MM 16: Invited Talk (Hauptvortrag): Takeuchi

Time: Tuesday 9:30–10:00 Location: H24

Invited Talk MM 16.1 Tue 9:30 H24
Combinatorial approach to multifunctional materials — •Ichiro Takeuchi — University of Maryland, College Park, MD, USA

We have developed a thin-film based high-throughput methodology for rapid screening of large compositional phase spaces in search of new compounds with enhanced physical properties. Pulsed laser deposition and co-sputtering serve as the main tools to generate combinatorial thin film library wafers. Various scanning and/or parallel measurement techniques are employed to obtain quantitative mapping of various physical properties across the libraries. Our primary targets are inorganic functional materials such as magnetic materials, piezoelectric materials, and superconductors. We map the structural properties across libraries and quickly cross-reference them with known phases in crystallographic databases. The need for such a study is common among combinatorial investigation of virtually all topics. Automated scanning X-ray diffraction across entire libraries is carried out at a synchrotron beamline as well as with in-house diffractomerers. Machine learning algorithms are used for materials property prediction and materials classification. The algorithms also provide a means for determining latent variables - primary predictors of material structure and properties that might otherwise be buried in the large datasets. Combinatorial investigation guided by theories will also be discussed.