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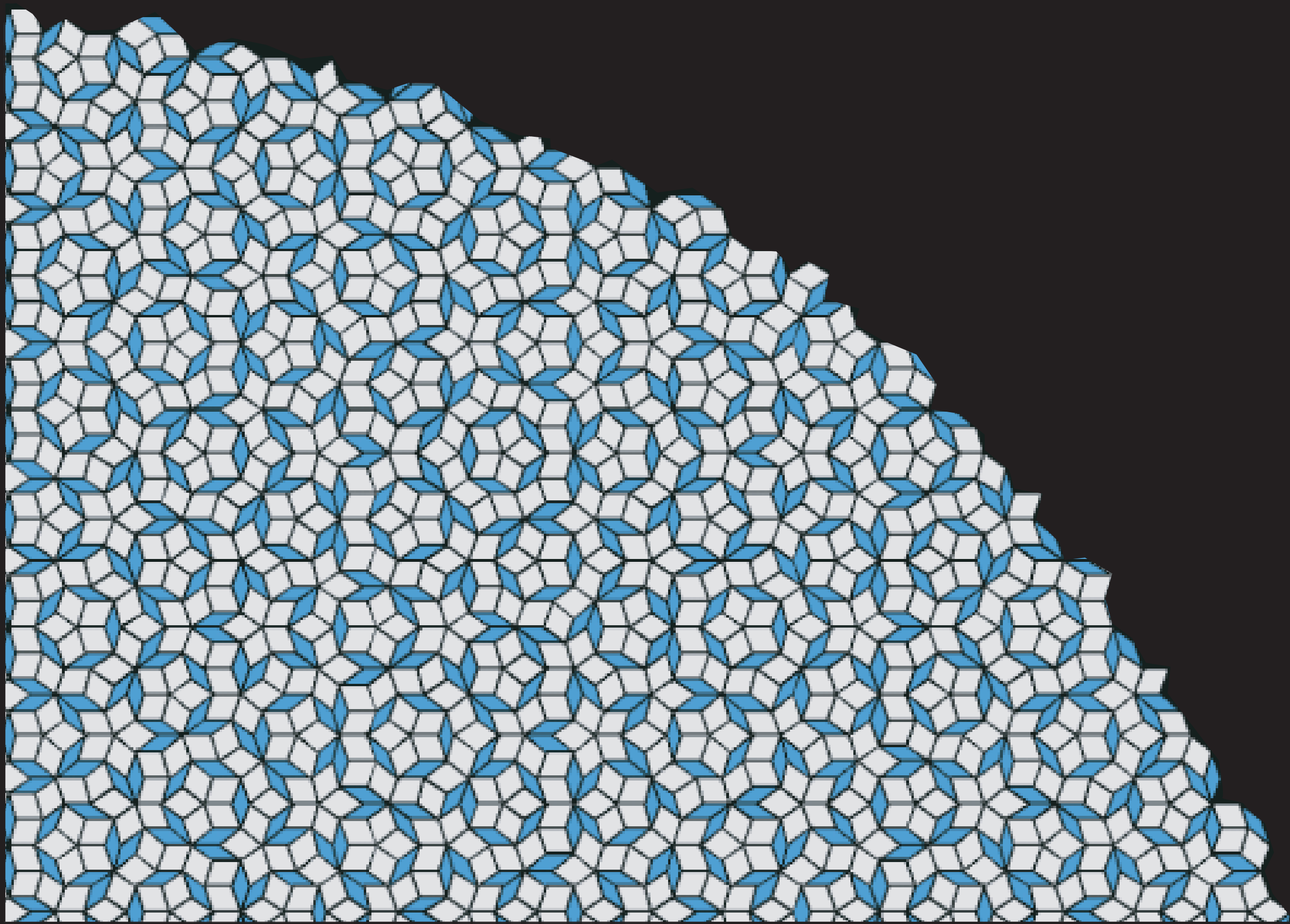
Special Issue: Crystallography at NBS/NIST



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- Computer Security
- Information Access
- Convergent Information Systems
- Information Services and Computing
- Software Diagnostics and Conformance Testing
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[1]At Boulder, CO 80303.
[2]Some elements at Boulder, CO.

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U.S. Department of Commerce—**Donald L. Evans,** Secretary
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National Institute of Standards and Technology—**Arden L. Bement, Jr.,** Director

Cover: The cover illustration, created by Denis Gratias, is a Penrose tiling, an example of an aperiodic tiling with 5-fold symmetry. It was created from a slice of a periodic arrangement of hypercubes. Just as three adjacent rhombs give the impression of a three dimensional cube, the five orientations of edges in this illustration can be seen as perpendicular to each other in a still higher dimension. Although the same groupings of tiles recur many times and are close to each other, their spacing is not regular and their surroundings are never exactly the same. This tiling is what is called quasiperiodic and its diffraction pattern would be quite similar to that of the aluminum-manganese quasicrystal along its 5-fold axis, displayed on p. 978 in the article on quasicrystals on p. 975. Cover illustration by C. Carey.

The *Journal of Research of the National Institute of Standards and Technology,* the flagship periodic publication of the national metrology institute of the United States, features advances in metrology and related fields of physical science, engineering, applied mathematics, statistics, biotechnology, and information technology that reflect the scientific and technical programs of the Institute. The *Journal* publishes papers on instrumentation for making accurate measurements, mathematical models of physical phenomena, including computational models, critical data, calibration techniques, well-characterized reference materials, and quality assurance programs that report the results of current NIST work in these areas. Occasionally, a Special Issue of the *Journal* is devoted to papers on a single topic. Also appearing on occasion are review articles and reports on conferences and workshops sponsored in whole or in part by NIST.

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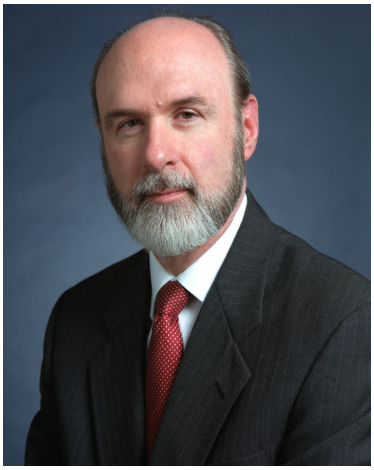
Richard D. Deslattes

On May 16, 2001, the National Institute of Standards and Technology lost a most illustrious career scientist in x-ray research. This volume is dedicated to honor the memory of Richard D. Deslattes and his lifetime of achievements at NIST. Deslattes' research in precision metrology, interferometry, and x-ray spectroscopy earned him worldwide recognition. Much of his research was directed toward the determination of fundamental physical constants and masses of elementary particles, and toward testing basic theories. Deslattes was the first to combine x-ray and optical interferometry, and in a famous experiment he used the remarkable instrument he created to link x-ray light to visible light and to precisely determine the spacing of atoms in a silicon crystal. This measurement was a key input needed to obtain an improved value for the Avogadro constant, a fundamental constant of nature related to the amount of substance, and which may one day lead to a new natural standard of mass. Deslattes also used the atom spacing measurement to establish more accurate x-ray and gamma ray wavelength standards. He played a major role in the development of the iodine stabilized laser, a precise light source that was a significant step in the evolution of the international standard for the meter. Deslattes was also well known for novel applications of x-ray diffraction. One of these applications was a precision calibration device that allowed radiologists to record better quality mammograms. His enormous energy, his ability to lead, and his remarkable creativity will be deeply missed.

Ernest Kessler
Gabrielle Long

Foreword



Leslie E. Smith

This *Special Issue,* which focuses on crystallography, is part of The Centennial Celebration of the National Institute of Standards and Technology (NIST), formerly known as the National Bureau of Standards (NBS). NBS/NIST has a long history (more than 50 years) of crystallographic research with contributions from many scientists from various divisions and diverse disciplines. The research was carried out as a fundamental part of the overall mission of NBS/NIST and its research programs. The mission of NBS/NIST enables its scientists to undertake large, long-term, research projects to develop fundamental understanding, data, and measurement methods that result in significant bodies of work and create a stimulating research environment. Crystallography represents one such area and this *Special Issue* was assembled to review work in this area by giving a brief overview of the role of crystallography at NBS/NIST—past, present, and future.

The articles cover a broad spectrum of topics including high-pressure crystallography, magnetic structure determinations, quasi-crystals, novel biomaterials, biological minerals, structure determination via neutron and x-ray diffraction, reduced cells, standard reference materials, phase equilibria and ceramic oxides, crystallographic texture, zeolitic materials, near perfect crystals, electron diffraction, crystallographic databases, protein crystallography, crystallography in construction, and synchrotron radiation. The articles are preceded by a memorial tribute to Richard Deslattes, a highly respected NBS/NIST scientist who is well known throughout the United States and the international scientific communities. His major scientific contributions were in the fields of x-ray physics, precision measurements and fundamental constants.

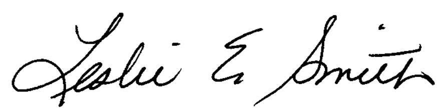
There is scientific diversity in the articles along with a number of fascinating highlights. For example, the article on quasi-crystals strikes at the fundamental definition of a crystal lattice. The article on bone cement shows that specialized crystalline materials can be designed to play a vital role in orthopedic surgical procedures. Several of the papers demonstrate that some of the outstanding achievements at NBS/NIST were arrived at by serendipity—not a direct part of a "defined" project, but arising from a creative and stimulating scientific environment. This type of research has long been an integral part of the synergistic NBS/NIST culture. For example, the diamond anvil pressure cell was invented "by scientists of different interests, different research activities and different backgrounds, who interacted on a professional level and recognized an opportunity to make a significant contribution to scientific research."

From these articles, it is obvious that crystallographic research at NBS/NIST will continue to play an important role in the future. The development of new and novel materials, material characterization techniques, standards, and standard reference materials will continue to be vital to the scientific community and the nation's economy. Several broad themes are apparent: (1) that collaborative efforts with outside organizations and individuals will continue to be an important part of the NBS/NIST research culture; (2) that instrumentation will continue to be emphasized; and (3) that work on databases will expand to meet the needs of the scientific community.

NBS/NIST has long supported collaborative research efforts with external groups. Accordingly, several such efforts are illustrated in the articles. For example, the Polymers Division and the American Dental Association have collaborated in research on dental materials for many years. An article on the development of a novel bone cement illustrates a medically important biomaterial that is a product of this collaboration. Another long-term and fruitful collaboration has been that between NBS/NIST and the International Centre for Diffraction Data (ICDD). This effort has focused on collecting and evaluating data for the Powder Diffraction File, a database that is used in laboratories worldwide for materials characterization. Finally, a "Research Collaboratory for Structural Bioinformatics (RCSB)," involving three groups, has recently been created.

An especially important NBS/NIST activity is the development of state-of-the-art instrumentation and making it available to the scientific community. In particular, articles on the NIST Center for Neutron Research capabilities describe the elegant instrumentation available for the rapid collection of neutron powder diffraction data and for property measurement. This equipment has provided the data required to solve and understand many unique structures of critical scientific importance, e.g., superconductors. These structure solutions have helped revolutionize concepts in inorganic chemistry. Similarly, another article gives a detailed discussion on the NBS/NIST synchrotron facilities for materials science.

Another theme embodied in this *Special Issue* is the increasing realization of the critical importance of crystallographic data centers to the needs of the scientific community. Concepts and software developed at NBS/NIST for the standardization of lattice parameters, for symmetry determination and for identification are widely used by the scientific community. In the future, computer-driven scientific instruments will funnel data into the public domain at an unprecedented rate. In response, there will be an increasing emphasis on computational techniques to work with and exploit this data. This trend is demonstrated by the creation of crystallographic databases in support of materials development. To handle the deluge of protein data, NIST, in partnership with Rutgers University and the UCSD, formed the RCSB, which acquired the Protein Data Bank in 1997. An important future role of NIST in crystallographic databases will be to set data standards, provide accessibility, interlink data, evaluate information, and create research and data mining software tools.



Leslie E. Smith

Director, Materials Science and Engineering Laboratory
Chair, NIST Centennial Committee

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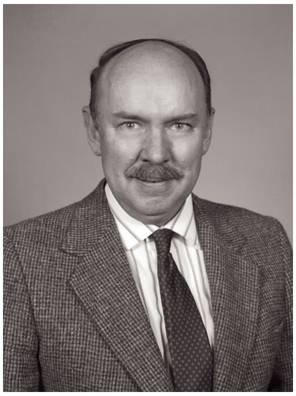
Crystallography at NBS/NIST

Preface

Winnie Wong-Ng



Alan D. Mighell

Special Issues of the Journal of Research of the National Institute of Standards and Technology are devoted to papers in a particular field of measurement science. The papers herein have been written by research scientists in the field and focus on the past accomplishments, present status, and future potential of crystallography at NBS/NIST. These papers, some of which were presented at the 2001 Los Angeles Meeting of the American Crystallographic Association, clearly show that crystallography at NBS/NIST has had, and will continue to have, a major impact on the advancement of science and technology. Over the years, many crystallographers at NBS/NIST, in addition to the authors, have participated in this research effort as demonstrated by the list following this Preface. The Special Issue Editors thank the authors for their sustained enthusiasm in recreating past events and in preparing this issue. Furthermore, the editors are very grateful to Julian M. Ives, Ronald Munro, Theodore V. Vorburger, and the NIST Publications Production Program for their dedicated work in producing this volume.

Alan D. Mighell
Winnie Wong-Ng

Special Issue Editors

Crystallographers at NBS/NIST

Crystallographic research at NBS/NIST began in the 1930s. Throughout the subsequent years, a large number of scientists have contributed to a long and distinguished history in this field. The following is a compilation of representative scientists who have pursued research in crystallography or closely related disciplines at NBS/NIST. It is not intended to be a complete list, but rather to provide an overview via the participants of the nature and diversity of crystallographic research at NBS/NIST. For each scientist, the list includes the name, the years of service and major research interests.

Andrew J. Allen (1991–present) Small-angle neutron and x-ray scattering, microstructure characterization, porous and nanocrystalline ceramics, thermal barrier coatings, cement systems, ceramic powders and suspensions.

John D. Barnes (1963–present) Polymer crystallization, quasielastic neutron scattering, lattice dynamics, molecular transport in polymers, small-angle scattering.

Alec J. Belsky (1999–present) Inorganic crystal data, data analysis, crystallographic software development.

Leonid A. Bendersky (1983–present) Electron microscopy, phase transformations, crystal structure.

Talapady N. Bhat (1999–present) Bioinformatics, Protein Data Bank, macro-molecular structures, software development, database.

David R. Black (1978–present) X-ray diffraction topography, synchrotron radiation instrumentation, x-ray optics, materials microstructure characterization.

Stanley Block (1954–1990) Diamond cell, ruby technique, x-ray diffraction at high pressures of single crystals, powders, polymers, RDF's, and IR spectroscopy.

Leonard H. Bolz (1948–1988) X-ray diffraction, free radical research.

Julie A. Borchers (1989–present) Neutron diffraction and reflectivity, magnetic thin films and multilayers.

Carroll S. Brickenkamp (1971–2001) Crystal structures using single crystal x-ray and neutron diffraction, NIST program planning, U.S. legal metrology, NIST calibration and other measurement services, measurement laboratory accreditation.

William S. Brower (1956–1980) Ceramic and crystal synthesis in energy related materials; crystal growth via melt, Czochralski, Bridgman, Verneuil techniques.

Walter E. Brown (1962–1993) Chemical physics, crystallography, calcium phosphate chemistry, thermodynamics.

Harold E. Burdette (1969–present) Synchrotron radiation instrumentation, x-ray topography, x-ray and real time imaging, crystal growth.

Gordon Burley (1954–1966) Silver iodide, rain making, crystallography.

Benjamin P. Burton (1983–present) First principle calculations, phase equilibria, crystal chemistry.

John W. Cahn (1977–present) Solid-state phase transformations, including ordering, crystal shapes, internal interfaces, surface anisotropy, rapid crystallization, and quasicrystals.

Chang S. Choi (1970–1995) Neutron diffraction, x-ray diffraction, energetic material structures, residual stress, texture.

Laurence C. Chow (1969–present) Calcium phosphates, solution chemistry, biomineralization, calcium phosphate biomaterials, dental caries.

James P. Cline (1986–present) X-ray powder diffraction, standard reference materials, instrumentation.

Sam R. Coriell (1961–present) Theory of crystal growth and alloy solidification, morphological and hydrodynamic instabilities.

Johan deGroot (1957–1979) Inorganic compound syntheses, standard powder diffraction patterns.

Richard D. Deslattes (1962–2001) Research in precision metrology, interferometry, and x-ray spectroscopy directed toward the determination of fundamental physical constants and masses of elementary particles, and toward testing basic theories.

Brian Dickens (1966–present) Groups I and II (particularly calcium) phosphates and carbonates, their hydrates, and related compounds, hydrogen bonding, water in crystal structures, epitaxy, low temperatures, impurities/mixed populations in crystalline sites, computer programming.

Ross W. Erwin (1985–present) Structure and dynamics of nanoscale magnetic structures, relaxor ferroelectrics.

Eloise Evans (1958–1989) High quality reference powder diffraction patterns.

Edward N. Farabaugh (1960–present) X-ray diffraction topography, powder x-ray diffraction, electron microscopy, crystal growth, diamond growth, phase equilibria.

Daniel A. Fischer (1991–present) Soft x-ray absorption spectroscopy, novel x-ray detectors, x-ray optics.

D. Travis Gallagher (1990–present) Protein and DNA crystallography, protein science, diffraction phase determination, macromolecular crystal growth.

Frank W. Gayle (1988–present) Physical metallurgy, electron microscopy, crystallography, aerospace alloys, and materials for microelectronics.

Gary L. Gilliland (1986–present) Protein crystallography, protein engineering, structural biology, structural biology databases (Biological Macromolecule Crystallization Database and Protein Data Bank).

Charles J. Glinka (1975–present) Small-angle neutron scattering, mesoporous materials, neutron optics and scattering instrumentation.

Thomas A. Hahn (1963–1981) Thermal expansion standards and reference data.

Qingzhen Huang (1990–present) X-ray and neutron powder diffraction, crystal structure, magnetic properties, Rietveld refinement.

Camden R. Hubbard (1971–1988) Single crystal and powder x-ray diffraction methods, software, standard reference materials, and reference patterns collection and evaluation.

Herbert Insley (1923–1953) Petrographic microscope, devitrification, composition of cement clinker, powder x-ray diffraction, initiated course in petrographic microscopy.

Debra L. Kaiser (1988–present) Single crystal growth, x-ray diffraction, high temperature superconductors.

Vicky L. Karen (1978–present) Crystallographic databases, lattice-theory, converse- transformation analysis, symmetry, x-ray and neutron diffraction, crystal structure determination, algorithm design.

Ernest G. Kessler, Jr. (1969–present) X-ray diffraction, precision x-ray wavelengths, x-ray wavelength database, crystal lattice parameter measurements.

Masao Kuriyama (1967–1990) Synchrotron radiation, x rays, dynamical diffraction, topography, inelastic scattering, real time imaging.

Jane E. Ladner (1992–present) Protein crystallography, structural biology, biological macromolecule crystallization database.

Ernest M. Levin (1945–1974) Phase equilibria, x-ray powder diffraction, phase diagrams for ceramists.

Igor Levin (1997–present) Crystal structures, phase transitions, transmission electron microscopy, x-ray and neutron powder diffraction.

Lyle E. Levine (1995–present) Ultra-small-angle x-ray scattering imaging, diffraction and small-angle-scattering from dislocations, fundamental theory of deformation, statistical physics.

David R. Lide (1954–present) Molecular spectroscopy, standard reference data and data evaluation methodology, development of electronic databases in crystallography, chemistry and physics.

Gabrielle G. Long (1980–present) X-ray and neutron scattering, x-ray optics, synchrotron radiation instrumentation, materials microstructure characterization.

Jeffrey W. Lynn (1976–present) Neutron diffraction and inelastic scattering phase transitions and critical phenomena.

Charles F. Majkrzak (1987–present) Neutron reflectometry studies of the chemical and magnetic nanostructures of thin films and multilayer materials.

Mathai Mathew (1975–present) Crystal chemistry of calcium phosphates, biomineralization, single crystal structural studies.

Floyd A. Mauer (1948–1989) Instrumentation for studies of the effects of temperature and pressure on the physical properties of solids.

Howard F. McMurdie (1928–present) Phase equilibria, x-ray diffraction, high temperature x-ray diffraction, phase diagrams for ceramists.

Alan D. Mighell (1964–present) Lattice analysis, symmetry determination, identification, structure determination, powder indexing, crystallographic databases.

Rose Mooney (1953–1956) Single crystal structure determination, phosphate structure analysis, initiated single crystal work at NBS.

Marlene Morris (1955–1986) High quality reference powder diffraction patterns, powder indexing.

Bernard Mozer (1968–1991) Neutron scattering, small-angle neutron-scattering, structure of quasicrystals, RDFs.

Ronald G. Munro (1976–present) Theory, high pressure RDFs, molecular dynamics, materials property relations, data evaluation methodology.

Mary M. Mrose (1983–1999) Phosphate minerals, powder diffraction, crystal data evaluation, single crystal diffraction.

Taki Negas (1968–1983) Electronic ceramics, high temperature defect chemistry, x-ray powder and single crystal diffraction, crystal structure and chemistry, analytical SEM/EDX, microstructure, phase diagrams.

Helen M. Ondik (1958–present) Phosphate crystal structures, Crystal Data compilation, data compilation of materials of construction for coal gasification plants, Phase Diagram data compilation, and database design.

Fred Ordway (1949–1964) Structural disorder, computer modeling, instrumentation, water structure.

Boris Paretzkin (1961–1994) X-ray powder diffraction, reference powder diffraction patterns.

Harry S. Parker (1951–1988) Crystal growth of ceramic materials from vapor and fluxes and synthesis of complex oxides, halides and chalcogenides.

H. Steffen Peiser (1957–present) Crystal growth, symmetry, and characterization for free-radical research, relative atomic mass values, and the fundamental constants.

Alvin Perloff (1951–1984) Single crystal x-ray analysis, phosphate and borate structure determination.

Gasper J. Piermarini (1957–present) Diamond anvil cell, ruby technique, high pressure x-ray diffraction of single crystals, powders, polymers, RDFs and IR spectroscopy at high pressures.

Aaron S. Posner (1950–1961) X-ray diffraction and IR absorption studies of the structure of calcium phosphates, bone and tooth mineral and collagen and related synthetic polymers, single crystal structure analysis, powder diffractometry and low angle x-ray scattering studies.

Henry J. Prask (1970–present) Neutron diffraction, energetic materials, residual stress, texture, coatings.

Edward Prince (1966–present) Neutron diffraction instrumentation, Rietveld method, maximum entropy, statistical methods.

Nikos P. Pyrros (1981–1983) Single crystal analysis, powder x-ray diffraction, software development, reference powder diffraction patterns.

Curt W. Reimann (1962–present) Structural and spectroscopic properties of transition metal complexes involving a variety of co-ordinate and hydrogen bonding arrangements creating unique environments.

Carl R. Robbins (1956–1986) Inorganic structural chemistry (e.g., oxides, silicates, germanates, aluminates), x-ray powder diffraction, single crystal, phase equilibria.

Robert S. Roth (1951–present) Phase equilibria of oxide ceramics, crystal chemistry, crystal structure analyses, x-ray powder diffraction, single crystal growth, single crystal structure analyses, neutron diffraction, electron diffraction, HREM lattice images.

John Rumble, Jr. (1980–present) Standard Reference Data, materials, chemistry and physics databases; crystallographic databases.

Antonio Santoro (1964–present) X-ray and neutron diffraction, crystal structure determination, lattice geometry, bond valence analysis.

Charles Saylor (1931–1968) Chemical microscopy relating to the formation of crystalline phases, crystalline rubber, optical properties of crystals.

LeRoy W. Schroeder (1969–1977) X-ray, Raman, and neutron scattering, hydrogen bonding, molecular motion in crystals, inter-layered structures, 2-D (surface) atom pair distributions.

Richard D. Spal (1969–present) Dynamical x-ray diffraction, x-ray optics, x-ray microradiography, x-ray microtomography, materials microstructure characterization, high temperature superconductor composite tape.

Judith K. Stalick (1975–present) Neutron powder diffraction, Rietveld method, quantitative phase determination, partial disorder in intermetallic structures.

Paul Stutzman (1987–present) Cement clinker, cement hydration products, concrete durability, compositional analysis, microstructure, Portland cement, x-ray powder diffraction, scanning electron microscopy.

Howard E. Swanson (1945–1974) High quality reference powder diffraction patterns, internal standards.

Shozo Takagi (1978–present) Calcium phosphate biomaterials, prevention of dental caries, quantitative digitized microradiography, single crystal and powder x-ray crystallography.

Robb Thomson (1971–present) Fundamental theory of fracture and deformation.

Brian H. Toby (1994–present) Powder diffraction crystallography, zeolitic materials, neutron diffraction, crystallographic software, local structure via PDF measurements.

John Torgesen (1948–1972) Growth and purification of large single crystals from aqueous solutions under extreme control of temperature and temperature gradients, measurement of impurity retention and resulting crystal habit modifications.

Samuel F. Trevino (1970–present) Neutron diffraction, small angle scattering and inelastic scattering, polymers, bio-materials, nano-particles, porous materials, quantum tunneling.

Shirley Turner (1986–present) Transmission electron microscopy, x-ray diffraction, manganese oxide minerals, asbestos.

Terrell Vanderah (1993–present) Phase equilibria, crystal chemistry, structure-property relationships, x-ray powder data.

Mark D. Vaudin (1986–present) Crystallographic texture analysis, x-ray diffraction, high temperature x-ray diffraction, electron backscattering diffraction.

Jennifer R. Verkouteren (1988–present) Micro XRD, electron backscattering diffraction, asbestos analysis by XRD.

Charles E. Weir (1943–1970) High pressure, diamond anvil cell, x-ray diffraction of single crystals and powders, high pressure instrumentation, polymers and IR spectroscopy at high pressure.

Alexander Wlodawer (1976–1987) Protein crystallography, neutron diffraction, synchrotron radiation, enzyme structure, AIDS drug design.

Joseph C. Woicik (1989–present) X-ray scattering, x-ray absorption, x-ray photoelectron emission, electronic and geometric structure of surfaces and interfaces.

Winnie Wong-Ng (1983–present) Crystal structure determination, crystal chemistry, phase equilibria, x-ray powder reference patterns, molecular orbital calculations, high temperature superconductors.

Marcello Zocchi (1964–1967) X-ray and neutron single crystal analysis, crystallographic computing, simultaneous diffraction.

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Special Issue: Crystallography at NBS/NIST

Alan D. Mighell and Winnie Wong-Ng, Editors

Articles

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