

MM 25: Transport (Diffusion, conductivity, heat)

Sessions: Transport I and II

Time: Wednesday 10:15–13:15

Location: H46

MM 25.1 Wed 10:15 H46

Strain induced atomic transport in ultra-fine grained Nickel — ●SHRADDHA SEVLIKAR¹, MAYUR VAIDYA¹, JONATHAN ZIMMERMANN², LISHAI SHOHAM², EUGEN RABKIN², GERHARD WILDE¹, and SERGIY DIVINSKI¹ — ¹Institute of Materials Physics, University of Muenster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — ²Department of Materials Science and Engineering, Israel Institute of Technology, Technion City, Haifa 3200003, Israel

Strain-induced atomic transport was investigated in coarse and ultra-fine grained (UFG) Nickel using the radiotracer analysis. UFG Ni was produced by high-pressure torsion (HPT) of high purity coarse-grained Ni samples using 10 rotations and 4 GPa pressure. X-ray analysis revealed a grain size of 100 nm for the HPT sample. The radioactive isotope ⁵⁷Co was deposited on the sample surface with mirror-finish obtained by mechanical polishing. The HPT sample was then carefully sandwiched between tantalum foils and subjected to cold rolling to 5/20% deformation. The tracer penetration achieved during rolling was measured by serial sectioning. A strain-induced tracer penetration was quantified and compared to thermally activated diffusion in coarse-grained and UFG Ni. Reducing the sample roughness during rolling and limiting the extent of deformation-induced porosity are identified as major challenges in developing this experimental setup. The impact of sample microstructure on deformation-induced atomic transport is discussed.

MM 25.2 Wed 10:30 H46

Understanding the bottlenecks of thermal transport in Metal-Organic Frameworks — ●SANDRO WIESER¹, TOMAS KAMENCEK¹, EGBERT ZOJER¹, ROCHUS SCHMID², JOHANNES PETER DÜRHOLOT², and NATALIA BEDOYA-MARTÍNEZ^{1,3} — ¹Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — ²Chair of Inorganic Chemistry 2, CMC Group, Ruhr-Universität Bochum, Germany — ³Materials Center Leoben, Austria

Metal-Organic Frameworks (MOFs) represent a family of highly porous materials that have shown promising properties for numerous applications including gas-storage and catalysis. As most of the applications for MOFs rely on the effectiveness of heat dissipation, it is crucial to investigate their thermal transport properties in detail. These materials allow for easy modifications in their structural composition and architecture. Thus, an in-depth understanding of the structure-to-property relationship will allow a precise tailoring of the material to meet individual requirements. Here we apply molecular dynamics (MD) simulations, in combination with the MOF-FF force field potential, to investigate the heat transport properties of MOFs with different composition (i.e. varying the organic and inorganic components). Special care is taken to analyze the periodic interfaces between the individual segments occurring in MOFs, as they are identified as a major limiting factor for heat transport. Furthermore, vibrational properties have been investigated in the framework of density-functional-theory, in order to provide further analysis leading to a more generally applicable prediction of the thermal conductivity for different MOF morphologies.

MM 25.3 Wed 10:45 H46

Determination of the correlation factor for Cd solute diffusion in Ni₃Al — ●BENGÜ TAS¹, RYAN MURRAY², GARY S. COLLINS², and SERGIY V. DIVINSKI¹ — ¹Institute of Materials Physics, University of Münster, Münster, Germany — ²Department of Physics and Astronomy, Washington State University, Pullman, WA, USA.

The correlation factor is an essential parameter for atomic transport in solids. In the case of self-diffusion, the correlation factor can be calculated easily from the lattice geometry, if the diffusion mechanism is known. Since the solute atoms modify the vacancy concentration and jump rates, measuring the solute diffusion correlation factor is a complicated task. While the first principles simulations have enabled computing the correlation factor within the framework of simplified models such as the five vacancy jump frequency model for fcc crystals, its experimental determination has never been performed. In this work, we contribute to the first measurements of the correlation factor of solute diffusion combining long-range diffusion measurements and perturbed angular correlation (PAC) experiments. The diffusion coef-

ficient of Cd was measured at a temperature of 1073 K within the cubic L1₂ ordered Ni₃Al crystal structure and the impurity jump frequency was determined at the same temperature. The experimental findings are finally combined to evaluate the correlation factor of Cd atoms in the Ni₃Al sublattice.

MM 25.4 Wed 11:00 H46

Spectral and transport properties of disordered Mott systems — ●HIMADRI BARMAN — Department of Physics, Zhejiang University, 38 Zheda Road, Hangzhou, Zhejiang 230027, China — Institute of Mathematical Sciences, 4th Cross, CIT Campus, Taramani, Chennai, Tamil Nadu 600113, India

We study the disordered Hubbard model within the dynamical mean-field theory (DMFT) framework using the coherent potential approximation (CPA). Despite similar studies have been performed in the earlier literature, for the first time, we looked at the finite temperature longitudinal and transverse (Hall) conductivity and discovered two different scattering rates: one following the Fermi-liquid's quadratic temperature (T) dependence and the other showing a non-Fermi-liquid like power-law behavior. Thus our theoretical results show that the interplay of disorder and Coulomb interaction may possess the answers to the long-standing unresolved problem of the two-scattering rates discovered in the cuprates, and subsequently in the bulk correlated oxide materials.

MM 25.5 Wed 11:15 H46

Low-energy electron attachment induced transport - conductivities and the role of blocking electrodes — ANNELI HEIN, MARTIN SCHÄFER, and ●KARL-MICHAEL WEITZEL — Philipps-Universität Marburg, Fachbereich Chemie

The charge carrier transport in an alkali ion conducting glass has been investigated by means of the charge attachment induced transport (CAIT) technique [1]. For the first time we describe the direct measurement of the absolute bulk conductivity and the activation energy for ion hopping in a glass by attachment of low-energy electrons to the front side of a glass, which is in contact with a single metal electrode at the backside [2]. The electron attachment experiment induces electrodiffusion of mobile cations towards the front side of the sample. In the limit of short time respectively little charge transported this approach allows measuring the conductivity as well as the activation energy of the glass, which agree well with reference measurements. In the limit of long time respectively considerable charge transported alkali depletion profiles evolve at the interface between the electrode and the glass. This eventually gives rise to the blocking of charge transport. A quantitative model for the evolution of "blocking electrode" characteristics is presented. The mechanism involves transient dielectric breakdown. [1] J. Martin, M. Gräf, T. Kramer, C. Jooss, M.J. Choe, K. Thornton, K.-M. Weitzel, PCCP, 19, 962, (2017) [2] A. Hein, M. Schäfer, K.-M. Weitzel, in preparation

15 min. break

MM 25.6 Wed 11:45 H46

Bulk diffusion of Mn in α -iron — ●VLADISLAV KULITCKII, SERGIY DIVINSKI, and GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany

The impact of a magnetic transition on bulk diffusion of Mn in α -iron is studied by microtome (higher temperatures) - and ion-beam sputtering (low temperatures) - sectioning using the radioactive isotope ⁵⁴Mn. The experiments were performed in the temperature range of 773 to 1173 K. In contrast to the case of self-diffusion [1, 2], a marginal * if any * impact of the magnetic transition in α -Fe on Mn bulk diffusion is observed with almost the same linear Arrhenius dependences below and above the Curie temperature. No distinct deviation from a linear Arrhenius temperature dependence is observed and the Mn bulk diffusion coefficient can be given by the pre-exponential factor $D_0 = 2.87 \cdot 10^{-2} \text{ m}^2/\text{s}$ and the activation enthalpy $Q = 282.8 \cdot 6.7 \text{ kJ/mol}$ in the whole temperature interval under investigation. [1] Y. Iijima, K. Kimura, K. Hirano. Acta Metall. 36 (1988) 2811-2820. [2] M. Lübbehusen, H. Mehrer. Acta Metall. 38 (1990) 283-292

MM 25.7 Wed 12:00 H46

Impact of paramagnetic excitations and relaxations on diffusion in Fe-Mn alloys — ●OMKAR HEGDE, OSAMU WASEDA, TILMANN HICKEL, CHRISTOPH FREYSOLDT, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Understanding the impact of paramagnetism on defect kinetics is, though conceptually and computationally challenging, important for designing Fe-based alloys. Since magnetic degrees of freedom change faster than atomic degrees of freedom in the paramagnetic state, the atoms move according to an averaged force instead of instantaneous forces attained from each spin configuration. Therefore, a new computationally efficient method based on spin-space averaging (SSA) has been developed to handle magnetic disorder next to defects. The method uses the spin constraint tool developed and implemented in the DFT code S/PHI/nX. The performance of the method is demonstrated for local atomic relaxations next to point defects. For α -Fe, we show that both magnetic disorder and local relaxations significantly affect vacancy formation and migration energies. Next, we focus on the FeMn system, for which the vacancy formation energy as a function of Mn concentration for both ferromagnetic and paramagnetic cases is presented. We demonstrate that paramagnetism significantly affects atomic relaxations as well as diffusion barriers and thereby explain why Mn diffusion shows a different temperature dependence than Fe-self diffusion in α -Fe.

MM 25.8 Wed 12:15 H46

On Stochastic Resonance in Double Resonance Models — ●AMIT CHATTOPADHYAY¹ and ELIAS AIFANTIS² — ¹Systems Analytics Research Institute, Mathematics, Aston University, Birmingham, UK — ²Laboratory of Mechanics and Materials, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece

Double diffusion as a model of transport involving two interacting species is essentially a continuum model with two local non-equilibrium concentration fields obeying separate mass and momentum balance equations, with a linear relation for the mass exchange term between them. Here we present results from two separate stochastic double-diffusion models involving two fluctuating phase densities, which represent the same system for two different symmetry cases. We show that presence of surface inhomogeneities and temporal delay have substantial impact at the interface of evolution for both models. The effect is most pronounced at a critical point, identified as the "stochastic resonance" [1,2] point where maximum energy transfer occurs that create complementary profiles for the spatial and temporal correlation functions. The symmetry difference between the two models lead to spatiotemporal patterns that are unique to each individual case. Model results verify a multitude of interface based experiments concerning nanomaterial dynamics.

References: [1] AKC & ECA; Physical Review E, vol 95, 052134 (2017). [2] AKC, et al; Materials Science and Technology, vol 34:13, 1606 (2018).

MM 25.9 Wed 12:30 H46

Low-temperature heat capacity of Fe-Mn alloys — ●MARIUS GERLITZ, MARTIN PETERLECHNER, SERGIY DIVINSKI, and GERHARD WILDE — Institute of Materials Physics, University of Münster, Germany

For a fundamental description of ferromagnetic materials, knowledge of characteristic thermodynamic properties is essential. The analysis of the magnetocaloric effect or magnetostriction is a significant step, feasible by specific heat measurements. The influence of magnetism, chemical composition and short-range order on the specific heat capacity of a series of Fe-Mn alloys (up to 9.5 at.% Mn) is systematically measured in the temperature interval between 1.9 K and 400

K. A physical properties measurement system (PPMS) is used and the 2-tau method is applied for the analysis. Additionally, a constant magnetic field of 3 T is applied to determine the impact of an external field. Furthermore, calorimetric measurements by differential scanning calorimetry (DSC) are performed using heating rates of 20 K/min in the temperature interval from 300 K to 723 K. Thermal - and magnetic entropy contributions are determined. The Debye temperatures and the electronic contribution to the specific heat are estimated. The results are discussed with respect to the chemical composition and probable short-range ordering.

MM 25.10 Wed 12:45 H46

Thermal properties of solids determined by lock-in infrared thermography — ●NILS ZIEGELER¹, PETER W. NOLTE², A. CHARLOTTE RIMBACH¹, and STEFAN SCHWEIZER^{1,2} — ¹South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — ²Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Lübecker Ring 2, 59494 Soest

As material science advances and more and more materials are developed, their use cases become increasingly specialized. In thermal design, a precise knowledge of the thermal parameters, such as the thermal diffusivity and the thermal conductivity, has to quickly be at hand if required.

Here, contactless lock-in infrared thermography is used to determine the thermal diffusivity value of a material. The method consists of a point-like heat source (such as a laser), which periodically heats the front side of the sample. The generated heat waves travel through the specimen and are detected on the backside by an infrared camera. In lock-in thermography, the phase delay between the periodic heating on the front and the temperature variations on the rear side is analyzed. Since the phase delay depends on the modulation frequency, a series of measurements is performed to determine the thermal diffusivity of the material. The principle is demonstrated on lithium borate glass of varying composition. The results show that even small changes in chemical composition can be detected.

MM 25.11 Wed 13:00 H46

Investigations of ionic transport in bicrystals of Sr-doped LaMnO₃ — ●JACQUELINE MARIE BÖRGERS^{1,2} and ROGER DE SOUZA¹ — ¹Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany — ²Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Jülich, Germany

Mixed-valence manganites are very promising candidates as materials for resistive switching due to the possibility to generate multilevel resistance states as well as area-dependent switching. This enables their use in future non-volatile memory or novel neuromorphic circuits.

It is widely accepted that ionic transport plays an important role in the field of resistive switching. Also for manganites the key mechanism is assumed to be drift and diffusion of oxygen vacancies. Additionally, by varying the composition and microstructure of manganites the electronic and ionic transport properties can be influenced. The aim of this study is to illuminate the relationship between structural factors of the material and its switching performance. Hereby, we are particularly interested in the influence of grain boundaries on the transport mechanisms.

Therefore, the ionic transport along grain-boundaries in Sr doped LaMnO₃ ((La_{1-x}Sr_x)MnO_{3±δ}, LSMO) is studied in order to gain further insight on its switching mechanisms. The migration of oxygen ions in bicrystals of LSMO is studied by Molecular Dynamics (MD) simulations employing empirical pair potentials. In addition, static atomistic simulations are used to gain further insights into defect formation processes.