



Baltimore-Washington SPECTRUM

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LOCAL SECTION NEWS

A note from John S. Canham, the Chairman of the Baltimore-Washington section of the Society for Applied Spectroscopy.

As we prepare for the upcoming year of meetings of the Baltimore-Washington section of the Society for Applied Spectroscopy, there are a wide variety of opportunities open to the section. These include outreach to the community, outreach to the federal, state, and local governments, supplying direction to the local society, and supplying direction to the Society for Applied Spectroscopy as a whole. These may seem to be grand goals, but we are in a unique position to put the variety of expertise in the society to good use.

At the community level, there are many opportunities to make a difference. These range from working as a judge at a Science Fair at local schools, being a guest speaker at a local school to provide insight to students, faculty, and parents into the varied roles of scientists. Writing a letter to the local school board, PTA or other organizations on topics of your expertise to interpret the huge amount of data from various sources that flood organizations. I have been involved, to a limited degree in several issues in the Howard County Maryland PTA, investigations of chemistry related issues, providing direction in the investigations. Often a trained scientific perspective is required, and not available.

The legislative bodies in this country have often responded to scientific issues without adequate scientific basis. We, as scientists have the ability to make a difference in issues being addressed by our governments. This can be as simple as making a phone

call, sending an e-mail, or as involved as you are inclined to be.

As the chairman of the Baltimore-Washington section of the SAS, I feel that I can speak for the remainder of the officers in saying that you can make a difference in the local section of the SAS. At present, I know I can use or need assistance in determining the direction, focus, and content of the meetings, as well as determining the direction, to the extent of my abilities, of the future of the section.

As a delegate to the national meetings of the Society for Applied Spectroscopy, you can make your ideas for the society heard at a national level. This year we did not have any delegates sent to the national meeting at the FACSS conference. This can and should change.

Society for Applied Spectroscopy

To advance and disseminate knowledge and information concerning the art and science of spectroscopy and other allied sciences.

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As a delegate to the national meetings of the Society for Applied Spectroscopy, you can make your ideas for the society heard at a national level. This year we did not have any delegates sent to the national meeting at the FACSS conference. This can and should change.

It is a good bet that I have not had the opportunity to meet or speak with you. I am relatively new to the community and there are a large number of the members of the Baltimore-Washington Section that I have not met. If you haven't made it to the meetings recently, take an evening to come to one of the meetings, for a nominal cost, you can come, talk to some interesting people in similar and different fields, and hear an interesting bit of science.

If there is some other reason that you don't come to the meetings, please let me know. If the cost of the meals is keeping you away, keep in mind that the speaker eats for free, and often gets to pick the location of the meeting and a date convenient to him/her. If you do not want to be the speaker, you can recommend people whom you would like to hear from, or topics that you would like to hear about.

I do not expect that I will receive a deluge of e-mails, phone calls and letters, but I hope that I hear from some of you, even if it is only to complain about the cost of gasoline, or the location of the section meetings. You can contact me by e-mail at John.S.Canham.1@gsc.nasa.gov or canham@erols.com, You can call me at work 301-286-8970, at home 410-480-2472. You can also write me at 2717 Brinkleigh Dr., Ellicott City, MD 21042.

Sincerely,

John S. Canham, Ph.D.

Meeting Announcement

- Date:** Wednesday November 15, 2000
- Place:** West End Grill
7904 Woodmont Ave., Bethesda, MD
301-951-9696
- Time:** 6 pm Social Hour, 7 pm Dinner, 8 pm Seminar.
- Cost:** \$20 -Choice of Pasta Entrees (You may choose at the restaurant) or Choice of: 1) Chicken Taverna (Chicken breast with eggplant, zucchini, tomato and cheese), 2) Grilled Salmon, or 3) Shrimp Francaise. Included with each meal is a House Salad, Coffee, Tea, or Soft Drink and Dessert.
- Reservations:** Please make your reservations by **NOON**, Monday, November 13, 2000 by calling John Canhan at work 301-286-8970 . **IF YOU RESPOND VIA E-MAIL, FOR THIS MEETING PLEASE SEND ELECTRONIC RSVP's TO:**
john.s.canham.1@gsc.nasa.gov.
- Directions:** From the Beltway take Wisconsin Ave. south past NIH. Take a right turn on Woodmont Ave. Restaurant is after the 4th light. Use street parking or the parking garage on the right in the next block.

Abstracts of Presentations

Simulation of Droplet Heating and Desolvation in an Inductively Coupled Plasma

Craig M. Benson, Sergey F. Gimelshein, Deborah A. Levin, and Akbar Montaser. Dept. of Chemistry, The George Washington University, Washington, DC 20052

The total desolvation rate of sample droplets in an argon inductively coupled plasma (Ar ICP) is investigated through the development of a two-phase flow computer model using the direct simulation Monte Carlo (DSMC) method. Particle evaporation equations are used to obtain desolvation rates for droplets under a variety of initial conditions. The desolvation model is supplemented by equations used to determine the trajectories of particles through the plasma. The model is used to calculate the behavior of aerosol droplets from a direct injection high efficiency nebulizer (DIHEN), a micronebulizer used to inject microliter quantities of samples that are toxic, expensive, or of limited volume. Although our primary objective has been to model the behavior of droplets from the DIHEN, the methodology is more general and can be applied to more rarefied flow conditions such as particle contamination in space plumes. We use the combination of desolvation and transport models to present the first predicted spatial distribution of droplet concentrations and evaporation rates in an ICP flow. This data is compared with the behavior of a DIHEN spray in an environment with no net argon gas flow to determine the importance of gas flow rates to overall droplet concentration profiles in the ICP. In addition, two separate techniques for determining droplet trajectories are contrasted.

Langmuir Probe Measurements of Plasma Properties in a Free-Running Helium Inductively Coupled Plasma

Craig S. Westphal, Akitoshi Okino, Lisa A. Iacone, Michael G. Minnich, Qun Jin, Hironobu Yabuta, and Akbar Montaser. Dept. of Chemistry, The George Washington University, Washington, DC 20052

A strong secondary discharge is observed at the mass spectrometer interface when helium inductively coupled plasmas (He ICPs) are used as ionization sources for mass spectrometry (MS). To reduce the ion kinetic energies and plasma potential, a free-running He ICP was developed for mass spectrometry. In this system, a balanced plasma can be obtained by adjustment of the center capacitor plate of the air capacitor located in the tank circuit of the generator. The effect of RF input power, capacitor plate position, and probe location on the plasma properties are examined. Electron temperature increases with RF input power from 400 W to 800 W. Measured electron temperature values range from 6,100 to 11,600 K and from 4,900 K to 8,900 K with the 13- and 18-mm torch, respectively. Measured electron number density values range from $1.1 \times 10^{14} \text{ cm}^{-3}$ to $1.6 \times 10^{14} \text{ cm}^{-3}$ and from $0.5 \times 10^{14} \text{ cm}^{-3}$ to $1.4 \times 10^{14} \text{ cm}^{-3}$ for plasmas in a 13- and 18-mm torch, respectively. The electron temperature of the He ICP at a capacitor plate setting of 0 mm (minimal secondary discharge in Ar ICPMS) is approximately 1.5 times greater than a setting (capacitor plate position = -11 mm) that offers minimal secondary discharge in He ICPMS. Relatedly, electron number density values in the He ICP at a capacitor position of 0 mm are 8 to 10 times greater compared to those measured at a capacitor plate position of -11 mm. Measured electron temperature values are also compared with the calculated local thermodynamic equilibrium (LTE) values.

Student Speakers

Craig M. Benson is a student at The George Washington University in Washington, DC. He holds a B.A. in Chemistry from Brandeis University in Massachusetts and anticipates finishing his Ph.D. in Physical Chemistry in June 2001. His past and present research interests, in addition to ICP-MS studies, have included synthesis and characterization of organonickel dimers that contain metal centers with different coordination numbers, determination of absolute lifetimes of atmospheric contaminants via UV absorption studies and subsequent computer modeling, and he has studied fluorinated compounds using IR line broadening to determine exact global warming potentials.

Craig S. Westphal is also a student at The George Washington University in Washington, DC. He holds a B.A. in Chemistry from Wittenberg University, Springfield, Ohio and anticipates finishing his Ph.D. in Analytical Chemistry in May 2004. In addition to the work he will be describing in his presentation, he has investigated and synthesized $\text{CB}_{11}\text{H}_{12}^-$ for potential use with boron neutron capture therapy, determined uranium levels and isotopic ratios in synthetic urine using the Large Bore-Direct Injection High Efficiency Nebulizer (LB-DIHEN), and been involved in the development of interfaces for coupling several chromatographic systems (capillary electrophoresis (CE), multicapillary-CE (MC-CE), gas chromatography (GC)) with ICP-MS.

October and November Historical Events In Spectroscopy

by Leopold May
Catholic University

- October 1, 1940** Air Products & Chemicals, Inc., was incorporated on this date.
- October 4 1957** Sputnik I, first artificial earth satellite, launched by USSR.
- October 7, 1885** The birthday of Niels Bohr who proposed the "solar system" model of atom to explain atomic spectra in 1913. He received the Nobel Prize in Physics in 1922.
- October 8, 1908** Roland C. Hawes, an Emeritus Member of SAS, was born on this day. He was the "co-discoverer" with Gordon Alles of the existence of an acetylcholine esterase. He worked on the design for many spectrophotometers at National Technical Laboratories and Applied Physics Corporation.
- October 9, 1879** Max von Laue, researcher in x-rays and crystal structure; suggested crystals diffract x-rays, 1912; Nobel prize in Physics (1914).
- October 10, 1920** Richard C. Lord, Jr., deceased Honorary Member of SAS, was born on this day. He did research in infrared spectroscopy.
- October 21, 1833** The birthday of Alfred Nobel who invented dynamite and established the Nobel Prizes.
- October 23, 1875** Gilbert N. Lewis who developed theories of chemical bond and valency, was born on this day.
- October 23, 2000** Mole Day, 6.02 a.m. through 6.02 p.m. (Mole Times); Mole Moment: 50.453 s after 6:42 p.m.
- November 4, 1958** The Society for Applied Spectroscopy, now the New York Section, was formed on this day in New York City.
- November 6, 1857** The first chief chemist of the US Bureau of Standards (now the National Institute of Standards and Testing), William A. Noyes, was born on this date. He served as editor of the Journal of the American Chemical Society from 1902 to 1917.
- November 7, 1888** Chandrasekhara V. Raman who discovered the Raman effect for which he received the Nobel Prize in 1930, was born on this day.
- November 11, 1925** The discovery of cosmic rays was announced on this day in Madison, Wisconsin.
- November 13, 1831** James Clerk Maxwell, who did research in electromagnetic theory and kinetic theory of gases, was born on this date.
- November 23, 1887** Henry G. J. Moseley, born on this day, discovered that the x-ray frequency is related to atomic number of the element in 1913. He was killed in World War I.
- November 26, 1934** Beckman Instruments, Inc. was incorporated on this day.
- November 27, 1914** Bryce Crawford, Honorary Member of SAS, was born on this day. He did research in infrared spectroscopy.
- November 29, 1936** The birthday of Yuan T. Lee who used a specially designed mass spectrometer that could separate and identify reaction products. He shared the Nobel Prize in 1986 with Dudley R. Herschbach and John C. Polanyi.

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