Combinatorial Methods

The Combinatorial Methods Program develops novel high-throughput measurement techniques and combinatorial experimental strategies specifically geared towards materials research. These tools enable the industrial and research communities to rapidly acquire and analyze physical and chemical data, thereby accelerating the pace of materials discovery and knowledge generation. By providing measurement infrastructure, standards, and protocols, and expanding existing capabilities relevant to combinatorial approaches, the Combinatorial Methods Program lowers barriers to the widespread industrial implementation of this new R&D paradigm.

The Combinatorial Methods Program has adopted a two-pronged strategy for meeting these goals. The first of these is an active research and development program designed to better tailor combinatorial methods for the materials sciences and extend the state of the art in combinatorial techniques. Measurement tools and techniques are developed to prepare and characterize combinatorial materials libraries, often by utilizing miniaturization, parallel experimentation, and a high degree of automation. A key concern in this effort is the validation of these new approaches with respect to traditional "one at a time" experimental strategies. Accordingly, demonstrations of the applicability of combinatorial methods to materials research problems provide the scientific credibility needed to engender wider acceptance of these techniques in the industrial and academic sectors. In addition, the successful adoption of the combinatorial approach involves a highly developed "workflow" scheme. All aspects of combinatorial research, from sample "library" design and library preparation to high-throughput assay and analysis, must be integrated through an informatics framework, which enables iterative refinement of measurements and experimental aims. Combinatorial Methods Program research projects give illustrations of how these processes are implemented effectively in a research setting.

NIST-wide research collaborations, facilitated by the Combinatorial Methods Program, have produced a wide range of new proficiencies in combinatorial techniques, which are detailed in a brochure, "Combinatorial Methods at NIST" (NISTIR 6730), and online at www.nist.gov/combi. Within MSEL, novel methods for combinatorial library preparation are designed to encompass variations of diverse physical and chemical properties, such as composition, film thickness, processing temperature, surface energy, chemical functionality, UV-exposure, and topographic patterning of organic and inorganic materials ranging from polymers to nanocomposites to ceramics. In addition, new instrumentation and techniques enable the high-throughput measurements of adhesion, mechanical properties, and failure mechanisms, among others. The combinatorial effort extends to multiphase, electronic, and magnetic materials, including biomaterials assays. On-line data analysis tools, process control methodology, and data archival methods are also being developed as part of the Program's informatics effort.

The second aspect of the Combinatorial Methods Program is an outreach effort designed to facilitate technology transfer with institutions interested in acquiring combinatorial capabilities. The centerpiece of this effort is the NIST Combinatorial Methods Center (NCMC), an industry-university-government consortium organized by MSEL that became operational on January 23, 2002 via a kick-off meeting in San Diego. Although it is still in the growth stage, the impact of NCMC activities is readily apparent, as 11 industrial partners and the Air Force Research Lab have already joined the NCMC membership program. The NCMC facilitates direct interaction between NIST staff and these industrial partners, and provides a conduit by which Combinatorial Methods Program research products, best practices and protocols, instrument schematics and specifications, and other combinatorial-related information can be effectively disseminated. This outreach is mediated in large part by a series of tri-annual workshops for NCMC members. The first NCMC meeting, "Library Design and Calibration", was held on April 26, 2002 at NIST, and provided information essential to starting a combinatorial research effort. The second meeting (October, 2002) will concentrate on combinatorial approaches to adhesion and mechanical properties. Further information on NCMC can be found on the web-site at www.nist.gov/combi.