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 by 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 accelerating the development and implementation of combinatorial approaches: an active intramural R&D program and an ambitious outreach activity. The intramural R&D program is 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. The successful adoption of the combinatorial approach also requires 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 combinatorial methodology is 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 the Materials Science and Engineering Laboratory (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 to metals. New instrumentation and techniques have been developed that enable the high-throughput measurements of adhesion, mechanical properties, failure mechanisms, film thicknesses, and refractive index, among others. The combinatorial effort extends to multiphase, electronic, optoelectronic, 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 extensive outreach activity in the Combinatorial Methods Program is 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. The recognized importance of NCMC activities is readily apparent, as 15 industrial partners, the Air Force Research Lab, and the University of Southern Mississippi are participating in the NCMC membership program. The membership continues to grow and 80 % of the members from last fiscal year have already renewed for this fiscal year. The NCMC facilitates direct interaction between NIST staff and these industrial partners, and it 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 semi-annual workshops for NCMC members. Indeed, since its inception, four NCMC workshops have been held at NIST. Further information on the NCMC can be found on the website at www.nist.gov/combi.

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