COMBINATORIAL APPROACH TO MATERIALS DISCOVERY AND THE MATERIALS GENOME INITIATIVE

Ichiro Takeuchi
Department of Materials Science and Engineering
University of Maryland

Throughout the history of mankind, scientists and engineers have relied on the slow and serendipitous trial-and-error approach for materials discovery. In the late 1980s, the combinatorial approach was pioneered in the pharmaceutical industry in order to dramatically increase the rate at which new chemicals are identified. The combinatorial concept is now widely being implemented in a variety of technological areas where new materials are urgently needed. The high-throughput strategy allows one to rapidly screen through a large composition phase space in search of compounds with enhanced physical properties. Combinatorial libraries also allow quick delineation of composition-property-structure relationships across compositional landscapes. Occurrence of enhanced physical properties is often accompanied by structural transitions, and therefore obtaining accurate information regarding structural phase distribution across libraries is crucial. In-house diffractometers as well as synchrotron diffraction are used for this purpose. I will discuss how we are using the large amount of diffraction data taken from libraries as the platform for developing various informatics tools and techniques including implementation of machine learning algorithms for rapid data analysis. The combinatorial approach is particularly powerful when guided by theoretical predictions. I will give examples of successfully carried out experiments where theoretical and experimental efforts were combined. The role of the combinatorial approach within the Materials Genome Initiative will also be discussed.