MM 7: Transport and Diffusion II

Time: Monday 11:30–12:45 Location: H 1029

MM 7.1 Mon 11:30 H 1029

First-principle study and modeling of strain dependent ionic migration on ZrO_2 — •Julian Hirschfeld and Hans Lustfeld — Forschungszentrum Jülich, IAS-1 and PGI-1, Jülich, Germany

Electrolytes with high ionic conductivity at lower temperatures are the prerequisite for the success of Solid Oxide Fuel Cells (SOFC). One promising candidate is doped zirconia. In the past its ionic conductivity has mainly been increased by decreasing its thickness. However, the influence of the thickness is only linear whereas the impact of migration barriers is exponential. Therefore understanding the oxygen transport in doped zirconia is of fundamental importance. In this work we pursue the approach of the strain dependent ionic migration in zirconia. We investigate how the migration barriers for oxygen ions respond to a change of the atomic strain. We employ the method of Density Functional Theory (DFT) to obtain the migration barrier of the oxygen ion jumps in zirconia for a given lattice constant. In contrast to other publications we find a migration barrier decrease for high compressive strains beyond a maximal height of the migration barrier at an intermediate compressive strain. We present a simple analytic model which by using interactions of the Lennard Jones type gives an explanation for this behavior.

MM 7.2 Mon 11:45 H 1029

The influence of Mg and Si atoms on the cluster formation process in Al-Mg-Si alloys studied by positron annihilation lifetime spectroscopy — •Meng Liu[1,2], Yong Yan[2], Zeqin Liang[1], Cynthia Chang[2], and John Banhart[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin — [2]Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin

After natural ageing (NA), Al-Mg-Si alloys with various Mg and Si contents exhibit either positive or negative strength response during subsequent artificial ageing, which is caused by clusters formed during NA. Previous studies focused on cluster formation in Al-Mg-Si alloys by using Positron Annihilation Lifetime Spectroscopy (which is uniquely sensitive to vacancies) found that the entire evolution consists of at least 4 stages. However, the exact interpretation of the underlying microscopic processes is still under dispute. Therefore, in-situ positron lifetime experiments were carried out for pure Al-Mg and Al-Si binary alloys with solute concentrations ranging from 0.005 at.% to 1 at.% in order to clarify the behaviour of Mg/Si atoms on the clustering formation processes from a vacancy perspective. The results show that in general, a decrease in positron lifetime to a stable value after a certain period of NA for both alloying systems can be observed. Lifetimes of Al-Mg samples are significantly higher than in Al-Si alloys for equal solute content. In addition, these results are compared to the Differential Scanning Calorimetry results for getting a better understanding of the different clustering stages in Al-Mg-Si alloys.

MM 7.3 Mon 12:00 H 1029

Simulation of internal nitradation phenomena with a cellular automata approach — •Katrin Jahns, Martin Landwehr, Jürgen Wübbelmann, and Ulrich Krupp — University of Applied Sciences Osnabrück, Faculty of Engineering and Computer Science, Albrechtstrasse 30, 49076 Osnabrück, Germany

In this study a simulation program is developed for predicting precipitation accompanying diffusion processes based on the method of cellular automata. Hereby, nitrogen diffusion and precipitate formation are simulated individually and in combination. Operation of high-temperature components as well as surface hardening processes, e.g., carburizing and nitridation, involve diffusion of gases in metals and alloying elements, precipitate nucleation and growth. The higher specific volume of the internal precipitates as compared to the substrate causes the generation of residual compressive stresses in the surface layer. Besides thermodynamics, these effects are taken into account when evolving the program. The simulation program is evaluated and verified by means of thermogravimetric nitridation and carburization experiments.

MM 7.4 Mon 12:15 H 1029

Transport Properties of In_2O_3 and its surface electron accumulation layer — •Natalie Preissler, Oliver Bierwagen, and James. S. Speck — preissler@pdi-berlin.de

We used variable temperature Hall measurements and room temperature thermoelectric measurements to determine the transport properties (mobility, sheet resistance, charge density, Seebeck-coefficient) of In_2O_3 thin films and their surface electron accumulation layers (SEALs). SEALs have an important impact on device applications and were shown already by x-ray photoelectron spectroscopy (XPS) and current-voltage (I-V) measurements, while their actual transport properties are still unknown. The investigated In_2O_3 samples were about 500 nm thick and were grown on insulating Yttria-stabilized zirconia (YSZ) by plasma-assisted molecular beam epitaxy. Unintentionally doped (uid) In_2O_3 exhibits n-type conductivity with a significantly lower volume electron concentration than in the SEAL. Acceptor doping by Mg turned the bulk of the samples insulating to maximize the relative contribution of the SEAL to the total conductivity. As a result we can estimate the sheet resistance of the SEAL to be greater than 46 kΩ. Current-voltage measurements with Hg contacts showed the existance of the SEAL. Temperature dependent Hall measurements were used to differentiate between the degenerate SEAL (high volume electron concentration, no freeze-out) and non-degenerate bulk (low concentration, freeze-out). While Hall measurements give a total sheet electron concentration, the Seebeck coefficient is related to the volume electron concentration and is used as another indicator for the SEAL.

MM 7.5 Mon 12:30 H 1029

Critical current noise in rough Josephson junctions — •Pierre-Luc Dallaire-Demers[1], Mohammad Ansari[2], and Frank Wilhelm-Mauch[1] — [1]Universität des Saarlandes, Saarbrücken, Deutschland — [2]University of Waterloo, Waterloo, Canada

While dissipationless, Josephson junctions as elements in superconducting nanocircuits are plagued by intrinsic noise mechanisms that will limit the coherence time of future high-precision quantum devices. Significant sources of current fluctuations may be caused by the noncristallinity and disorder of the oxide layer separating the two superconducting leads. A microscopic calculation of the spectral density of noise of a rough superconducting tunnel junction is presented in this work. To account for disorder, a Josephson junction is modelled as a set of pinholes with a universal bimodal distribution of transmission eigenvalues that add their noise power incoherently. Each pinhole is treated as a ballistic point contact with an intrinsic thin barrier that modulates the transmission coefficient. The noise spectrum is computed using the quasiclassical Green's function method for non-equilibrium superconductivity. This formalism allows us to investigate high and low transmission limits at finite temperature for any relevant frequency. As suggested by experiments, low transmission pinholes generate shot noise while fast switching between the subgap states of high transmission channels create a strong non-poissonian low-frequency noise yet to be measured. The fluctuation of the low-frequency noise from one sample to the other is also found to be significant when the phase of the order-parameter is anti-symmetric across the junction.