Data and Data Delivery

The economic importance of technical data has grown steadily over the past three decades. NBS/NIST took an important lead early in the effort to emphasize the pervasive use and increase the impact of reliable materials property data. As early as 1985, former NBS Director E. Ambler noted that the need for property data had become a "national priority," while the National Research Council repeatedly observed that there is a persistent "critical national need" for materials property data.

The NIST Materials Science and Engineering Laboratory (MSEL) has been a prominent leader in responding to this national need. By design, the scope of the MSEL effort is evolutionary and responds to the ever-increasing advances in technology. Currently, MSEL has six project areas in the Data and Data Delivery program.

- ***Crystallographic and Phase Equilibria Databases*** *[Project Leader — V. Karen]:* This project encompasses the two most venerable efforts in MSEL, each of which recently has had a major new release. In collaboration with Fachinformationszentrum Karlsruhe (FIZ, Germany), a CDROM version of the FIZ/NIST Inorganic Crystal Structure Database (ICSD) has been released providing the full structural data, *i.e*., lattice parameters and atomic coordinates, for approximately 60,000 compounds. The long-standing collaboration between NIST and the American Ceramic Society (ACerS) has continued with the completion of a new topical volume in the NIST/ACerS Phase Equilibria Diagrams series, the first of two planned volumes on electronic ceramics.

- ***Phase Equilibria and Properties of Dielectric Ceramics*** *[Project Leader — T. Vanderah]:* An integrated theoretical and experimental effort is underway to predict and measure phase equilibria and electronic behavior in dielectric oxide systems. This work includes relaxor ferroelectrics, dielectrics for cellular infrastructure and hand-held devices, and dielectrics for low temperature co-fired ceramics for applications in multilayer ceramic integrated circuit technology. The impact of this work was evident in Dr. Vanderah's invited perspective article, "Talking Ceramics," which appeared in the journal *Science*. The timeliness of this work was emphasized further by its subsequent feature in the science section of the *New York Times*.

- ***Phase Relationships in High Temperature Superconductors*** *[Project Leader — W. Wong-Ng]:* MSEL's meticulous effort to provide phase information critical to the development of practical superconductors is currently directed towards two important systems: $Ba_2RCu_3O_{7-x}$, where R is yttrium or a lanthanide, and MgB_2. For $Ba_2RCu_3O_{7-x}$, work has focused on the phase relations in BaF_2-BaO-Y_2O_3-CuO_x-H_2O and the interactions of $Ba_2RCu_3O_{6+x}$ with buffer layers, both of which are important for advances in the "BaF_2 *ex situ*" process and the "liquid-phase-epitaxy" process. For MgB_2, the enthalpy of formation, vapor pressure, and sources of variability have been determined.

- ***Reaction Path Analysis in Multicomponent Systems*** *[Project Leader — C. Campbell]:* Many industrial processes rely on multicomponent diffusion to control the formation and dissolution of precipitate phases. MSEL is developing a multicomponent diffusion mobility database for Ni-base superalloys that will be used, for example, to predict the formation of the γ' (ordered FCC) phase during the solidification of superalloys. A workshop, "High Throughput Analysis of Multicomponent Multiphase Diffusion Data," was held in March 2003 to focus on the development of methods to extract diffusion data from multicomponent diffusion couples.

- ***Evaluated Materials Property Data*** *[Project Leader — R. Munro]:* Engineering designs utilizing advanced materials require reliable data. Elasticity, strength, toughness, hardness, creep, thermal expansion, conductivity, diffusivity, and durability are prominent among the data categories needed and desired for materials applications and development. This project is directed both towards the development of evaluated databases of these properties for structural and superconducting ceramics and towards the establishment of the evaluation methodologies that form the foundation of reliable materials property data systems. A significant achievement in this effort is "Data Evaluation Theory and Practice for Materials Properties," SP960-11, the eleventh NIST Recommended Practice Guide produced by MSEL.

- ***Informatics and Visualization in Materials Data Delivery*** *[Project Leader — C. Beauchamp]:* The internet, and the World Wide Web in particular, has become a dominant resource medium for technical information. MSEL has undertaken a major commitment to make its extensive data collections available *via* this medium. New efforts, now underway, will provide web access to the MSEL lead-free solder materials property database and the diffusion data archive that is important for the processing of metal alloys. Additionally, the internet will be used increasingly as a means of disseminating MSEL's prodigious technical publications in the form of electronic manuscripts.

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