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Hysteresis Design of Magnetic Materials for Efficient Energy Conversion

Tuesday, 1 February 2022, 9:00 s.t., TU Darmstadt, Zoom

Foto: K. Marquard, RUB

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Thin-film materials libraries for the data-driven discovery and investigation of compositionally complex materials

Abstract:

Discovery of new materials is a key challenge in materials science: e.g. new materials for sustainable production/storage/conversion of energy carriers are necessary to improve existing and to enable future energy systems. Efficient methods for discovery and optimization of new materials are necessary: Thin-film combinatorial materials science (1) is presented as an effective means to produce large datasets on new materials. This approach is useful for validation of theoretical predictions (e.g. from high-throughput computations), and production of large, consistent and complete experimental datasets which can be used for materials informatics. The approach comprises fabrication and processing of thin-film materials libraries by combinatorial sputter deposition processes and optional post-deposition treatments, followed by the high-throughput characterization of the different thin-film samples contained in these libraries, and finally the organization of the acquired multi-dimensional data in adequate databases as well their effective computational analysis and visualization. The importance of defining adequate screening parameters and according designs of materials libraries is addressed. High-throughput material characterization methods are automated, fast, and mostly non-destructive: examples are EDX and RBS for composition, XRD for crystal structure, high-throughput test stands for temperature-dependent resistance (phase transformation), magnetic, optical and mechanical properties as well as scanning droplet cells for (photo)electrochemical properties screening. Results for up to quinary systems are visualized in the form of composition-processing-structure-function diagrams, interlinking compositional data with structural and functional properties. The talk will cover and discuss examples of combinatorial discoveries and development of new materials in different materials classes and forms (films, nanoparticles) with a focus on compositionally complex materials (e.g. (2)). Furthermore, a new approach (3) to accelerate atomic-scale measurements for complex alloys is presented as well as applications of materials informatics to accelerate and improve the materials discovery process (4, 5). Finally, challenges and opportunities of applying combinatorial materials science to magnetic materials are addressed.

(1) A. Ludwig (2019) *Discovery of new materials using combinatorial synthesis and high-throughput characterization of thin-film materials libraries combined with computational methods*, npj computational materials 5, 70

(2) T. Löffler, H. Meyer, A. Savan, P. Wilde, A. Garzón Manjón, Y. T. Chen, E. Ventosa, C. Scheu, A. Ludwig, W. Schuhmann (2018) *Discovery of a multinary noble metal free oxygen reduction catalyst*, Adv. Energy Mater. 8, 1802269

(3) Y. J. Li, A. Savan, A. Kostka, H. S. Stein, A. Ludwig (2018) *Accelerated atomic-scale exploration of phase evolution in compositionally complex materials*, Materials Horizons 5, 86 - 92

(4) P. M. Maffettone, L. Banko, P. Cui, Y. Lysogorskiy, M. Little, D. Olds, A. Ludwig, A. I. Cooper (2021) *Crystallography companion agent for high-throughput materials discovery*, Nature Computational Science 1, 290 – 297.

(5) L. Banko, O. A. Krysiak, J. K. Pedersen, B. Xiao, A. Savan, T. Löffler, S. Baha, J. Rossmeisl, W. Schuhmann, A. Ludwig (2022) *Unravelling composition-activity-stability trends in high entropy alloy electrocatalysts by using a data-guided combinatorial synthesis strategy and computational modelling*, Adv. Energy Mater., 2103312

About the speaker:

Alfred Ludwig is Professor for Materials Discovery and Interfaces at the Institute for Materials of Ruhr University Bochum (RUB). In 1999 he received his Ph.D. in mechanical engineering from University of Karlsruhe. He then worked at the caesar research center in Bonn and became head of the research group "Combinatorial Materials Science" in 2002. At the same time, he started at RUB as junior professor and became full professor in 2012. He initiated and organised the research center ZGH (Center for Interface-Dominated High Performance Materials) of which he is the scientific director. In 2021 he became as well one of the founding directors of the Research Alliance Ruhr research center “Future Energy Materials and Systems”. His research interests include combinatorial materials science, high-throughput experimentation, material informatics, autonomous experimentation, materials for nano/microsystems, thin films and multinary nanoparticles, with a focus on multifunctional materials for future energy systems, e.g. novel electrocatalysts.

Zoom information: Meeting-ID: 850 8986 6688, Kenncode: 967238