I. Physikalisches Institut (IA)
Phasenwechselmaterialien
Prof. Dr. rer. nat. Matthias Wuttig

Master Thesis in Physics

Investigating metavalent materials by Field Ion Microscopy

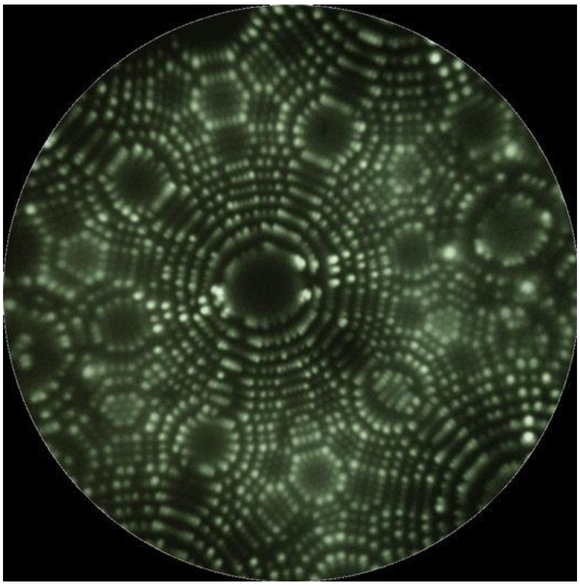

Fig 1: Example of a FIM image with atomic resolution

Field ion microscopy (FIM) was the first method enabling the imaging of single atoms.[1,2] Nowadays, it is possible to reach atomic resolution in three dimensions with 100 % positional detection efficiency by using the state of the art 3D-FIM technique. A high electric field is applied on the surface of a sharp (r < 100 nm) needle-shaped specimen under a certain constant pressure of imaging gas (e.g. He or Ne) at base temperatures between 20 – 80 K. During the experiment the imaging gas gets ionized in the vicinity of the specimen (which acts as a field-emitter) as a consequence of the locally high electric field. The objective of this project is to analyze metavalent materials using the 3D-FIM method. Metavalent materials belong to a new material class, which contains solids with a distinct bonding mechanism (metavalent bonding) and both, a unique set of physical properties and bond breaking behavior observed by atom probe tomography (APT). In local electrode atom probe tomography (LEAPT), a DC potential of 3-8 kV is applied between the sample and the local electrode. Field evaporation of single (or multiple) atoms is achieved through successive laser or voltage pulses. The field evaporated atoms get ionized and accelerated through a mass spectrometer towards a delay line detector. This allows to obtain a 3D tomographic reconstruction of the specimen including the chemical identity of the atoms with almost atomic resolution. The effect of detecting a single ion after a successful laser pulse signifies a single event, while the detection of multiple ions (emitted during the same pulse) defines a multiple event. One key characteristic of metavalent materials is the unusually high intrinsic probability of detecting multiple events, i.e. the field evaporation process at the surface is anticipated to be fundamentally different compared to classical covalent or metallic materials. The successful candidate will perform FIM measurements on a variety of metavalent and non-metavalent materials and compare the results with the goal of finding systematic differences in the field evaporation process in order to reach a better understanding of the unusually high detection probability of multiple events, observed for metavalent materials. A typical sample size analyzed in 3D-FIM results in tomographic datasets of ca. 2 x 10^5 images containing information on sequential atomic positions. Handling and analyzing such large datasets is one of the major challenges of 3D-FIM. There are currently two data analysis methods: atom by atom and geometrical approaches. The first method is based on the layer by layer evaporation, where the atoms are identified based on a threshold intensity. The geometrical approach uses a stacking of the digital images. The image stack is then corrected, assuming a known projection law, a specimen`s geometry and a constant evaporation rate. With the recent developments of Artificial intelligence, especially in computer vision, modern machine learning algorithms were developed, enabling a fully automated detection and classification of objects in an image. Such algorithms can be used to derive systematic insights from very rich experimental datasets such as the datasets obtained from a 3D-FIM experiment. One main goal of the project is to successfully analyze 3D-FIM datasets by employing one of the data analysis methods described above.

Requirements for the candidate:

- Profound knowledge in data analysis methods (e.g. with Python and/or MatLab)
- Programming skills (e.g. in Python or MatLab) are highly appreciated
- Ability to work structured, independently and responsibly
- Good scientific practice

Dr. Stefan Maier
✉ s.maier@physik.rwth-aachen.de
28 A 509 0241 / 80 27175