High-throughput XRD and Analysis for Rapid Determination of Phase Distribution Across Combinatorial Libraries

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We have developed techniques to handle large numbers of diffraction data from measurements performed on combinatorial libraries of functional thin film materials. In order to rapidly indentify new functional materials with enhanced physical properties, we screen thin film combinatorial libraries and composition spreads spanning large segments of binary and ternary compositional phase diagrams. The library wafers are fabricated by pulsed laser deposition or co-sputtering. Among various properties to be mapped for hundreds of spots across a library, structural phases or structural evolution across phase diagrams is of particular interest since properties such as mechanical actuation and electromechanical coupling can be substantially enhanced at structural boundaries for smart materials. We use an in-house diffractometer as well as synchrotron microdiffraction to collect a large number of 2D diffraction images per library. We have developed several visualization schemes which allow us to rapidly plot, view, and analyze up to hundreds of diffraction spectra simultaneously. The ultimate goal in this practice is to rapidly map the structural phase diagrams. We have demonstrated that for some materials systems, cluster analysis techniques are useful for quickly deciphering the distribution of phases from diffraction spectra taken from ternary composition spreads. Using this method together with reference diffraction patterns from crystallographic databases, the arduous analysis and classification of hundreds of diffraction spectra is reduced to a much shorter analysis of only a few spectra. Our recent work on application of non-negative matrix factorization to handle spectra with mixed phases will also be discussed. This work is performed in collaboration with Chris Long and Vicky Karen and is supported by NSF MRSEC at UMD ((DMR 0520471) and NIST.