

MM 3: Topical Session: Sustainable metallurgy

Time: Monday 10:15–13:00

Location: C 130

Topical Talk

MM 3.1 Mon 10:15 C 130

Sustainable Green Ceramics: Future and Perspectives — ●JENNIFER L.M. RUPP — Technische Universität München, Lehrstuhl für Chemie der Festkörperelektrolyte, Lichtenbergstraße 4, 85748 Garching

Next generation of functional ceramics rely on new ways to not only exchange single elements but looking ahead at redefining sustainable synthesis at low energy and CO₂ footprint. The ways we have synthesized functional ceramics for energy storage and conversion devices like batteries, fuel cells, electrolyzers, and commodities such as gas turbine, construction, medical and other sectors has been very much laid out over the last 50 years to tackle mostly price. However, as climate change progresses and with 25% of our CO₂ footprint stemming solely from transportation and material making and assembly in steel and ceramic industry, we need to consider what are alternative and new synthesis ways that drastically reduce our needs in material making. Aspects like socio-economic equality on green materials made at lower footprints and also supply chain security are of essence and we as scientist have to step up the game to propose hods on how solid state chemistry, physics and synthesis can be altered to meet sustainability goals. Through the talks examples on functional ceramic trends for physics and chemistry application and devices will be selected per material class, and we will exemplify on the show case of Li⁺ ion batteries current tech trends and how novel solid state chemistry and physics can support to offer alternatives for a new generation of green functional ceramics at work.

MM 3.2 Mon 10:45 C 130

Data-Driven Design of Recycling Processes for Lithium Ion Batteries — ●NIMA EMAMI¹, LUIS GOMEZ-MORENO², ANNA KEMETTINEN², RODRIGO SERNA-GUERRERO², and MILICA TODOROVIC¹ — ¹University of Turku, Turku, Finland — ²Aalto University, Espoo, Finland

Shifting our focus from mining to extracting materials from waste is essential for sustainable and environmental resource management. We combine lithium-ion battery recycling process simulations with data science to redesign the process for optimal materials recovery, prior to experimental validation. Starting with a model process, we altered processing parameters to simulate 10,000 process outcomes and monitored material flow to identify which parameters maximize the recovery of materials mass for graphite and LiNiMnCoO₂ (NMC).

The data analysis shows that the first selected design was suboptimal: while up to 91% of graphite mass could be recovered, its purity was lacking at 70%, and NMC average mass recovery was only 6%. Given that no parameter combination could resolve this problem, we modified the processing stages and repeated the simulations with the enhanced process. We now observed the average graphene purity rise to 99%, while a much broader range of NMC mass outputs indicated that recovery of up to 92% of input mass was possible. Data analysis allowed us to determine parameter combinations that simultaneously optimise the recovery of both graphite and NMC. This study demonstrates that data-driven approaches provide new insights into recycling processes and can facilitate systemic optimisation and design.

MM 3.3 Mon 11:00 C 130

On the origin of embrittlement in Mn containing and Zn-coated steels — ●REZA DARVISHI KAMACHALI — Federal Institute for Materials Research and Testing (BAM)

Grain boundary embrittlement in medium-Mn steels and liquid metal embrittlement (LME) in Zn-coated high strength steels are among key challenges on the way of safe application of sustainable steels for automotive industry. Using a novel density-based model for grain boundaries, we reveal that the affinity of a grain boundary to attract Mn and Zn atoms result in a segregation transition accompanied by interfacial structural changes. In case of the Zn, the simulations show that the amount of segregation abruptly increases with decreasing temperature, while the Zn content in the alloy, required for triggering the segregation transition, decreases. The results are discussed in the context of CALPHAD-integrated density-based grain boundary phase diagrams.

MM 3.4 Mon 11:15 C 130

Development of an interatomic potential for iron and its ox-

ides for direct reduction applications — ●BAPTISTE BIENVENU¹, MIRA TODOROVA¹, JÖRG NEUGEBAUER¹, MATOUS MROVEC², YURY LYSOGORSKIY², RALF DRAUTZ², and DIERK RAABE¹ — ¹Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — ²Interdisciplinary Centre for Advanced Materials Simulation, Ruhr Universität Bochum, 44780 Bochum, Germany

Atomistic modeling of iron oxides poses many great challenges, due to their combined structural and electronic complexities, down at the level of electronic structure calculations and up to the length and time scales relevant for the study of mechanisms involved, for instance, in the process of their direct reduction. To leverage these limitations in terms of accessible scales, one requires a physically justified interatomic potential with sufficient accuracy to correctly account for the complexity of iron-oxygen systems, which is not yet available in the literature. In this work, we propose a machine-learning potential based on the Atomic Cluster Expansion for modeling the iron-oxygen system, with an explicit account of magnetism. The model is fitted on an extensive density functional theory database encompassing pure iron and the whole range of possible oxygen containing structures. We test the potential on a wide range of properties of iron and its oxides, including defects and relative stability between different crystal structures and magnetic orders, and demonstrate its ability to describe the thermodynamics of systems spanning the whole range of oxygen content and including magnetic degrees of freedom.

15 min. break

MM 3.5 Mon 11:45 C 130

Artificial negative pressure in DFT+U calculations for iron oxides — ●HAO CHEN, CHRISTOPH FREYSOLDT, MIRA TODOROVA, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Off-stoichiometric iron oxides play a crucial role in the process of iron ore reduction. The thermal stability and transformation kinetics of relevant iron oxides depend sensitively on magnetic, configurational, and vibrational degrees of freedom and their interplay, but our understanding in this regard is still limited. In addressing this issue, it's imperative to first achieve a precise and reliable description of the iron oxides, in particular their electronic properties and stability. We employ DFT+U, which is an efficient tool for studying strongly correlated systems, to investigate the stability of Hematite (Fe₂O₃), Magnetite (Fe₃O₄), and Wüstite (FeO). We find that the Hubbard U parameter and details of how the projection onto the correlated subspace is implemented may modify even basic materials parameters such as the equilibrium volume by several percent, indicating that the actual ad-hoc choices influence the prediction of lattice constants and bond lengths. We analyze in detail the factors that may contribute to and influence this phenomenon, and explore possible solutions to mitigate the dependence of volume on U.

MM 3.6 Mon 12:00 C 130

Multi-technique investigation of Fe-rich intermetallic compounds for more impurity-tolerant Al alloys — ●SHIKANG FENG¹, YILUN GONG², JÖRG NEUGEBAUER², DIERK RAABE², ENZO LIOTTI¹, and PATRICK S. GRANT¹ — ¹University of Oxford, UK — ²Max-Planck-Institut für Eisenforschung GmbH, Germany

During Al alloy solidification, Fe impurities precipitate as coarse (up to millimetres), anisotropic Fe-rich intermetallic compounds (IMCs), severely undermining tensile ductility and toughness, hindering Al recycling. Increasing effort is made to understanding the formation and growth of these IMCs, for a better control of their type, morphology, size and distribution for more sustainable, impurity-tolerant Al recycling processes. In this work, we use *in situ* synchrotron X-ray radiography to study systematically the formation and growth kinetics of Al₁₃Fe₄ in a model Al-3wt.%Fe alloy, at cooling rates 0.5–20 Ks⁻¹, representative of industrial conditions. These are then combined with post-solidification electron backscattered diffraction, X-ray computed tomography and atomic-resolution scanning transmission electron microscopy to elaborate on the role of twinning in Al₁₃Fe₄ formation and growth mechanisms. Finally, we show how we fuse the multi-technique insights to control the size and morphology of otherwise coarse, plate-like Al₁₃Fe₄ using twinning-based modification. The role of targeted

alloying additions in the modification and their interplay with twin boundaries is rationalised by density functional theory calculations and atomistic simulations. The work paves a potential pathway to designing next-generation, impurity-tolerant recycled Al alloys.

MM 3.7 Mon 12:15 C 130

On the development of Ni-Fe-Cu anodes for sustainable, CO₂-free aluminium electrolysis — •TOM JAMIESON¹, RALF BUSCH¹, ANDREI IASINSKII², JON MAGNUSON³, GUDMUNDUR GUNNARSSON⁴, PEER DECKER⁵, ROMAN DUESSEL⁵, and ISABELLA GALLINO¹ — ¹University of Saarland, Saarbruecken, Germany — ²RWTH Aachen University, Aachen, Germany — ³IceTec, Reykjavik, Iceland — ⁴Arctus Metals Ltd, Reykjavik, Iceland — ⁵TRIMET Aluminium SE, Germany

CO₂-free aluminium could be produced from renewable energy sources through an electrolytic process by using inert anodes and wetted drained cathodes as a sustainable substitute to the Hall-Héroult process. Primary aluminium production is a worldwide, energy intensive industry with estimates suggesting the contribution to the global tonnage of greenhouse gas emissions is as high as 1%. The use of consumable carbon anodes in the Hall-Héroult process is a significant contributor to greenhouse gas production, with 1.5t of CO₂ produced per tonne of aluminium.

Ni-Fe-Cu alloys have emerged as a strong candidate for inert anodes with a study spanning large parts of the composition space currently lacking. Our work aims to undertake a systematic investigation of the key anodic properties (corrosion resistance, cell stability, purity of resultant aluminium) as a function of the alloy composition to determine an optimal composition range for electrolysis cell performance.

MM 3.8 Mon 12:30 C 130

Order-disorder transitions on alloy surfaces: Full Monte Carlo thermodynamic averages versus Calphad inspired analytical models — JING YANG, •MIRA TODOROVA, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, D-40237 Düsseldorf, Germany

In this work, we propose an analytical thermodynamic model to de-

scribe the order-disorder transition on the surface of a metal alloy with substitutional defects. We apply this model on the system of Mg surface with Ca substitutions. First, we show the occurrence of a surface phase transition by using Monte Carlo simulations coupled with cluster expansion. Specifically, the system undergoes a transition from a disordered phase at high temperature and Ca-poor conditions to an ordered phase with 1/3 monolayer Ca coverage at low temperature and Ca-rich conditions. Then we show that with an analytical model which assumes Boltzmann distribution of the phase fractions, it is possible to accurately reproduce the critical transition condition. Last, we compare our method to the sublattice model, which is commonly used in the CALPHAD approach to describe solution phases with ordering. The proposed method provides a simplified model for describing order-disorder transition and is potentially applicable also to constructing bulk phase diagrams.

MM 3.9 Mon 12:45 C 130

Segregation behavior in Ni-based superalloys — •AHMED ABDELKAWY, MIRA TODOROVA, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Max-Planck-Str.1, 40470 Düsseldorf

Precipitation-hardened nickel-based superalloys are widely used in aerospace and oil and gas industries due to their high strength and corrosion resistance properties that are retained even at elevated temperatures. The exceptional high-temperature strength characteristics are due to the dispersion of intermetallic phases, such as γ' (Ni₃(Al, Ti)) and γ'' (Ni₃Nb), within the γ (Ni) Matrix. The corrosion resistance is attributed to the presence of Cr, Nb, and Mo as solid solution within the matrix. The interplay between the matrix, the intermetallic phases, and the dispersed solid solution elements may influence the alloys' properties but remains largely unexplored due to the complexity of the multicomponent nature of these systems. In this study, we examine the segregation behavior of the alloying elements into and around the intermetallic phases and its effect on the corrosion-resistant characteristics of the superalloys. Moreover, we systemically study the thermodynamic stability of the various defects and formed interfaces by constructing defect phase diagrams.