner, and Gerhard Wilde — Institut für Materialphysik, WWU Münster

Experimental calorimetric data obtained by differential thermal analysis on the nucleation of undercooled Cu-Ge melts are presented. Deep undercooling levels have been reached throughout the entire composition range of this binary alloy in an experimental setup using an inorganic glass as an embedding medium. The heating and cooling cycles are statistically analyzed and lead to quantitatively determining nucleation rates independent of a specific nucleation kinetics model. Parameters of the classical nucleation theory, such as the kinetic prefactor and nucleation work, are extracted. We further discuss the data using different solution models for the alloy melts and consider their impact on nucleation kinetics. Thus, the nucleation kinetics parameters for the binary alloy system have been determined as a function of composition throughout the entire composition range and allow comparison with simplified models for concentration-dependent nucleation kinetics.

MM 3.3 Mon 10:45 H45

Experimental investigation of the early stage precipitation reactions in Al-Cu alloys — •Johannes Berlin, Tobias Stegmüller, and Ferdinand Haider — Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsburg

Due to their superior strength to weight ratio heat treatable Al-Cu alloys (2XXX-Series) are widely used particularly in aerospace industry. Although the hardening precipitates in these alloys are well-known, the very early stages of decomposition are still topic of ongoing research. Based on state-of-the-art scanning transmission electron microscopy, single Cu atoms can be imaged and natural ageing in form of Guinier*Preston zone formation accelerated by excess vacancies can be investigated, which was possible before only by diffraction experiments. Scanning transmission electron microscopy is used to investigate the influence of different parameters, such as thermal history, on early-stage precipitation in Al. The growth of GP I Zones is followed by ex-situ recording of a detailed time series during natural aging. In addition, resistivity and hardness measurements are performed to evaluate the temper state of the specimens. The results are compared to numerical simulations. A better understanding of the mechanisms leading to precipitate formation in these alloys for light-weight construction could be tuned more precisely regarding their intended use.

MM 3.4 Mon 11:00 H45

2D precipitate growth in a 3D matrix – Revealing the kinetics of Guinier–Preston zone formation in Al–Cu from atomic Monte Carlo — •Tobias Stegmüller and Ferdinand Haider — University of Augsburg, Universitätsstr. 1, 86159 Augsburg, Germany

Guinier–Preston zones (GPZ) in Al–Cu, constituting the precipitate phase that was already responsible for the hardness increase in the first age-hardenable Al-alloy about 115 years go, still attract attention first because of their special atomic mono- up to multilayer structure of Cu atoms and second due to their even at room temperature occurring formation, requiring an unexpected fast Cu diffusion.

To understand the origin of the GPZ structure, we performed Monte Carlo (MC) simulations mimicking precipitate growth by applying a Cluster Expansion (CE) for Al–Cu. From this we were able to identify an energy barrier above and below the layers of GPZ that is hardly overcome by migrating Cu. With this barrier we are able to explain the morphology of GPZ from a perspective focussing on the growth kinetics. On the one hand, the barrier guides migrating Cu to the layers' edges, supporting 2D growth. On the other hand, Cu atoms moving towards the layers' faces are stopped by the barrier, leading to nucleation of further Cu layers and explaining the multilayer shape.

To study the origin of the high Cu mobility, we recently included vacancies into simulations by switching from the CE based rigid lattice MC to a MC method allowing lattice relaxations by using a neural network interatomic potential. We present first results from this approach with regard to the interaction of vacancies with GPZ.

MM 3.5 Mon 11:15 H45

Atomic-scale observation of silver segregation in a high angle grain boundary in copper — •Lena Frommeyer, Tobias Brink, Gerhard Dehm, and Christian Liebscher — Max-Planck-Str. 1, 40213 Düsseldorf

Although it is well recognized that segregation to grain boundaries (GBs) influences mechanical and electrical properties of materials, the impact of segregation on individual GB phases is poorly understood on the atomic level. Thermodynamic models are established to describe equilibrium segregation, but the atomistic origins and direct observation of solute segregation inside the GB core structure are seldomly investigated since high resolution imaging and spectroscopy are required.

Lately, we were able to resolve the atomic structure of a symmetric Σ 37c <111> {3 4 7} tilt GB in a Cu thin film using aberration-corrected high angle annular dark field scanning transmission electron microscopy (HAADF-STEM). By depositing a 100 nm thin Ag layer on top of our 2 μm-thick Cu thin film and subsequent annealing at 600°C, we could investigate the effect of Ag segregation on these GBs. Interestingly, the structure of the GB remains unchanged. Ag atoms solely substitute specific sites in the GB. If the Ag content in the GB is increased, one atomic column in the GB structure is filled up first, followed by four other columns. A combination of atomic resolution energy dispersive X-ray spectrometry, HAADF-STEM experiments and atomistic simulations were used to explore the underlying mechanisms leading to the observed Ag segregation pattern.

15 min. break

MM 3.6 Mon 11:45 H45

Grain boundary phase transitions and patterning in a copper tilt grain boundary — •Tobias Brink[1], Lena Frommeyer[1], Rodrigo Freitas[2], Timofey Frolov[3], Christian H. Liebscher[1], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Germany — [2]MIT, USA — [3]LLNL, USA

The atomic structure of grain boundaries (GBs) can exhibit different "phases" (also called complexions), which undergo thermodynamic phase transitions, but which have been observed in just a few simulation studies. Experimental confirmation often remains indirect. Here, we report on such a transition investigated by molecular dynamics computer simulations and supported by direct evidence from STEM imaging [1]. Two distinct atomistic structures could be found in a Σ37c [111] tilt GB by a search with an evolutionary algorithm. Free energy calculations using the quasi-harmonic approximation predict a GB phase transition at 460 K. In the experiment, both phases also occur, but exhibit a pattern at room temperature in which the two

phases alternate. We present a hypothesis to explain this thermodynamically unexpected phenomenon by elastic interactions of the phase junctions, which are line defects with partial dislocation character.

Acknowledgment: This result is part of a project that has received funding from the ERC under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 787446).

[1] Frommeyer, Brink et al., "Dual phase patterning during a congruent grain boundary phase transition in elemental copper" Nat. Commun. (accepted, 2022)

MM 3.7 Mon 12:00 H45

Structural and thermal characterisation of a AuGe alloy via electron microscopy and fast differential scanning calorimetry — •Štefan Stanko[1], Jürgen Schawe[1,2], and Jörg Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Mettler-Toledo GmbH, Analytical, 8606 Nänikon, Switzerland

A device combining scanning electron microscopy (SEM) and fast differential scanning calorimetry (FDSC) was developed to perform *in situ* characterisation of metastable phase transformations. The potential of this device is demonstrated on the example of a AuGe eutectic alloy. Upon rapid cooling, the alloy forms the metastable crystalline phases β and γ and an amorphous phase. A thin lamella for transmission electron microscopy (TEM) was produced from a sample prepared in FDSC to further characterise the microstructure of the alloy beyond the capabilities of the *in situ* device. *Ex situ* FDSC experiments were performed using cooling and heating rates of several 1000 K/s to characterise the thermal behaviour of the β and γ phase. The transformation kinetics of the metastable phases was investigated. Finally, we show that we can prepare the glassy phase in FDSC and determine its thermophysical properties.

MM 3.8 Mon 12:15 H45

Phase decomposition in nanoporous Au-Pt — •Maowen Liu[1,2] and Jörg Weissmüller[1,2] — [1]Institute of Materials Mechanics, Helmholtz-Zentrum Hereon — [2]Institute of Materials Physics and Technology, Hamburg University of Technology

Nanostructured Au-Pt system has attracted great attention for its broad applications in catalysis. Due to the miscibility gap for a large range of composition and temperature in bulk Au-Pt system, a comprehensive understanding of the structure transformation at various temperatures is necessitated. In the present work, nanoporous Au-Pt prepared by dealloying is selected for the investigation of the microstructure evolution during annealing. Dealloying transforms the homogeneous, ternary bulk solid solution Ag-Au-Pt into a nanoporous Au-Pt solution that would be immiscible at thermodynamic equilibrium. Remarkably, in view of the substantial atomic-scale rearrangement at the dissolution front, our experiments confirm a homogeneous Au-Pt solid solution. Upon annealing-induced coarsening, the phase structure evolves to semicoherent two-phase by way of an intermediate, coherent two-phase state.

MM 3.9 Mon 12:30 H45

Microstructural characteristics of lean magnesium alloys — •Tatiana Akhmetshina, Leopold Berger, Samuel Montibeller, Robin E. Schäublin, and Jörg F. Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Lean magnesium alloys with less than 1 at.% of alloying elements are of high interest for biodegradable implant applications, where the implant remains only temporarily in the body, but degrades after it has fulfilled its task. With a specific combination of requirements, such as biocompatibility, appropriate mechanical properties and low degradation rate, such alloy development is still challenging. Here, we tailored the mechanical properties of lean Mg-Ca alloys by hot extrusion. The optimal alloying range was obtained via thermodynamic calculations using Pandat. The alloys were cast and extruded at the same ratio with different speeds and temperatures. A tensile toughness of up to 76 MJ/m^3 was obtained, indicating a superior combination of strength and ductility. Depending on the extrusion parameters, the alloys exhibit a tensile strength of more than 420 MPa or, alternatively, a high ductility of up to 35% elongation at fracture. To obtain a clear understanding of the relationship between mechanical properties and microstructure, the latter was investigated by SEM, TEM and EBSD, focusing on precipitation, grain morphology, and dislocation structure. The grain size varied from submicrometer to several tens of micrometers. Apart from weak texture, the most ductile materials revealed an intriguing activation of <c+a> pyramidal slip.