High-Throughput μXRD² Mapping and Analysis of Combinatorial Thin Films

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When multiple elements are co-sputtered onto a flat substrate from different angles, they form a thin film with a composition that varies continuously across the surface. A single combinatorial thin-film sample can therefore encompass thousands of distinct alloy compositions, providing a powerful platform for high-throughput screening of composition–microstructure–processing–property relationships.

We are developing *SwissMapper* (Figure 1), a fully automated single-platform instrument that integrates μXRD² and μXRF with nanoindentation, light microscopy, electrical probing, reflectometry, and ellipsometry. All techniques probe the exact same raster grid across the full area of 4-inch substrates at a lateral resolution of approximately 500 μm, yielding perfectly spatially aligned multimodal datasets over night. The platform is complemented by in-house developed software for "mapping-native" data processing, featurization, visualization, correlation, and interactive exploration, designed to provide intuitive and low-barrier no-code analysis.

At the core of the data workflow is an advanced XRD/XRF analysis pipeline for the efficient evaluation of combinatorial datasets with more than 1000 measurement points. The combined use of diffraction and fluorescence data provides a strong foundation for deriving phase-diagram-like information across composition space. The workflow follows a hybrid strategy that combines similarity-based unsupervised machine learning with expert interpretation, allowing transferability across chemical space without the need for material-specific supervised model training. First, the diffraction map is segmented into regions of homogeneous signal using methods that are robust against peak shifts caused by continuous compositional variation while respecting simple yet powerful graph-network-based constraints. Structural model hypotheses established on representative patterns from each subset are then propagated and refined through batch Rietveld refinement across the full dataset, enabling efficient and consistent analysis of the entire combinatorial map. Where appropriate, the 2D diffraction data can further be interrogated to assess crystallographic texture, crystallite size, lattice strain, and related microstructural features.

The combination of fully integrated, automated multi-technique data acquisition with a bespoke modern software stack substantially accelerates the exploration of complex materials spaces. By enabling spatially aligned characterization, rapid data reduction, and scalable analysis of large combinatorial datasets, SwissMapper provides an efficient route from thin-film synthesis to phase and property mapping. At the same time, the resulting structured and traceable datasets create a durable basis for data-driven materials research, institutional knowledge retention, and the future development of machine-learning methods.

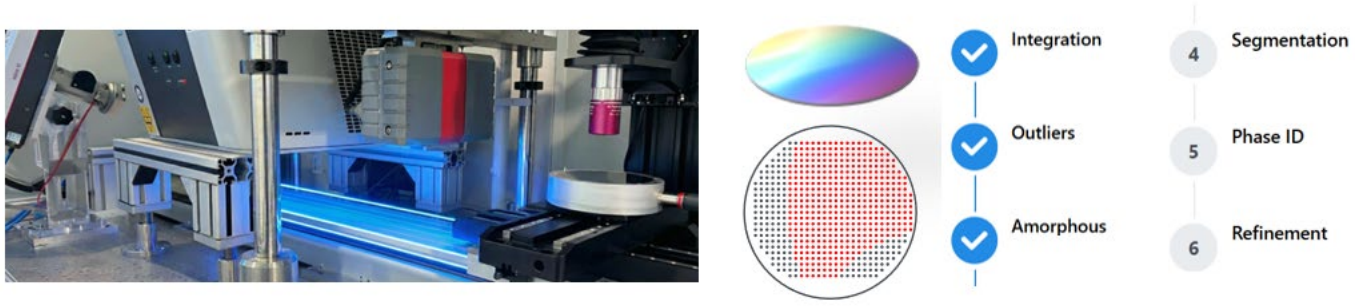


Figure 1. *SwissMapper, a high-throughput combinatorial thin film characterisation system*