MM 63: Transport (Diffusion, conductivity, heat)

Transport I

Time: Thursday 15:45–17:00 Location: TC 010

MM 63.1 Thu 15:45 TC 010

Atomic transport in Si/Al interfaces — •Kevin-Patrick Treder, Efi Hadjixenophontos, Sebastian Eich, and Guido Schmitz — Institut für Materialwissenschaft, Lehrstuhl für Materialphysik, Stuttgart, Deutschland

The crystallization temperature for semiconductors such as Si and Ge can be drastically lowered when in contact with a metal. Metal induced crystallization (MIC) or the layer-exchange processes were tried to be understood by different thermodynamic or kinetic approaches in the recent years. The direct comparison of the reactions of amorphous or crystalline Si with Al inside a single sample may provide further insight into the mechanisms. In a new experimental approach, we produce artificial nano-sized triple junctions at which the Al/c-Si, the Al/a-Si and the c-Si/a-Si interfaces merge. Samples are prepared via RF-Sputtering, followed by ex-situ annealing in Ar-atmosphere and subsequent post processing via FIB-lift-outs. Full cross-section characterization and analysis was provided by HRTEM and local EDX-analysis. Clear evidence is provided for ~ 2 nm temperature-independent amorphous interlayer formed at the c-Si/Al interface. The diffusion phenomena across and along the related interfaces are demonstrated and measured in direct comparison.

MM 63.2 Thu 16:00 TC 010

Magnetotransport and Quantum Oscillation Phenomena in Dirac Semimetal Na_3Bi — •Mohammad Pakdaman, Alimamy Bangura, Claus Mühle, and Hidenori Takagi — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

Three dimensional Dirac semimetals are a three dimension analogue of Graphene where the conduction band and valance band touch at discrete points in reciprocal space with linear dispersion. In this class of materials Na_3Bi has a uniquely simple band structure compared to other example discovered so far. A consequence of this unique band structure is the realization of unusual electronic properties that are predicted to be manifest in the transport properties. In order to probe the exotic electronic properties of this material, the magnetotransport measurement have been done on single crystal of Na_3Bi. The results were compared to the *ab initio* calculations and predictions of the physical properties for this recently predicted state of matter, and these experiments give further evidence for the realisation of this exotic state of matter.

MM 63.3 Thu 16:15 TC 010

Plasma charge carrier attachment induced transport in electrolytes — •Jan Wiemer and Karl-Michael Weitzel — Philipps Universität Marburg, Chemistry Department

A new approach for measuring the electrical conductivity properties of solid electrolytes over a wide range of total pressures applicable for any thickness of the sample is presented. The approach is based on generating a plasma by femtosecond laser ionization of e.g. air. Charge carriers of different polarity are separated in a static electric field. Charge carriers of the selected polarity are attached to the front side of a sample which is in contact with a single metal electrode inducing a well defined surface potential. This induces charge carrier transport in the sample which is detected at the metal electrode. We present different examples of glasses demonstrating that the approach allows measuring conductivities and activation energies in full agreement with reference measurements. The advantages are that the sample is i.) only in contact with a single electrode, ii.) the pressure range is from fine vacuum up to high pressures, iii.) the chemical identity of the charge carrier can be chosen by choosing the plasma medium and iv.) the polarity can be easily switched by switching static fields.

MM 63.4 Thu 16:30 TC 010

On bottleneck areas for ionic transport in NASICON materials — •Kaustubh Bhat, Stefan Blügel, and Hans Lustfeld — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Among ionic conductors, NASICON [1] materials are receiving attention for large-scale energy storage applications. We first use the Nudged Elastic Band (NEB) method for calculating the energy barrier for sodium ion transport in $Na_6Sc_4(PO_4)_6$ (NSP). Experimental results point towards the existence of certain bottlenecks which reportedly determine the ionic conductivity of a given material [2]. We have developed a novel method using second order force constants to model the influence of these bottlenecks – interionic distances and in particular areas – to the migration barriers of sodium ions. Using our model we test the bottleneck hypothesis [3]. Furthermore, we use the information gained from the model to identify ionic substitutions to NSP that reduce the energy barrier.

[1] H.Y.P. Hong, Mat. Res. Bull. **11**, 173 (1976).
[2] M. Guin and F. Tietz, J. Power Sources **273**, 1056 (2015).
[3] M. Guin, PhD Thesis, ISBN 978-3-95806-229-0 (2017)

MM 63.5 Thu 16:45 TC 010

Improvements in thermoelectric material performance — •Genadi Naydenov, Philip Hasnip, Vlado Lazarov, and Matthew Probert — Department of Physics, University of York, York, YO10 5DD, UK

Thermoelectric technology has the potential to convert waste heat into useful electricity, dramatically improving energy efficiency. Optimising thermoelectric materials focuses on increasing their power factor and decreasing their thermal conductivity. Recent experimental and theoretical studies have shown that half-Heusler systems, e.g. NbFeSb, can reach a high power factor ($\sim$10 $m\mathrm{Wm}^{-1}\mathrm{K}^{-1}$) even at room temperature, and that the thermal transport is dominated by phonons. The phonon thermal conductivity may be lowered by substitution with heavier elements, which introduce point scatterers. Recently the half-Heusler TaFeSb has also been predicted to be an excellent thermoelectric material, but has yet to be investigated thoroughly. We will present the results of our first-principles materials modelling investigation into the thermoelectric properties of pure TaFeSb, NbFeSb and $Ta_xNb_{1-x}FeSb$, and show how the power factor and ZT may be optimised by judicious choices of x and doping concentration. We show that p-type $Ta_xNb_{1-x}FeSb$ is an excellent candidate thermoelectric material.