

## Outputs and Interactions - Surface and Microanalysis Science Division

### 1. Publications

#### 1a. Publications in Print

- Carpick, R.W., and Batteas, J.D., "*Scanning Probe Studies of Nanoscale Adhesion Between Slides in the Presence of Liquids and Monolayers Films*," Springer Handbook of Nanotechnology, B. Bhushan (ed.), Springer-Verlag, Heidelberg, Germany, 605-629, (2004).
- Castle, J.E., and Powell, C.J., "*Report on the IUVSTA Workshop 'XPS: From Spectra to Results – Towards an Expert System'*," Surf. Interface Anal. 36, 225-237 (2004).
- Currie, L.A., "*The Remarkable Metrological History of Radiocarbon Dating [III]*" Journal Research of the National Institute of Standards and Technology, 109, 185-217 (2004).
- Currie, L.A., "*Detection and quantification limits: basic concepts, international harmonization, and outstanding ("low level") issues*," Applied Radiation and Isotopes 61, 145-149 (2004).
- Currie, L.A., "*Uncertainty in Measurements Close to Detection Limits: Detection and Quantification Capabilities*," IAEA-TECDOC-1401(R. Parr, P. Povinec, A. Fajgelj, and P. DeRegge, eds.) Quantifying uncertainty in nuclear analytical measurements 9-34 (2004).
- Danzer, K., Otto, M., and Currie, L.A., "*Guidelines for Calibration in Analytical Chemistry; Part 2: Multispecies Calibration*," Pure and ad Appl. Chem., 76, 1215-1225 (2004).
- Drain, C.M., Smeareanu, G., Batteas, J.D., and Patel, S., "*Self-Assembled Porphyrinic Arrays on Surfaces*," Dekker Encyclopedia of Nanotechnology, J.A. Schwartz, C.I. Contescu, K. Putyera, Eds., Marcel Dekker, Inc.: Vol 5. 3481-3502. New York, (2004).
- Drain, C.M., Milic, T., Garno, J.C., Smeureanu, G. and Batteas, J.D., "*Organizing Self-Assembled Porphyrin Arrays on Metal and Glass Surfaces*," Polymer Preprints 45, 346 (2004).
- Egelhoff, W. F., Jr., Gan, L., Etedgui, H., Kadmon, Y., Powell, C. J., Chen, P. J., Shapiro, A. J., McMichael, R. D., Mallett, J. J., Moffat, T. P., Stiles, M. D., and Svedberg, E. B., "*Artifacts in Ballistic Magnetoresistance Measurements*," J. Appl. Phys. 95, 7554-7559 (2004).
- Hacker, C.A., Batteas, J.D., Garno, J.C., Marquez, M., Richter, C.A., Richter, L.J., vanZee, R.D., and Zangmeister, C.D., "*Structural and Chemical Characterization of Monofluoro-Substituted Oligo (Phenylene-Ethynylene) Thiolate Self-Assembled Monolayers on Gold*," Langmuir, 20 (15): 6195-6205 (2004).

- Helt, J.M., and Batteas, J.D., "***Mica Surfaces: Charge Nucleation and Wear.***" Dekker Encyclopedia of Nanoscience and Nanotechnology, James A. Schwarz, Cristian I. Contescu, and Karol Putyera, Eds.; Marcel Dekker, Inc.: Vol 3: 1947-1966, New York, (2004).
- Hernandez, R.M., Richter, L.J., Semancik, S., Stranick, S.J., and Mallouk, T.E., "***Template Fabrication of Protein-Functionalized Gold-Polypyrrole-Gold Segmented Nanowire,***" Chemistry of Materials, 16 (18): 3431-3438 (2004).
- Hidy, G.M., Eatough, D.J., and Klouda, G.A., "***Design Scenario for the Radioisotopic Estimation of the Biogenic Component of Airborne Particles,***" J. Air and Waste Manage. Assoc., Vol. 54, 600-613 (2004).
- Jablonski, A., Salvat, F., and Powell, C. J., "***Comparison of Electron Elastic-Scattering Cross Sections Calculated from Two Commonly Used Atomic Potentials,***" J. Phys. Chem. Ref. Data, 33, 2, 409-451, (2004).
- Jablonski, A., and Powell, C. J., "***Effect of Different Electron Elastic-Scattering Cross Sections on Inelastic Mean Free Paths Obtained from Elastic-Backscattering Experiments,***" Microchimica Acta, 145, 78-80, (2004).
- Jablonski, A., Salvat, F., and Powell, C. J., "***Differential Cross Sections for Elastic Scattering of electrons by Atoms and Solids,***" J. Electron Spectroscopy and Related Phenomena, 137-140, 299-303, (2004).
- Jach, T.J., Dura, J.A., Nguyen, N.V., Swider, J.R., Cappello, G., and Richter, C.A., "***Comparative Measurements of SiO<sub>2</sub>/Si Films for Thickness Less than 10 nm,***" Surface and Interface Analysis, 36, 23<sup>2</sup> (2004).
- Jach, T.J., Kim, S., Gopalan, V., Durbin, S.M., and Bright, D.S., "***Long-Range Strains and the Effects of Applied Field at 180° Ferroelectric Domain Walls in Lithium Niobate,***" Physical Review B, 69, 064113 (2004).
- Klouda, G.A., Filliben, J.J., Chow, J.C., and Cary, R., "***Reference Material 8785: Air Particulate Matter on Filter Media,***" Symposium on Air Quality Measurement Methods and Technology 2004 Conference Proceedings, April 20-22, 2004, CD-ROM, ISBN 0-923204-62-8 (2004).
- Klouda, G.A., Gillen, J.G., Fletcher, R.A., Etz, E.S., Verkouteren, J.R., Verkouteren, R.M., and Ferguson, E.R., "***Metrology in Support of Trace Explosive Detection Equipment for Homeland Security Applications,***" Symposium on Air Quality Measurement Methods and Technology 2004 Conference Proceedings, April 20-22, 2004, CD-ROM, ISBN 0-923204-62-8 (2004).

- Lewis, C.W., Klouda, G.A., and Ellenson, W.D., "**Radiocarbon Measurement of the Biogenic Contribution to Summertime PM-2.5 Ambient Aerosol in Nashville, TN**," Atmospheric Environment, Vol. 38, 6053-6061 (2004).
- Marinenko, R.B., "**Hetrogeneity Evaluation of Research Materials for Standards Certification**," Microscopy and Microanalysis Journal 10, 491-506, (2004).
- Michaels, C.A., Gu, X., Chase, D.B., and Stranick, S.J., "**Near-Field Infrared Imaging and Spectroscopy of a Thin Film PS/PEA Blend**," Appl. Spec., 58, 257 (2004)
- Newbury, D.E., "**Improving the Sensitivity of Electron Beam Microanalytical Techniques by Enhanced X-ray Spectrometry: X-ray Microcalorimetry, Silicon Drift Detector Energy Dispersive X-ray Spectrometry, and Polycapillary X-ray Optics**," e-journal of Surface Science and Nanotechnology, (<http://www.sssj.org/ejsnt/>) (<http://www.sssj.org/ejsnt/ALC03Contents.html>) (2004).
- Newbury, D.E., "**Quantitative Electron Probe Microanalysis of Rough Targets: Testing the Peak-to-Local Background Method**," SCANNING, v 26, 103-114, (2004).
- Newbury, D.E., "**Energy Dispersive X-ray Spectrometry in the Scanning Electron Microscope**," Micros. Microanal. 10 (Suppl 2) 126-127, (2004).
- Nikoobakht, B., Michaels, C.A., Vaudin, M.D., and Stranick, S.J., "**Horizontal Growth and In Situ Assembly of Oriented Zinc Oxide Nanowires**," Appl. Phys. Lett., Vol.85, 3244 (2004).
- Nikoobakht, B., Davydov, A., and Stranick, S.J., "**Controlling the Growth Direction of ZnO Nanowires on C-Plane Sapphire**," 2004 Materials Research Symposium Proceedings, Vol. 818, M.8.25.1 (2004).
- Powell, C. J., "**Growth and Trends in Surface Analysis and its Applications**," Journal of Vacuum Science and Technology. A 21 (5) Sep/Oct, S42-S53, (2003).
- Powell, C. J., and Jablonski, A., "**Measurement of Gate-Oxide Film Thicknesses by X-ray Photoelectron Spectroscopy**," Characterization and Metrology for ULSI Technology 2003 International Conference, 321-325, (2003).
- Powell, C. J., "**Effect of Backscattered Electrons on the Analysis Area in Scanning Auger Microscopy**," Appl. Surf. Science 230, 327-333, (2004).
- Richter, C.A., Hacker, C.A., Richter, L.J., and Vogel, E.M., "**Molecular Devices Formed by Direct Monolayer Attachment to Silicon**," (2003). Solid-State Electronics, 48 (10-11): 1747-1752
- Richter, L.J., Yang, C.S.C., Wilson, P.T., and Hacker, C.A., "**Optical Charaterization of Oligo (phenylene-ethynylene) Self-Assembled Monolayers on Gold Monolayers on Gold**," J. Physics Chem B, 108, (33):12547-12559 (2004).

- Stranick, S.J., ***“Fabrication and Characterization of Protein Functionalized Gold-Poly (pyrrole)-Gold Nanowires,”*** Chemistry of Materials, 16, 3431-3438 2004, (2004).
- Stranick, S.J., ***“Controlling the Growth Directions of ZnO Nanowires (NWs) on c and a Plane Sapphire,”*** Electronic Publication, November 1 issue of Virtual Journal of Nanoscale Science and Technology, (2004).
- Xu, C., Wu, T., Drain, C.M., Batteas J.D., and Beers, K.L., ***“Synthesis of Gradient Copolymer Brushes via Surface Initiated Atom Transfer Radical C. Copolymerization,”*** Polymer Preprints 45 677 (2004).
- Yang, C.S.C., Wilson, P.T., and Richter, L.J. ***“The Structure of Polystyrene at the interface with various Liquids,”*** Macromolecules, 37 (20): 7742-7746, (2004).
- Yao, H., Michaels, C.A., Stranick, S.J., Isohashi, T., and Kimura, K., ***“Collapse and Self-reconstruction of Mesoscopic Architectures of Supramolecular J Aggregates in Solution: From Strings to Tubular Rods,”*** Lett. Org. Chem. 1, 280 (2004).
- 1b. Manuscripts in review (manuscripts that have been approved by the NIST internal review process and submitted for publication, but have not yet appeared in print).**
- Bright, D.S., and Newbury, D.E., ***“Maximum Pixel Spectrum: A New Tool for Detecting and Recovering Rare, Unanticipated Features from Spectrum Image Data Cubes,”*** Journal of Microscopy, (in press).
- Buchanan, J. D. R., Hase, T. P. A., Tanner, B. K., Powell, C. J., and Egelhoff, W. F., Jr., ***“Interface Intermixing and In-Plane Grain Size in Aluminum-Transition Metal Bilayers,”*** J. Appl. Phys. (submitted).
- Chi, P.H., and Gillen, J. G., ***“Positive Secondary Ion Yields Enhancement on Metal Elements Using Trichlorotrifluoroethane and Tetrachloroethene.”*** Proceeding of the SIMS XIV Conference, San Diego, CA., (in press).
- Coakley, K.J., Simons, D.S., and Leifer, A.M., ***“Secondary Ion Mass Spectrometry Measurements of Isotopic Ratios: Correction for Time Varying Count Rate,”*** Int. J. Mass Spectrum, (in press).
- Conny, J.M., ***“How Does Thermal-Optical Analysis for Atmospheric Elemental Carbon Behave Optically? Investigations of the Apparent Specific Absorption Cross Section,”*** Aerosol Science Technology, (in press).
- Currie, L.A., Kessler, J.D., Fletcher, R.A., and Dibb, J.E., ***“Long Range Transport of Biomass Aerosol to Greenland: Multi-Spectroscopic Investigation of Particles Deposited in the Snow,”*** Journal of Radioanalytical and Nuclear Chemistry, 263 (2005) (in press).

- Egelhoff, W. F., Jr., Gan, L., Etedgui, H., Kadmon, Y., Powell, C. J., Chen, P. J., Shapiro, A. J., McMichael, R. D., Mallett, J. J., Moffat, T. P., Stiles, M. D., and Svedberg, E. B., **"Artifacts That Mimic Ballistic Magnetoresistance,"** J. Magnetism Mag. Materials, (in press).
- Etz, E.S., **"Development and Certification of NIST Standard Reference Materials for Relative Raman Intensity Calibration,"** Microchimica Acta, 2004, (in press).
- Gadzuk, J.W., and Plihal, M., **"Vibrational Quantum Mirages in Scanning Tunneling Spectroscopy,"** Physical Review B, (in press).
- Gillen, J.G., Wight, S.A., Chi, P.H., and Fahey, A. J., **"Bevel Depth Profiling SIMS for Analysis of Layer Structures,"** Characterization and Metrology for Ultra Large Scale Integration, American Institute of Physics, (in press).
- Gillen J.G., **"Automated Analysis of Organic Particles using Cluster SIMS,"** Applied Surface Science, (in press).
- Gonzalez, C., Simón-Manso, Y., Batteas, J.D., Marquez, M., Ratner, M., and Mujica, V., **"A Quasi-molecular Approach to the Conductance of Molecule-Metal Junctions: Theory and Application to Voltage-Induced Conductance Switching,"** J. Phys. Chem. B, (in press).
- Holbrook, R.D., Wagner, M.S., Mahoney, C.M., and Wight, S.A., **"Investigating Activated Sludge Flocs Using Microanalytical Techniques: Demonstration of ESEM and TOF-SIMS for Wasterwater Applications,"** Water Environment Research, (in press).
- Jablonski, A., and Powell, C. J., **"Electron Effective Attenuation Lengths in Electron Spectroscopies,"** Int. J. Compounds & Alloys, (in press).
- Jablonski, A., and Powell, C. J., **"The Information Depth for Elastic-Peak Electron Spectroscopy,"** Surf. Science, (in press).
- Jablonski, A., Powell, C.J., **"Monte Carlo Simulations of Electron Transport in Solids: Applications to Electron Backscattering from Surfaces,"** Applied Surface Science, (in press).
- Jablonski, A., and Powell, C.J., **"The Backscattering Factor in Auger Electron Spectroscopy: New Approach for an Old Subject,"** Applied Surface Science, (in press).
- Jach, T.J., **"Improving Energy Stability in the NIST Microcalorimeter X-Ray Detector,"** Advances in X-ray Analysis, 48, (in press).

- Kim, S.H., Fletcher, R.A., and Zacharia, M.R., ***“The Role of Metals of the Difference in Oxidative Properties between Flame and Diesel Soot Nanoparticles,”*** Environmental Science and Technol., (in press).
- Kopanski, J.J., Marchiando, J.F., Rennex, B.G., Simons, D. and Chau, Q., ***“Towards Reproducible SCM Image Interpretation,”*** J. Vac. Sci Technol. B, in review, (in press).
- Mahoney, C.M., Gillen, J.G., and Roberson, S.V., ***“Dynamic SIMS Utilizing SF<sub>5</sub><sup>+</sup> Polyatomic Primary Ion Beams for Drug Delivery Applications,”*** Applied Surface Science, (in press).
- Mahoney, C.M., Roberson, S.V., and Gillen, J.G., ***“Depth Profiling of 4-Actamidophenol Doped Poly(lactic acid) Films using Cluster SIMS,”*** Analytical Chemistry, (in press).
- Michaels, C.A., Chase, D.B., and Stranick, S.J., ***“Chemical Imaging of Heterogeneous Polymeric Materials With Near-Field IR Microscopy,”*** Applications of Scanning Probe Microscopy to Polymers, J. Batteas, C.A. Michaels, G.C. Walker, Eds. : ACS Symposium Series, Vol. 897, 2004, (in press).
- Powell, C. J., ***“Improvements in the Reliability of X-ray Photoelectron Spectroscopy for Surface Analysis,”*** J. Chem. Education, (in press).
- Powell, C.J., Jablonski, A., Salvat, F., Tanuma, S., and Penn, D.R., ***“New Developments in Data for Auger Electron Spectroscopy and X-ray Photoelectron Spectroscopy,”*** Journal of Surface Analysis, (in press).
- Powell, C.J., Jablonski, A., Werner, W.S., Smekal, W., ***“Characterization of Thin Films on the Nanometer Scale by Auger Electron Spectroscopy and X-ray Photoelectron Spectroscopy,”*** Applied Surface Science, (in press).
- Powell, C.J., ***“Summary of ISO/TC 201 Technical Report: ISO/TR 19319: 2003 – Surface Chemical Analysis – Auger Electron Spectroscopy and X-ray Photoelectron Spectroscopy – Determination of Lateral Resolution, Analysis Area, and Sample Area Viewed by the Analyser,”*** Surface and Interface Analysis, (in press).
- Robey, S.W., (Co-authors) ***“Fermi Level Alignment and Electronic Levels in “Molecular Wire” Self-Assembled Monolayers on Au,”*** Journal of Physical Chemistry B, 2004, (in press).
- Salvat, F., Jablonski, A., and Powell, C.J., ***“ELSEPA-Dirac partial –wave calculation of elastic scattering of electrons and positrons by atoms, positive ions and molecules,”*** Computer Physics Communications, (in press).
- Tanuma, S., Powell, C.J., and Penn, D.R., ***“Calculations of Electron Inelastic Mean Free Paths. VIII. Data for 15 Elemental Solids over the 50 eV to 2000 eV Range,”*** Surface and Interface Analysis, (in press).

- Wagner, M.S., and Gillen, J.G., "***Impact Energy Dependence of SF<sub>5</sub><sup>+</sup> Ion Beam Damage of Poly(Methyl Methacrylate) Studied by Time-of-Flight Secondary Ion Mass Spectrometry,***" Applied Surface Science, (in press).
- Wagner, M.S., Pasche, S., Textor, M., and Castner, D.G., "***Characterization of Poly(L-Lysine)-graft Poly (Ethylene Glycol) Assembled Monolayers on Niobium Pentoxide Substrates using Time of Flight Secondary Ion Mass Spectrometry and Multivariate Analysis,***" Analytical Chemistry, (in press).
- Werner, W. S. M., Smekal, W., and Powell, C. J., "***Simulation of Spectra for Surface Analysis,***" Version 1.0 (SRD 100) (in press).
- Wylie, A.G., Greenwood, W., and Verkouteren, J.R., "***Mineralogical Characterization of Fibrous Talc,***" Canadian Mineralogist, (in press).
- Widmann, J.F., Duchez, J. Yang, J.C., Conny, J.M., and Mulholland, G.W., "***Measurement of the Optical Extinction Coefficient of Combustion-Generated Aerosol,***" J. Aerosol Sci., (in press).

## 2. Talks

- Batteas, J.D., "***Self Organizing Materials for Nanoscale Devices,***" University of California at Davis, Davis, CA, October 14, 2003.
- Batteas, J.D., "***Organizing Nanoscale Devices on Surfaces,***" University of California at Berkeley, Berkeley, CA, October 16, 2003.
- Batteas, J. D., "***Molecular Electronics Metrology: Organizing Characterizing Nanoscale Materials and Devices,***" Drexel University, Philadelphia, PA, November 19, 2003.
- Batteas, J.D., "***Charge Transport in Alkanethiols and Molecular Wires,***" American Chemical Society National Meeting, Anaheim, CA, April 1, 2004.
- Buntin, S.A., "***Nanoscale Chemical and Materials Characterization with Near-Field Microscopy and Spectroscopy,***" American Chemical Society National Meeting, Anaheim, CA, March 30, 2004.
- Chi, P.H., "***Thermal Stability of Si,Mg-implanted GaAs and InP as evaluated by SIMS,***" 17<sup>th</sup> Annual SIMS Workshop, Westminster, CO, May 19, 2004.
- Conny, J.M., "***How Does Thermal-Optical Analysis for Atmospheric Elemental Carbon Behave Optically? Investigations of the Apparent Specific Absorption Cross Section,***" EPA Office of Research and Development, Research Triangle Park, NC, September 21, 2004.

- Currie, L.A., *"Detection and quantification limits: basic concepts, international harmonization, and outstanding ("low-level") issues,"* ICRM Conference on Low-level radioactivity measurement techniques, Vienna, Austria, October 14, 2003.
- Currie, L.A., *"Biomass Aerosol Transported to Greenland: A Multi-Spectroscopic Study of Particles Deposited in the Snow"* Technical University of Vienna, Vienna, Austria, October 17, 2003, invited.
- Currie, L.A., *"Some Basic Assumptions and Limiting Factors in Very Low-Level Measurement"* IAEA Marine Environment Laboratory, Monaco, October 20, 2003, invited.
- Currie, L.A., *"On the isolation of elemental carbon for micro-molar  $^{14}\text{C}$  accelerator mass spectrometry; impact of isotopic heterogeneity, and accuracy assurance through isotopic particulate carbon standards,"* 8<sup>th</sup> International Conference on Carbonaceous Particles in the Atmosphere, Vienna, September 14, 2004.
- Etz, E.S., *"Micro-Raman Spectroscopy for Materials Characterization at NIST,"* Microscopy Society of Northeastern Ohio, Akron, OH, April 27, 2004.
- Fahey, A.F., *"Isotopic Measurements of Uranium,"* 17<sup>th</sup> Annual SIMS Workshop, Westminster, CO, May 18, 2004.
- Fletcher, R.A., *"A Comparison of Polycyclic Aromatic Hydrocarbons,"* American Association for Aerosol Research, Anaheim, CA, October 22, 2003.
- Fletcher, R.A., *"Particle removal by air jets,"* 8<sup>th</sup> International Symposium on the Analysis and Detection of Explosives, Ottawa, Canada, June 8, 2004.
- Gadzuk, J.W., *"Scanning Tunneling Spectroscopy of Nanostructures: From Analytic Models to Computer Simulations,"* Workshop on "Fundamental Physical Issues in Nonequilibrium Interface Dynamics, University of Maryland, College Park, MD, October 21, 2003.
- Gadzuk, J.W., *"Electrostatic Potential Profile within a Biased Molecular Electronics Device: A Cavity QED Approach,"* American Vacuum Society 50<sup>th</sup> International Symposium, Baltimore, MD, November 5, 2003.
- Gadzuk, J.W., *"Surface Reaction Generated Chemicurrents: From Core Level Spectroscopy to Chemical Sensors,"* University of Virginia, Charlottesville, VA, December 18, 2003.
- Gadzuk, J.W., *"Scanning Tunneling Spectroscopy of Nanostructures: Mirages in Quantum Corrals,"* University of Virginia, Charlottesville, VA, December 18, 2003.
- Gadzuk, J.W., *"Production and Detection of Chemically Induced Hot Electrons in Surface Processes: X-Ray Edges, Driven Oscillators, Friction,"* Ein Gedi Workshop on Non Adiabatic Processes at Surfaces, Ein Gedi, ISRAEL, January 11, 2004.

- Gadzuk, J.W., "**Scanning Tunneling Spectroscopy of Nanostructures: Mirages in Quantum Corrals**," National Science Foundation, Arlington, VA, February 4, 2004.
- Gadzuk, J.W., "**Scanning Tunneling Spectroscopy of Localized States and Nanoparticles: Ligands on Molecular Wires**," American Physical Society, Montreal, Canada, March 24, 2004.
- Garno, J.C., "**AFM Based Lithography and Conductive Probe Measurements with Substituted Oligo (Phenylene Ethynylene) Molecular Wire on Au (111)**," AVS International Symposium, Baltimore, MD, November 6, 2003.
- Garno, J.C., "**Measuring Electrical Properties from Single Molecules to Moletronic Devices**," Materials Research Society Meeting, San Francisco, CA, April 14, 2004.
- Gillen, J.G., "**Biomaterials Surface Characterization at NIST**," 17<sup>th</sup> Annual SIMS Workshop, Westminster, CO, May 18, 2004.
- Gillen, J.G., "**3D Image Depth Profiling of Molecular Solids Using Cluster SIMS**," 17<sup>th</sup> Annual SIMS Workshop, Westminster, CO, May 18, 2004.
- Gillen, J.G., "**Inkjet Printed Explosive Standards**," 8<sup>th</sup> International Symposium on Analysis and Detection of Explosives, Ottawa, Canada, June 8, 2004.
- Gillen, J.G., "**Automated Analysis of Explosive Particles Using Cluster SIMS**," 8<sup>th</sup> International Symposium on Analysis and Detection of Explosives, Ottawa, Canada, June 8, 2004.
- Gillen, J.G., "**Trace Explosive Detection Research Program at NIST**," 8<sup>th</sup> International Symposium on Analysis and Detection of Explosives, Ottawa, Canada, June 8, 2004.
- Jach, T.J., "**Comparative thickness measurements of SiO<sub>2</sub>/Si films**," American Vacuum Society Symposium, Baltimore, MD, November 3, 2003.
- Jach, T.J., "**Improving Energy Stability in the NIST Microcalorimeter**," 2004 Denver X-Ray Conference, Steamboat Springs, CO, August 5, 2004.
- Klouda, G.A., "**Reference Material 8785; Air Particulate Matter on Filter Media**," Symposium on Air Quality Measurement Methods and Technology 2004, Research Triangle Park, NC, April 21, 2004.
- Klouda, G.A., "**Metrology in Support of Trace Explosive Detection Equipment for Homeland Security Applications**," Symposium on Air Quality Measurement Methods and Technology 2004, Research Triangle Park, NC, April 21, 2004.

Klouda, G.A., "***Evaluation of Swipes and Surfaces in Sampling Explosives Residues,***" 8<sup>th</sup> International Symposium on the Analysis and Detection of Explosives, Ottawa, Canada, June 8, 2004.

Klouda, G.A., "***Particle Collection Efficiency of Two Metal-Fiber Filters Used in Portal,***" 8<sup>th</sup> International Symposium on the Analysis and Detection of Explosives, Ottawa, Canada, June 8, 2004.

Mahoney, C.M., "***Depth Profiling in PLLA/Pluronic Blends Using T-o-F/SIMS,***" 17<sup>th</sup> Annual SIMS Workshop, Westminster, CO, May 18, 2004.

Mahoney, C.M., "***Characterization of Gunpowder Samples using T-o-F SIMS,***" 8<sup>th</sup> International Symposium on the Analysis and Detection of Explosives, Ottawa, Canada, June 8, 2004.

Marinenko, R.B., "***A New NIST SRM for Microanalysis and X-Ray Fluorescence,***" Microscopy and Microanalysis 2004 Meeting, Savannah, GA, August 3, 2004.

Michaels, C.A., "***Confocal Raman Imaging of Heterogeneous Polymeric Materials,***" Pittcon 2004, Chicago, IL, March 11, 2004.

Michaels, C.A., "***Confocal Raman Imaging of Heterogeneous Polymeric Materials,***" Society of Plastic Engineers, Chicago, IL, May 19, 2004.

Michaels, C.A., "***Chemical Imaging of Thermoplastic Olefins and Fluoropolymer Blend Films,***" Dow Chemical, Auburn Hills, MI, July 29, 2004.

Michaels, C.A., "***Chemical Imaging of Thermoplastic Olefins and Fluoropolymer Blend Films,***" MTS Systems, Oak Ridge, TN, September 26, 2004.

Newbury, D.E., "***Improving the Sensitivity of Electron Beam Microanalytical Techniques by enhanced X-ray Spectrometry: X-ray microcalorimetry, silicon drift detector energy dispersive X-ray spectrometry, and polycapillary X-ray optics,***" 4<sup>th</sup> International Symposium on Atomic Level Characterizations for New Materials and Devices, Kauai, HI, October 5, 2003, Invited.

Newbury, D.E., "***The impact of Environmental Scanning Electron Microscopy in Materials Science,***" Eastern Analytical Symposium, Somerset, NJ, November 20, 2003, invited.

Newbury, D.E., Bright, D.S., "***Gleaning the Cube: Developing Tools to Find the Unexpected in X-ray Spectrum Images,***" NIST Statistical Engineering Division Seminar, Gaithersburg, MD, March 9, 2004, invited.

- Newbury, D.E., ***“X-ray mapping for microstructural characterization: a convergence of advances in spectrometry technology and computer aided imaging/analysis,”*** Dept. of Mineral Sciences, National Museum of Natural History, Smithsonian Institution, Washington, DC, March 11, 2004, invited.
- Newbury, D.E., ***“Quantitative Electron Probe Microanalysis (EPMA): Doing It Right and Doing It Wrong!,”*** NIST Diffusion Workshop, Gaithersburg, MD, April 1, 2004, invited.
- Newbury, D.E., ***“Particle X-ray Microanalysis in the Variable Pressure SEM/Environmental SEM,”*** SCANNING 2004 Conference, Washington, DC, April 29, 2004, invited.
- Newbury, D.E., ***“Gleaning the Cube: Interactive NIST LISPIX Tools for Examining Large Spectral Databases from Compositional Mapping,”*** SCANNING 2004 Conference, Washington, DC, April 29, 2004, invited.
- Newbury, D.E., ***“X-ray Mapping for Microstructural Characterization: a Convergence of Advances in Spectrometry Technology and Computer Aided Imaging/Analysis,”*** Freer Gallery of the Smithsonian Institution, Washington, DC, May 10, 2004, invited.
- Newbury, D.E., ***“X-ray Mapping for Microstructural Characterization: a Convergence of Advances in Spectrometry Technology and Computer Aided Imaging/Analysis,”*** New York Society of Microscopists, New York, NY, May 21, 2004, invited.
- Newbury, D.E., ***“Blunders in automatic qualitative analysis: an emerging crisis in energy dispersive x-ray microanalysis,”*** Microscopy and Microanalysis 2004 Conference, Savannah, GA, August 2, 2004, invited.
- Newbury, D.E., ***“Maximum Channel Spectrum” An Intuitive Software Tool for Detecting and Recovering Rare Features in Spectrum Image Datacubes,*** Microscopy and Microanalysis 2004 Conference, Savannah, GA, August 3, 2004, invited.
- Newbury, D.E., ***“Spectrum Image Mapping with a Silicon Drift Detector (SDD) in an SEM,”*** Microscopy and Microanalysis 2004 Conference, Savannah, GA, August 4, 2004, invited.
- Newbury, D.E., ***“Energy Dispersive X-ray Spectrometry in the Scanning Electron Microscope (SEM): A Tutorial on EDS Qualitative Analysis,”*** Microscopy and Microanalysis 2004 Conference, Savannah, GA, August 4, 2004, invited.
- Newbury, D.E., ***“Silicon Drift Detectors (SDD): spectrometry and x-ray spectrum imaging above 100,000 cps, and what to do with all this data,”*** High Temperature Materials Group Seminar, Oak Ridge National Laboratory, Oak Ridge, TN, September 14, 2004, invited.
- Nikoobakht, B., ***“Controlling the Growth Direction of ZnO Nanowires on C-Plane Sapphire,”*** 2004 Materials Research Symposium, San Francisco, CA, April 13, 2004.

- Powell, C.J., "***Effect of Backscattered Electrons on the Analysis Area in Scanning Auger Microscopy***," Tenth European Conference of Surface and Interface Analysis, Berlin, Germany, October 6, 2003, invited.
- Powell, C.J., "***Measurement of Gate-Oxide Film Thicknesses by X-Ray Photoelectron Spectroscopy***," Tenth European Conference of Surface and Interface Analysis, Berlin, Germany, October 9, 2003, invited.
- Powell, C.J., "***The Development of Documentary Standards for Surface Chemical Analysis***," Tenth European Conference of Surface and Interface Analysis, Berlin, Germany, October 10, 2003, invited.
- Powell, C. J., "***The Electron Attenuation Length in Auger-Electron Spectroscopy and X-Ray Photoelectron Spectroscopy: New Approaches for an Old Subject***," International Workshop on Applied Surface and Interface Analysis: Past, Present and Future, Miraflores de la Sierra, Madrid, Spain, October 17, 2003, invited.
- Powell, C.J., "***Role of Vacuum Technology and Other Drivers in the Development of Surface Analysis***," AVS International Symposium, Baltimore, MD, November 6, 2003, invited.
- Powell, C.J., "***Characterization of Thin Films on the Nanometer Scale by Auger Electron Spectroscopy and X-ray Photoelectron Spectroscopy***," Ninth International Symposium on Advanced Physical Fields: Characterization of Artificial Nanostructures and Nanomaterials, Tokyo, Japan, March 2-4, 2004, invited.
- Powell, C. J., "***The Backscattering Factor in Auger Electron Spectroscopy: New Approach for an Old Subject***," Scanning 2004, Washington, D.C., April 28, 2004.
- Powell, C.J., "***A New NIST Database for the Simulation of Electron Spectra Analysis: Application to Angle-Resolved X-ray Photoelectron Spectroscopy of Hafnium Dioxide Films on Silicon***," 26<sup>th</sup> Annual Symposium on Applied Surface Analysis, Richland, WA, June 16, 2004.
- Powell, C.J., "***NIST Databases for Applications in Electron Spectroscopy***," International Workshop on "Electron Scattering Solids: From Fundamental Concepts to Practical Applications," Debrecen, Hungary, July 5, 2004, invited.
- Powell, C.J., "***Calculations of Electron Inelastic Mean Free Paths from Optical Data: Limitations and Comparison with Experiments***," International Workshop on "Electron Scattering Solids: From Fundamental Concepts to Practical Applications," Debrecen, Hungary, July 6, 2004, invited.
- Ritchie, N.W., "***Stability of Microcalorimeter with Transition Edge Sensor for X-Ray Detection***," Microscopy and Microanalysis 2004, Savannah, GA, August 3, 2004.

- Richter, L.J., "***Vibrationally Resonant Sum Frequency Generation Studies of Buried Interfaces,***" Exxon Mobil, Clinton, NJ, October 24, 2003.
- Richter, L.J., "***In-Situ Characterization of Hybrid Bilayer Membranes,***" American Chemical Society National Meeting, Anaheim, CA, March 28, 2004.
- Robey, S.W., "***Electronic Structure/Hole Injection Barriers in Phenylene Ethynylene Oligomer Self Assembled Monolayers,***" American Vacuum Society International Symposium, Baltimore, MD, November 3, 2003.
- Robey, S.W., "***Electronic Structure and Fermi Level Alignment in Phenylene Ethynylene Self Assembled Monolayers,***" Rutgers University, New Brunswick, NJ, March 4, 2004.
- Robey, S.W., "***Electronic Structure and Fermi Level Alignment in Phenylene Ethynylene Self Assembled Monolayers,***" Princeton University, Princeton, NJ, March 5, 2004.
- Robey, S.W., "***Occupied and Unoccupied States in Phenylene Ethynylene Oligomer Monolayers,***" American Physical Society, Montreal, Canada, March 25, 2004.
- Robey, S.W., "***Fermi Level Alignment in Prototype Molecular Wire Systems,***" Gordon Research Conference on Electronic Processes in Organic Materials, Mount Holyoke College, South Hadley, MA, July 27, 2004.
- Scott, J.H., "***Practical Ultramicroanalysis in the Analytical Electron,***" Pittcon 2004, Chicago, IL, March 11, 2004.
- Scott, J.H., "***Measuring Spectral Variation in XEDS Spectrum Images,***" Microscopy and Microanalysis Conference 2004, Savannah, GA, August 2, 2004.
- Scott, J.H., "***Advanced Analytical Electron Microscopy for Materials,***" Department of Materials Science and Engineering, College Park, MD, September 10, 2004.
- Simons, D.S., "***Application of Time Interpolation in SIMS Isotopic Ratio Measurements,***" 17<sup>th</sup> Annual SIMS Workshop, Westminster, CO, May 18, 2004.
- Small, J.A., "***Quantitative Analysis of Nanoparticles in SEM,***" American Chemical Society National Meeting, Anaheim, CA, March 30, 2004.
- Stranick, S.J., "***Near Field Microscopies for Chemical and Material Analysis,***" Federation of Analytical Chemistry and Spectroscopy Societies, Ft. Lauderdale, FL, October 20, 2003.
- Stranick, S.J., "***Near Field Microscopies for Chemical and Material Analysis,***" Center for Nanoscale Materials, Argonne National Labs, Chicago, IL, February 5, 2004.
- Stranick, S.J., "***Near Field Microscopies for Chemical and Material Analysis on the Nanoscale,***" American Chemical Society National Meeting, Anaheim, CA, March 28, 2004.

- Stranick, S.J., “*Near Field Microscopies for Chemical and Material Analysis on the Nanoscale*,” American Chemical Society National Meeting, Philadelphia, PA, August 25, 2004.
- Verkouteren, J.R., “*Particle Characteristics of Trace High Explosives: RDX and PETN*,” 8<sup>th</sup> International Symposium of the Analysis and Detection of Explosives,” Ottawa, Canada, June 8, 2004.
- Verkouteren, R.M., “*Advanced Metrology for IMS Trace Explosive Detection*,” 13<sup>th</sup> International Society for ION Mobility Spectrometer, Gatlinburg, TN, July 26, 2004.
- Wagner, M.S., “*SF5+ Ion Beam Damage of Poly (acrylates) Studied*,” American Vacuum Society Symposium, Baltimore, MD, November 11, 2003.
- Wagner, M.S., “*Molecular Depth Profiling of Polymer Multilayers Using T-o-F/SIMS*,” 17<sup>th</sup> Annual SIMS Workshop, Westminster, CO, May 18, 2004.
- Walker, M.L., “*In-Situ Ellipsometric Study of Peg/CL-Co Adsorption on Cu, Ag, and Au*,” Gordon Research Conference on Electrodeposition, Colby-Sawyer College, New London, NH, August 10, 2004.
- Windsor, E.S., “*SIMS Backside Analysis: Sample Preparation and Application*,” 17<sup>th</sup> Annual Workshop on SIMS, Westminster, CO, May 18, 2004.

### **3. Cooperative Research and Development Agreements (CRADAs) and Consortia**

“Evaluation of Near-Field Spectroscopic Probes of Polymeric and Catalytic Materials,” with Dow Chemical Company, Stephan J. Stranick and Chris A. Michaels

“Dielectric Measurement of Particles,” with Pfizer Inc. and Stephan J. Stranick

“Nano-Particle Characterization,” with Pfizer Inc. and Stephan J. Stranick

“Characterization and Modeling of Interfaces and Interphases between Polymer Coatings and Substrates,” with MTS Systems Corporation, Chris Michaels, Charles Han, Tinh Nguyen, and Nick Martys

### **4. Patents Issued**

### **5. Measurement Services**

#### **5a. SRM Activities**

SRM 2806 Recertification, Medium Test Dust in Hydraulic Fluid

SRM 2061 Titanium Aluminum Alloy for Microanalysis

SRM 2062 Titanium Aluminum Alloy for Microanalysis

## **5b. SRD Activities**

SRD 20 X-ray Photoelectron Spectroscopy Database (Versions 3.4 released August, 2003) C.J. Powell

SRD 64 NIST Elastic-Electron Scattering Cross-Section (Database Users' Guide for Version 3.1 released August, 2003) C. J. Powell

SRD 71 Electron Inelastic-mean-free-path database, Powell, C.J.

SRD 82 NIST Electron Effective-Attenuation-Length Database (Version 1.1 released 2003) C.J. Powell

SRD 100 Simulation of Spectra for Surface Analysis (Version 1.0, in final preparation, to be released early 2005) Powell, C.J.

SEE ME ON THE SRD

## **5c. Calibrations**

None

## **6. Committee Assignments**

### **Batteas, J.D.**

Board of Directors for the Polymer Analysis Division (PAD) of the Society of Plastics Engineers

### **Cavanagh, R.R.**

NIST Homeland Security Strategic Working Group

Organizing Committee – NNI Interagency Workshop on Instrumentation and Metrology for Nanotechnology

Organizing Committee – NanoCommerce2003

### **Conny, J.M.**

ASTM D-22 Sampling and Analysis of Atmospheres (Member)

### **Currie, L.A.**

International Union of Pure and Applied Chemistry

Attribution Science Panel

### **Etz, E.S.**

ASTM E-13 Molecular Spectroscopy and Chromatography (Member)

ASTM E-13.08 Raman Spectroscopy (Member)

ASTM E-13.10 Molecular Spectroscopic Optical Imaging (Member)

Microbeam Analysis Society (President 2002-2003)

Organization for the Prohibition of Chemical Weapons (OPCW): U.S. Representative to the Task Force on Analytical Database to the Verification Division of the OPCW, The Hague, The Netherlands

### **Fahey, A.J.**

NASA Planetary Instrument Definitions Proposal Review Panel

ASTM E-42 Surface Analysis (Member)  
ASTM E-42.06 Secondary Ion Mass Spectrometry (Member)

**Fletcher, R.A.**

NFPA T2.9 Contamination Control Committee  
U.S. TAG ISO/TC 131 Fluid Power Systems (Technical Advisor)  
U.S. TAG ISO/TC 131SC6 on Contamination Control and Hydraulic Fluids  
(Technical Advisor)

**Gadzuk, J.W.**

Office of Information Services/Library (CSTL Subject Specialist/Advisor)  
Washington Editorial Review Board (CSTL representative)

**Gillen J.G.**

ASTM E42 Surface Analysis  
ASTM E42.06 Subcommittee on Secondary Ion Mass Spectrometry (Chairman)

**Jach, T.J.**

Synchrotron Radiation Instrumentation Collaborative Access Team, Applied Photon  
Source, Argonne National Laboratory (Member);  
X24A Beamline, National Synchrotron Light Source, Brookhaven National Laboratory  
(Director and Spokesperson);

**Klouda, G.A.**

Equal Employment Opportunity Counselor

**Marinenko, R.B.**

Advisory Group for ISO TC202 on Microbeam Analysis (Member)  
ASTM E42 Surface Analysis  
ASTM E42.15 Electron Probe Microanalysis/Electron Microscopy (Member)  
ASTM E42.96 US TAG for ISO TC202/SC2 on Microbeam Analysis (Member), US  
TAG Chairman for TC202  
Microbeam Analysis Society, Editor of MicroNews (Newsletter, pub. 3 times/yr)

**Newbury, D.E.**

ASTM E42 Surface Analysis (Member)  
ISO TC202 on Microbeam Analysis (Member)  
CSTL/837: Committee to Organize Workshop on Limits to Accuracy in Quantitative  
Electron Probe Microanalysis

**Powell, C.J.**

ASTM Committee E-42 on Surface Analysis (Member)  
ASTM Subcommittee E-42.02 on Terminology (Member)  
ASTM Subcommittee E-42.03 on Auger-Electron Spectroscopy and X-Ray

Photoelectron Spectroscopy (Member)  
International Advisory Board, European Conference on Application of Surface and Interface Analysis (Member)  
Organizing Committee, 10<sup>th</sup> Topical Conference on Quantitative Surface Analysis (Chairman)  
Report Committee on Elastic Scattering of Electrons and Positrons, International Commission on Radiation Units and Measurement (Member)  
SEMATECH Analytical Laboratory Managers Council (Member)  
Surface Chemical Analysis Technical Working Area, Versailles Project on Advanced Materials and Standards (U.S. Representative and Chairman)  
Technical Committee 201 on Surface Chemical Analysis of the International Organization for Standards (U.S. Delegate)  
Subcommittee 5 on Auger Electron Spectroscopy of ISO/TC 201 (Chairman)  
U.S. Technical Advisory Group for ISO/TC 201 on Surface Chemical Analysis (Member)  
International Advisory Committee, Second International Symposium on Practical Surface Analysis (Member)  
Workshop on Electron Scattering in Solids: From Fundamental Concepts to Practical Applications of the International Union of Vacuum Science, Technique, and Applications (co-chairman)  
NIST Workshop on Modeling Electron Transport for Applications in Electron and X-ray Analysis and Metrology (co-chairman)

**Richter, L.J.**

Division Representative to the CSTL Colloquium Committee

**Scott, J.H.**

ASTM E42-15 Electron Probe Microanalysis/Electron Microscopy (Member)  
ASTM E42.96 US Tag for ISO/TC202/SC2 on Microbeam Analysis (Member)  
ISO/Technical Committee 202/Subcommittee 3 (Secretary)

**Simons, D.S.**

ASTM E-42 Surface Analysis  
ASTM E42.06 Secondary Ion Mass Spectrometry  
ISO TC201 Surface Chemical Analysis – SC6 Secondary Ion Mass Spectrometry (Chairman of U.S. Delegation)  
NIST Ionizing Radiation Safety Committee  
Surface Science Spectra (Editorial Board)

**Small, J.A.**

Advisory Group for ISO TC202 on Microbeam Analysis (Member)  
ASTM D22 Sampling and Analysis of Atmospheres (Member)  
ASTM D22-05 Indoor Air (Member)  
ASTM D22-05.01 Working Group Asbestos (Member)  
ASTM E42-15 Electron Probe Microanalysis/Electron Microscopy (Chair)

**Steel, E.B.**

ASTM D22 Sampling and Analysis of Atmospheres (Member)  
ASTM D22.05 Indoor Air

**Stranick, S.J.**

Division Laser Safety Officer  
NFO-7 Near-Field Optics and Related Techniques (Co-Chairman)  
Committee: MRS Information Services Committee, Member 2003-2005  
Committee: MRS Academic Affairs Committee, Member 2003-2005  
Committee: ACS Awards Committee, Member 2002-2004  
Committee: NFO Near-field Optics and Related Techniques Conference, International Advisory Panel. 2001-2005.

**Turner, S.**

ASTM D22 Sampling and Analysis of Atmospheres (Member)  
ASTM D22.07 Sampling and Analysis of Asbestos (Member)

**Verkouteren, J.R.**

International Center for Diffraction Data (ICDD), Secretary, Ceramics Subcommittee

**Verkouteren R.M.**

IAEA Stable Isotope Reference Materials Committee  
Water and Environmental Samples  
STP/CENR Air Quality Research Subcommittee

**Wight, S.A.**

ASTM Committee E-42 on Surface Analysis  
ASTM E42.15 Electron Probe Microanalysis/Electron Microscopy (Member)  
ASTM E42.96 U.S. TA/ISO/TC202 Microbeam Analysis (Member)

**Windsor, E.S.**

Division 837 Safety Representative

**Zeissler, C.J.**

NIST Ionizing Radiation Safety Committee Substitute Member  
Safety Representative for Ionizing Radiation, Division 837

**7. Editorships**

**Michael, C.A.**

“Chemical Imaging of Thin Film Polymer Blends with Near-Field IR Microscopy,”  
Applications of Scanning Probe Microscopy to Polymers

**Newbury, D.E.**

Journal of Microscopy  
Microscopy and Microanalysis

## SCANNING

### **Simons, D. S.**

Surface Science Spectra (Editorial Board)

### **Stranick, S.J.**

Encyclopedia of Nanosciences and Nanotechnology,” (Editorial Board)

## **8. Seminars**

### **October 31, 2003**

Dr. Lucile Teague, Trinity College, “STM and DFT Studies of Cycloaddition Reactions on Si(100)” (Division Sponsor: J. Batteas)

### **November 6, 2003**

Dr. Miquel Salmeron, Lawrence Berkeley National Laboratory, “Elementary Mechanisms of Energy Dissipation in Nanoscale Friction,” (Division Sponsor: J. Batteas)

### **November 21, 2003**

Dr. Jamie Kim, Lawrence Berkeley National Laboratory, “Investigation of Macromolecular Adsorption at the Solid/Liquid Interface,” (Division Sponsor: J. Batteas)

### **February 18, 2004**

Professor Paul Cremer, Texas A&M University, “Multivalent Binding Studies on a Chip,” (Division Sponsor: J. Batteas)

### **February 24, 2004**

Professor George Flynn, Columbia University, “Self Assembly at Liquid-Solid and Vacuum-Solid Interfaces,” (Division Sponsor: J. Batteas)

### **February 26, 2004**

Professor Donna Chen, University of South Carolina, “Studies of the Growth and Reactivity of Oxide-Supported Metal Nanoparticles as Models for Heterogeneous Catalysts,” (Division Sponsor: J. Batteas)

### **March 5, 2004**

Dr. Marc Gurau, Texas A&M University, “Monolayer and Water Structure at Langmuir Monolayers Probed with Vibrational Sum Frequency Spectroscopy,” (Division Sponsor: L. Richter)

### **May 27, 2004**

Dr. Mohsen Yeganeh, Exxon Mobil Corporate Strategic Research Laboratories, “Sum Frequency Generation Study of High-Surface-Area Materials,” (Division Sponsor: L. Richter)

**August 25, 2004**

Dr. Colin Bain, University of Oxford, “Interfacial Phase Transitions of Surfactants at Aqueous Interfaces,” (Division Sponsor: L. Richter)

**September 17, 2004**

L. Niewohner, Ph.D, Forensic Science Institute of the Bundeskriminalamt Section Gunshot Traces, Wiesbaden, “The GSR Particle Standard – A Useful Tool for Validation and Proficiency Testing,” (Division Sponsor: C. Zeissler)

**9. Conferences/Workshops/Sessions Sponsored/Co-Sponsored**

10<sup>th</sup> Topical Conference on Quantitative Surface Analysis, Baltimore, MD, November 3, 2003 (C.J. Powell).

High Resolution Polymer Microscopy Session, ANTEC 2004 Meeting, Chicago, IL, May 19, 2004 (C. Michaels).

Electron Scattering in Solids: From Fundamental Concepts to Practical Applications, Debrecen, Hungary, July 5<sup>th</sup>–8<sup>th</sup>, 2004 (C.J. Powell, Co-Chair).

Organized and presented “X-ray Physics” workshop, 2004 Denver X-ray Conference, Steamboat Springs, CO, August 2, 2004 (T. Jach).