Seminar announcement

Tuesday, June 18, 2024
1:30 pm
WSI, Seminar room S 101
Exclusively in person

“Accelerating the development of novel semiconductor thin films through advanced automated characterization”

The discovery of new functional materials remains a key challenge in the development of next-generation sustainable technologies. Fueled by advances in high-throughput computation, new exciting materials are being predicted at an ever-increasing rate. Combinatorial high-throughput materials science techniques hold the promise to match this rate by facilitating the rapid exploration of complex phase spaces. Today, combinatorial materials science workflows are employed in many laboratories around the world. While gradient deposition of combinatorial thin-film libraries can be implemented in most standard deposition equipment, a comprehensive toolbox for rapid materials characterization, which is just as crucial, is often harder to realize. In this presentation, it will be shown how accelerated thin-film materials development is performed in the Coating Technologies group at Empa. We employ a workflow consisting of reactive combinatorial physical vapor deposition, automated characterization and semi-automated data analysis, which covers most common thin-film characterization techniques as well as functional property mapping. In recent years, we extended this infrastructure to include high-throughput surface analysis, but also optical measurement setups for accelerated aging studies. This extension not only complements the existing workflows, but provides additional insights that were previously much harder to obtain. It will be shown how surface analysis mapping can facilitate the discovery of new semiconductor materials in complex phase spaces, such as the wide band gap nitride semiconductors Zn2VN3[1,2] or Zn2TaN3[3]. In addition, it will be shown how accelerated optical aging studies combined with machine-learning assisted data analysis can generate insights into the operational stability and degradation kinetics of more volatile materials.[4] The results presented here showcase the potential of integrating advanced characterization techniques into high-throughput materials science workflows for the rapid development of new energy materials.

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[2] S. Zhuk, S. Siol, Appl. Surf. Sci. 2022, 601, 154172.
[3] S. Zhuk, A. Wieczorek, A. Sharma, J. Patidar, K. Thorwarth, J. Michler, S. Siol, Chem. Mater. 2023, 35, 17, 7069–7078
[4] A. Wieczorek, A. Kuba, J. Sommerhäuser, L. N. Caceres, Q. Guesnay, C. Wolff, S. Siol, J. Mater. Chem. A, 2024, 12, 7025-7035

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