KFM 17: Functional Materials: Performance, Reliability and Degradation; and Complex Materials (joint session MM/KFM)

Time: Thursday 11:45–13:00 Location: H23

KFM 17.1 Thu 11:45 H23

Untersuchungen des Bruchverhaltens im Bereich der Ultra-Langzeitfestigkeit von Federstählen — •Jörg Gollnick — THM, FB ME, Wiesenstr. 14, 35390 Gießen

In einer hochfrequenten resonanten Anwendung als Spiegel für Laserscanner werden Federstähle des Typs Ck101 im Grenzbereich belastet. Im Rahmen eines Forschungsvorhabens wurden die spezifischen Möglichkeiten untersucht, die Lebensdauer dieser Bauteile zu steigern. Bislang wurden nur unzureichende Lebensdauern erreicht.

Bemerkenswert war die Ausprägung des Versagensverhaltens, dass in Zusammenhang mit der Fertigungstechnologie einem Sprödbruch unter Mode III nach den bruchmechanischen Ansätzen gemäß Griffith entspricht. Aus der Erklärung der Schädigungen wurden weitere Möglichkeiten untersucht, die Lebensdauer nicht nur zu steigern sondern weiterhin die nach Paris-Erdogan zu erwartende Dauerfestigkeit genau zu bestimmen.

Mit hohen Frequenzen im Bereich bis zu 10000kHz werden Bauteile bis zu 10 Milliarden Schwingungen im Grenzbereich betrieben. Eine mehrstufige Auswertung nach dem Treppenstufenverfahren zeigt, dass eine Auswertung in diesem Segment nicht nur möglich ist, sondern als geeignete Strategie angesehen werden darf, die Erkenntnisse der Ultra-Langzeitfestigkeit diesbezüglich zu erweitern.

Weitergehende Versuche werden vorgestellt.

Falls gewünscht kann der Vortrag und Beitrag gerne auch auf englisch abgefasst werden.

KFM 17.2 Thu 12:00 H23

Searching for ferroelectric porous metal organic frameworks using machine-learning and Monte-Carlo-simulations — •Thomas Bergler[1,2], Harald Oberhofer[1,2], and Dirk Volkmer[3] — [1]University of Bayreuth, Germany — [2]Bavarian Center for Battery Technologies — [3]University of Augsburg, Germany

Metal organic frameworks (MOFs) have so far found a number of successful applications, among them as storage for gasses and filter for gas mixtures. So far these mostly incorporated them as passive materials, but recent research points the way towards a more active role, possibly through the external manipulation of the materials' internal properties. One recent example for such a property is the susceptibility of the lattice parameters of a number of MOFs towards electric fields. Inspired by this, the aim of our project is to further investigate this behavior and potentially design ferroelectric MOFs. Using a hierarchy of Monte-Carlo-simulations aided by Machine-Learning (ML) we sample the design space MOFs augmented by rotatable polar groups. In succession, we first sample a huge space of rotors in a simplified point-dipole model. A selection of thus uncovered MOF geometries is then investigated with a specially parameterized atomistic model to confirm earlier predictions. Using this data, an ML model is trained to predict the dielectric properties of such polar rotor-augmented MOFs. The best candidates extracted with this procedure are finally evaluated with density functional theory. MOF geometries surviving this funnel-like approach can finally be checked experimentally for a variety of applications, ranging from data-storage to gas nano-funnelling.

KFM 17.3 Thu 12:15 H23

Atomic Scale Insights into A-site Deficient Perovskite Catalysts:$La_{0.7}Fe_{0.7}Mn_{0.3}O_3$ — •Roham Talei Jeid — Institute for Material Physics, University of Stuttgart, Deutschland

This study investigates the atomic-scale properties of the A-site-deficient perovskite catalyst $La_{0.7}Fe_{0.7}Mn_{0.3}O_3$ (La07FM), emphasizing the role of iron oxide (FeO) in redox reactions. Advanced techniques, including scanning transmission electron microscopy (STEM), energy-dispersive X-ray spectroscopy (EDXS), and a custom Python-based strain mapping tool linked to chemical analysis reveal nanoscale La deficiencies and Fe enrichments at grain boundaries as key for catalytic activity. Post-catalysis studies identify Fe-rich, FeO-like nanoparticles at strained, defective grain boundaries, underscoring the impact of A-site deficiencies on performance in NOx denitrification (DeNOx). These findings highlight how A-site deficiencies and Fe-rich nanostructures enhance catalytic efficiency, offering broader insights into electrochemistry and heterogeneous catalysis.

KFM 17.4 Thu 12:30 H23

Use of LiMn2O4 for switching applications in silicon waveguide circuits — •Vinit Agarwalla[1], Yug Joshi[2], and Guido Schmitz[1] — [1]Insitut für Materialwissenschaft, Universität Stuttgart, Heisenbergstr.3, 70569 Stuttgart — [2]Max-Planck-Institut für Nachhaltige Materialien, Max-Planck-Straße 1, 40237, Düsseldorf

Lithium ion intercalation and deintercalation play an important role in determining the storage performance of cathode materials for lithium ion batteries. However, intercalation of ions also regularly modifies electron structure and optical properties of the materials. This study explores the possibility of exploiting the optical properties of the cathode material LiMn2O4 (LMO) for optical switching applications in silicon waveguide circuits. For this, LMO is coated as a cladding around Si waveguides suitable for the 1550 nm wavelength of optical telecommunication. To stabilize the interface a thin intermediate Si oxide film is tested as an optical transparent reaction barrier. Our TEM images and the EDX mapping show that the Si does not react with LMO for oxide layer thickness as low as 10 nm. Previous work has explored the change in resonance wavelength of reflectance spectra with lithiation/delithiation in the visible region[1]. In extension, we have measured FTIR reflectance spectra in the near IR region. They show a fairly continuous spectrum between visible and IR region with reflectance going to 100 % and a gradual shift in resonance wavelength in the IR region with Li intercalation. The optical response on light transmission along the wave guides has been determined in dependence on the degree of lithiation. [1]. DOI:10.1002/adom.201701362

KFM 17.5 Thu 12:45 H23

Chemical short-range order and local lattice distortions in High-Entropy Alloys: state of the art — •Andrea Fantin, Anna Maria Manzoni, Reza Darvishi Kamachali, and Robert Maass — Bundesanstalt fuer Materialforschung und -pruefung, Unter den Eichen 87, 12205 Berlin, Germany

Understanding the intricate atomic-scale structures within High-Entropy Alloys (HEAs) is crucial for tailoring their properties for diverse applications. This contribution tries to provide a brief overview of the state-of-the-art experimental techniques employed to probe local lattice distortions and chemical short-range order in HEAs, with specific focus on X-ray absorption spectroscopy and total scattering. The main problem to overcome in multi-component alloys is the intrinsic reduced scattering contrast between nearest neighbors in the periodic table, which limits the amount of information that can be extracted from the data. This statement remains valid when employing transmission electron microscopy, as well. Specific examples such as the Al-Co-Cr-Cu-Fe-Ni fcc system [Small Science 4(2), 2300225 (2024); Nature Communications 15(1), 7815 (2024)] and the MoNbTaW bcc system [Materials Research Letters 12(5), 346-354 (2024)] will be outlined. It comes clear that rather than specific techniques, it is only the combination of several experiments, supported by simulations and multi-technique simultaneous structural refinements, that can help in disentangling the different contributions to performances of each element within the alloy solid solution, with strength and weaknesses depending on the specific experimental measurements.