MM 24: Non-equilibrium Phenomena in Materials Induced by Electrical and Magnetic Fields 4

Crystal structures

Time: Wednesday 15:45–18:30 Location: H45

Topical Talk MM 24.1 Wed 15:45 H45

Electromigration effects on the atomic ordering process in hard magnetic $L1_0$ intermetallic phases — •Daniel Urban[1,2] and Christian Elsässer[1,2] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg — [2]Freiburger Materialforschungszentrum, Stefan-Meier-Straße 21, 79104 Freiburg

High-performance permanent magnets are needed for many applications in energy and information technology. The $L1_0$ phase of FeNi is a promising candidate for a sustainable material that is free of rare-earth elements. However, on earth FeNi can only be found in the disordered A1 crystal structure, although the layered $L1_0$ structure is lower in energy. By contrast, the latter was found in meteorites, proving the astronomical long timescales required for the dynamical ordering of the material.

We investigate the atomic migration processes in binary intermetallic $L1_0$ phases within the framework of density functional theory. Our main objectives are (i) to develop a thorough understanding of the possibilities to enhance the thermally activated diffusion processes at the atomic scale by electric fields and currents and (ii) an assessment in how far electromigration effects can be effective in processing hard magnetic materials. We extend the scope to the hard magnetic $L1_0$ phases of FePt, FePd, MnAl and MnGa as well as ternary Fe(Pt,Ni). These alloys cover a wide range of thermal ordering time scales and related experimental feasibilities.

MM 24.2 Wed 16:15 H45

Deriving Macroscopic Diffusivity from a Microscopic Master Equation Approach — •Daniel Pfalzgraf[1,2], Daniel Urban[1,2], and Christian Elsässer[1,2] — [1]Freiburg Materials Research Center (FMF), University of Freiburg, Stefan-Meier-Straße 21, 79104 Freiburg, Germany — [2]Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

We present our generalisation of a model formalism that allows the derivation of macroscopic diffusion properties of a crystalline material from jump rates of individual atoms or ions. This work is based on a mathematical formalism modelling the uncorrelated motion of particles on a lattice by a Markov chain, from which a master equation in time and space is constructed. This approach is discussed, reformulated, and generalised to be applicable to any three-dimensional crystal system. Specifically, it is capable of describing the diffusion and drift of particles in a tilted potential landscape, as e.g. induced by electric fields. We sketch multiple use cases for systems involving point defects and grain boundaries and use the derived framework to discuss the diffusion of oxygen vacancies in strontium titanate.

MM 24.3 Wed 16:30 H45

Atomistic calculations of charged point defects at grain boundaries in $SrTiO_3$ — •Cong Tao[1], Daniel Mutter[1], Daniel Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

Oxygen vacancies have been identified to play an important role in accelerating grain growth in polycrystalline perovskite-oxide ceramics. To advance the fundamental understanding of growth mechanisms at the atomic scale, we performed classical atomistic simulations to investigate the atomistic structures and oxygen vacancy formation energies at grain boundaries in the prototypical perovskite-oxide material $SrTiO_3$ [1]. We focus on two symmetric tilt grain boundaries, namely $\Sigma5(310)[001]$ and $\Sigma5(210)[001]$. Electrostatic potentials are present in supercells containing alternatingly charged lattice planes and grain boundaries. We derive analytic solutions for these potentials for both open and periodic boundary conditions and apply them to our atomistic model structures. In this way, simulation artifacts resulting from the interaction of the electrostatic potential with charged point defects can be corrected, leading to physically reasonable defect energies. We report calculated formation energies of oxygen vacancies on all possible sites across boundaries between the two misoriented grains, and we analyze the values with respect to local charge densities at the vacant sites. The developed calculation procedure can be transferred to more complicated interfaces such as asymmetric tilt grain boundaries [2].

[1] C. Tao, et. al., Phys. Rev. B 104, 054114 (2021).

[2] C. Tao, et. al., arxiv.org/abs/2110.02118.

MM 24.4 Wed 16:45 H45

Field assisted sintering of piezoelectric-bioactive scaffolds for bone tissue engineering — •Abdullah Riaz[1], Christian Polley[1], Eberhard Burkel[2], and Hermann Seitz[1] — [1]Chair of Microfluidics, Faculty of Mechanical Engineering and Marine Technology, University of Rostock, Rostock, Germany — [2]Institute of Physics, University of Rostock, Rostock, Germany

The treatment of critical size bone defects is still a challenge. The external material is often needed to support bone and guide tissue regeneration by physical stimulation. Promising effects of electrical stimulation on bone cell growth have led to an interest in using piezoelectric ceramics for tissue repair. Nevertheless, it is still concerning due to the toxicity of ceramics, which exhibit ion dissolution in biological fluids. In this study, nanostructured pure and doped calcium titanate is prepared by sol-gel synthesis and field assisted sintering. The piezoelectric behaviour is observed in calcium titanate, which is also a non-cytotoxic compound. This behaviour is referred to as pseudo-piezoelectricity since it is generated by the distorted structure which is formed during densification by field assisted sintering. Additionally, piezoelectric barium titanate-45S5 bioactive glass composites are combined with titanium alloy Ti6Al4V for the potential implantation of piezoelectric-bioactive scaffolds in load-bearing areas. For the engineering of these bulk scaffolds, electron beam melting is utilized for manufacturing metallic load-bearing lattice structures and combined with piezoelectric-bioactive composites for the joint processing via field assisted sintering.

15 min. break

MM 24.5 Wed 17:15 H45

Microstructure and hardness of self-passivating SMART alloys manufactured via field assisted sintering technology — •Jie Chen[1], Andrey Litnovsky[1], Xiaoyue Tan[2], and Christian Linsmeier[1] — [1]Forschungszentrum Jülich GmbH, IEK-4, 52425 Jülich, Germany — [2]School of Materials Science and Engineering, Hefei University of Technology, 230009 Hefei, China

Self-passivating Metal Alloys with Reduced Thermo-oxidation (SMART) with a composition of W-11.4wt%Cr-0.6Y% is a promising candidate for plasma facing material of a future fusion power plant. In addition to sputtering resistance under plasma exposure, the laboratory-made bulk SMART system has exhibited excellent antioxidation performance at 1273K in humid environment relevant to accident conditions. The field assisted sintering technology is applied to manufacture SMART alloy. The microstructure of SMART alloy is intimately related to production parameters including heating ramp, sintering temperature, thermal holding time and applied pressure. Heating rate and appropriate sintering temperature are considered important to obtain ultrafine or nanosized grain. The machinability of sintered SMART alloy is under investigation in which hardness and thermal conductivity are of particular interest. The as-sintered SMART alloy with 1217 HV0.5 is obtaned by heating at a rate of 200K/min to 1460*C and applying pressure of 50 MPa. There is an attempt to reduce the material*s hardness to facilitate its application in fusion reactor. Details of the work are presented in the contribution.

Topical Talk MM 24.6 Wed 17:30 H45

From Uncovering the Mechanisms of Flash Sintering to Realizing Ultrafast Sintering without Electric Fields and Discovering Electrochemically Driven Microstructural Evolution — •Jian Luo — University of California San Diego, U.S.A.

This talk will first review our recent studies on understanding the scientific questions and technological opportunities of flash sintering [Scripta 146: 260 (2018); MRS Bulletin 46: 26 (2021)]. We originally proposed that flash sintering generally starts a thermal runaway [Acta 94:87 (2015)], but it can also be activated by bulk phase and grain boundary complexion transitions [Acta 181:544 (2019)]. We further proved that ultrafast densification is enabled by ultrahigh heating rates of ~100 K/s [Acta 125:465 (2017)]. Subsequently, a generic ultrafast high-temperature sintering was reported in a collaborative study [Science 368:521 (2020)]. Other related technologies include water-assisted flash sintering (WAFS) to flash ZnO at room temperature [Scripta 142:79 (2018)] and two-step flash sintering (TSFS) to densify ceramics with suppressed grain growth [Scripta 141:6 (2017)]. Recent research discovered electrochemically induced grain boundary transitions that can cause enhanced or abnormal grain growth [Nature Communications 12:2374 (2021)]. Subsequently, I will discuss a series of on-going studies to further investigate electrochemically controlled microstructural evolution and tailor the microstructural evolution with applied electric fields in various systems and schemes [Yan et al., unpublished work].

Topical Talk MM 24.7 Wed 18:00 H45

Electric fields effects in ionic conductors during flash sintering and ion exchange — •Mattia Biesuz, Gian Domenico Soraru, and Vincenzo Maria Sglavo — University of Trento, Trento, Italy

Electric fields can drive ceramic ionic conductors out of the equilibrium dictated by temperature, composition, and pressure. These phenomena can be used to promote ceramics sintering or ion exchange.

Herein, we explore flash sintering in oxygen ionic conductors (YSZ and GDC) evidencing the presence of some electrochemical effects producing alterations of the defect chemistry and activating n-type electronic conductivity. This enhances the conductivity of the green sample, increases the electric power dissipation and contributes to the activation of the flash leading to sudden densification of ceramics. The pivotal role of electrochemical reduction during DC-flash sintering impacts the thermal history of the flashed samples generating strong thermal gradients between the cathode and anode which can be enhanced or removed by changing the quality and type of the used electrodes. The electrochemical description of flash sintering in oxygen ion conductors well explains the electrode configuration and atmosphere effects on the flash processes.

Electrochemical phenomena are, however, pivotal also in other ionic conductor systems subjected to flash-like processes. It is shown that the electrode material choice strongly affects the flash behavior and modifies the glass composition in the vicinity of electrodes. Hence, electric fields can be to modify the surface glass or ceramics composition improving mechanical and functional properties.