Automating Powder Pattern Interpretation with High-Throughput Measurements and Artificial Intelligence

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Phase mapping is a long standing challenge in automated data interpretation. This talk presents innovative uses of machine learning and artificial intelligence to fully automate phase mapping enabled by high-throughput experimentation and data management. As materials scientists explore higher dimensional composition spaces (ternary or higher) to discover and optimize functional materials, establishing composition-structure-processing-property relationships becomes increasingly difficult because (i) many high order phase diagrams have yet to be explored; (ii) there are many known low-order (e.g. binary) phases that may form, possibly including unknown phases, and (iii) the syntheses used for rapid materials exploration often yield non-equilibrium phase behavior, especially alloying over broad composition ranges. Compounding these data interpretation challenges is the limited ability of humans to perform manual analysis due to the need to dissect many mixed-phase patterns and track phase concentrations through multi-dimensional composition spaces. Phase mapping algorithms inherently need to provide super-human analysis capabilities, which will be demonstrated using several ternary datasets from combinatorial materials discovery research.