PNNL-23870

ICP-MS Workshop

November 2014

GC Eiden

AJ Carman

U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
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Pacific Northwest National Laboratory
Richland, Washington 99352

Abstract

Sponsored by DOE's National Nuclear Security Administration (NNSA) Office of Defense Nuclear Nonproliferation Research and Development Office of Proliferation Detection, the FY14 Mass Spectrometry Workshop, hosted by Pacific Northwest National Laboratory, focused on Inductively Coupled Plasma Mass Spectrometry (ICP-MS). *Thermal Ionization Mass Spectrometry* (TIMS) was featured at the 2013 workshop hosted by Idaho National Laboratory; *Secondary Ionization Mass Spectrometry* (SIMS) is planned for the 2015 workshop hosted by Lawrence Livermore National Laboratory.

This report brings together the final components of the planning effort for the FY14 ICP-MS Workshop. The workshop consisted of a two day open short course on various topics of ICP-MS followed by a third day closed session. A separate report on the outcomes of the closed session will be submitted. This report serves to assemble all of the planning materials in one place.

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1.0 Participants

Prospective participants were identified through the TIMS course invitations assembled by INL, through professional contacts from staff at PNNL and through various academic, government, industry and stake holder networks. The following Tables are shown here:

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- Table 2: Government and Industry Invite List. This information is also found in the separate "Excel" document "Government Invite List.xlsx"
- Table 3: Attendee List. This information is also found in the separate "Excel" document "Attendance List FY14.xlsx"
- Table 4: Closed Session Attendees. This information is also found in the separate "Excel" document "Attendance List FY14.xlsx"
- Table 5: Student and Stipend Award List. Note that the yellow highlighted students were foreign nationals and therefore not eligible for stipend.. This information is also found in the separate "Excel" document "Attendance List FY14.xlsx"

Table 1: Academic Invite List

University	Name	Email
Washington State University	John Wolff (Petrologist)	jawolff@wsu.edu
	Jeff Vervoort (Isotope Geochemist)	vervoort@wsu.edu
University of Washington	Bruce Nelson (Isotope Geochemist)	bnelson@uw.edu
BYU	Paul Farnsworth (Analytical Chemist)	pbfarnsw@chem.byu.edu
Indiana University	Gary Hieftje	hieftje@indiana.edu
Universtiy of Maryland - College Park	Bill McDonough	mcdonough@geol.umd.edu
University of Houston	Alan Brandon	abrandon@uh.edu
	Thomas Lapen	tjlapen@uh.edu
	Peter Copeland	copeland@uh.edu
University of Wisconsin - Madison	John Valley	valley@geology.wisc.edu
	Clark Johnson	clarkj@geology.wisc.edu
University of Arizona	George Gehrels	ggehrels@email.arizona.edu
	Bonner Denton	mbdenton@u.arizona.edu
Miami Ohio	Michael Crowder	crowdemw@MiamiOH.edu
	Elisabeth Widom	widome@MiamiOh.edu
Arizona State	Peter Williams	pw@asu.edu
	Daniel Buttry	Dan.Buttry@asu.edu
	GEOPIG ICP-MS Facility	panjai@asu.edu
University of Illinois - Urbana/Champaign	Isotope Geochemistry Lab MC-ICPMS	geology@illinois.edu
	Craig Lundstrom	lundstro@illinois.edu
	Rudiger Laufhutte	laufhutt@illinois.edu
	Robert Hudson	rjhudson@illinois.edu
Columbia University	ICPMS Lab - Lamont Doherty Earth Observatory	
	Envtl Tracers Group	etg@ldeo.columbia.edu
	Sean Solomon	director@ldeo.columbia.edu
Woods Hole Oceanographic Institute (MIT)	Daniel Repeta	drepeta@whoi.edu
	Jerzy Blusztajn	jblusztajn@whoi.edu
Union Collge	Kurt Hollocher	hollochk@union.edu
Berkeley	Paul Brooks	icp@berkeley.edu
	Donald DePaolo	depaolo@eps.berkeley.edu

	Dan Neumark	chemchair@cchem.berkeley.edu
	Bruce Buffett	bbuffett@berkeley.edu
	Paul Renne	prenne@bgc.org
Air Force Institute of Technology	James Petrosky	James.Petrosky@afit.edu
Caltech/JPL	James Chen	james.h.chen@jpl.nasa.gov
Caltech/JPL	Dimitri Papanastassiou	dimitri.a.papanastassiou@jpl.nasa.gov
Clemson University	Ken Marcus	marcusr@clemson.edu
Georgia Tech	Glenn Sjoden	sjoden@gatech.edu
Indiana University	Steve Ray	sjray@indiana.edu
Iowa State University	Sam Houl	rshouk@iastate.edu
Northern Arizona University	Michael Ketterer	michael.ketterer@nau.edu
Purdue University	Graham Cooks	cooks@purdue.edu
University of California - Berkeley	Karl van Bibber	karl.van.bibber@nuc.berkeley.edu
	Jasmina Vujic	vujic@nuc.berkeley.edu
	Paul Brooks	icp@berkeley.edu
	Donald DePaolo	depaolo@eps.berkeley.edu
	Dan Neumark	chemchair@cchem.berkeley.edu
	Paul Renne	prenne@bgc.org
University of Cincinnati	Joe Caruso	joseph.caruso@uc.edu
University of Nevada - Las Vegas	Ken Czerwinski	czerwin2@unlv.nevada.edu
	Ralf Sudowe	ralf.sudowe@unlv.edu
West Virginia University	Glen Jackson	glen.jackson@mail.wvu.edu

Table 2: Government and Industry Invite List

LAST NAME	FIRST NAME	ORGANIZATION	EMAIL
McClory	John	AFIT	John.McClory@afit.edu
Baldwin	David	Ames Laboratory	dbaldwin@ameslab.gov
Ulicny	Bill	DNDO	william.ulicny@hq.dhs.gov
Morrison	Jeffrey	DNDO	jeffrey.morrison@hq.dhs.gov
Sassin	Nick	DoD	Nicholas.Sassin@dodiis.mil
Lamont	Steven	DOE-IN	stephen.lamont@in.doe.gov
Wilk	Sarah	DTRA	sarah.wilk@dtra.mil
Smith	Donna	DTRA	
Hague	Robert	INL	robert.hague@inl.gov
Chamberlin	Becky	LANL	rmchamberlin@lanl.gov
Steiner	Robert	LANL	steiner@lanl.gov
Oldham	Warren	LANL	
Brooks	George	LANL	gbrooks@lanl.gov
Jarvinen	Gordon	LANL	gjarvinen@lanl.gov
Russo	Rick	LBNL	rerusso@lbl.gov
Ramon	Erick	LLNL	ramon1@llnl.gov
Kristo	Mike	LLNL	kristo2@llnl.gov
Ingeneri	Kris	McCrone Associates Inc.	kingeneri@mccrone.com
Hoff	John	McCrone Associates Inc.	jhoff@mccrone.com
Rhodes	Kent	McCrone Associates Inc.	krhodes@mccrone.com
Dolan	Jennifer	NA-22 NGP Fellow	jennifer.dolan@nnsa.doe.gov
Fay	Alexander	NA-22 NGP Fellow	alexander.fay@nnsa.doe.gov
Miller	James	NA-22 NGP Fellow	james.miller@nnsa.doe.gov
Dixon	Elenor	NA-221	eleanor.dixon@nnsa.doe.gov
Kim	Won	NA-221	won.kim@nnsa.doe.gov
Franques	Victoria	NA-221	Victoria.Franques@nnsa.doe.gov
Broadhead	Bryan	NA-221	Bryan.Broadhead@nnsa.doe.gov
Johnson	Jared	NA-221	Jared.Johnson@nnsa.doe.gov
Frederiksen	Steven	NA-221	Steven.frederiksen@nnsa.doe.gov
Dougan	Arden	NA-221	arden.dougan@nnsa.doe.gov
Musk	COL Jeff	NA-221	jeffery.musk@nnsa.doe.gov
LaGraffe	David	NA-221	david.lagraffe@nnsa.doe.gov

Kiess	Thomas	NA-222	thomas.kiess@nnsa.doe.gov
Goldberg	Steven	NA-45	steven.goldberg@nnsa.doe.gov
Simons	David	NIST	david.simons@nist.gov
Nelson	Chris	NSTec	nelsonc1@nv.doe.gov
Klingensmith	Amanda	NSTec	klingeal@nv.doe.gov
Cable-Dunlap	Paula	ORNL	cabledunlapr@ornl.gov
Hexel	Cole	ORNL	hexelcr@ornl.gov
Roback	Jason	ORNL	robackjw@ornl.gov
Arnquist	Isaac	PNNL	isaac.arnquist@pnnl.gov
Berry	Pam	PNNL	pam.berry@pnnl.gov
Bos	Stan	PNNL	stanley.bos@pnnl.gov
Carman	April	PNNL	april.carman@pnnl.gov
Duckworth	Doug	PNNL	douglas.duckworth@pnnl.gov
Duffin	Andrew	PNNL	andrew.duffin@pnnl.gov
Eiden	Greg	PNNL	greg.eiden@pnnl.gov
Grate	Jay	PNNL	jay.grate@pnnl.gov
Hagar	Sara	PNNL	sara.hagar@pnnl.gov
Hanlen	Rich	PNNL	rich.hanlen@pnnl.gov
Hart	Garret	PNNL	garret.hart@pnnl.gov
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Kreuzer	Helen	PNNL	helen.kreuzer@pnnl.gov
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Moran	Jim	PNNL	james.moran@pnnl.gov
Petersen	Steven	PNNL	steven.petersen@pnnl.gov
Reilly	Dallas	PNNL	dallas.reilly@pnnl.gov
Sorensen	Chris	PNNL	christina.sorensen@pnnl.gov
Springer	Kellen	PNNL	kellen.springer@pnnl.gov
Taylor	Nick	PNNL	nicholas.taylor@pnnl.gov
Vickery	Buzz	PNNL	buzz.vickery@pnnl.gov
Wacker	John	PNNL	john.wacker@pnnl.gov
Ward	Jesse	PNNL	jesse.ward@pnnl.gov
Wunschel	David	PNNL	david.wunschel@pnnl.gov
Tachau	Rob	SNL	rdtacha@sandia.gov
Spahn	Olga	SNL	oblum@sandia.gov
Rogers	Karen	SNL	ksroger@sandia.gov

Martin	Jeff	SNL	jbmart@sandia.gov
Blair	Dianna	SNL	dsblair@sandia.gov
Zemyan	Michael	Schafer Vallecitos	mzemyan@schaferlabs.com
Farkas	Dave	Shafer Vallecitos	
Stein	John	Shafer Vallecitos	john.stein@schafercorp.com
Fugate	Glenn	SRNL	glenn.fugate@srnl.doe.gov
Griggs	Dan	SRNL	dan.griggs@srnl.doe.gov
Halverson	Justin	SRNL	justin.halverson@srnl.doe.gov
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Rybicki	George	US Air Force	george.rybicki@patrick.af.mil
Lessard	Oscar	US Air Force	oscar.lessard@patrick.af.mil
Smith	Scott	US Air Force	Scott.Smith.23@us.af.mil
Cheney	Eugene	US Air Force	Eugene.Cheney@us.af.mil
Shuford	John	US Air Force	John.Shuford.1@us.af.mil
Hofstetter	Theresa	US Air Force	theresa.hofstetter@us.af.mil
Appelhans	Tony	Walsh Engineering	tony.appelhans@gmail.com

Table 3: Attendee List

Last Name	First Name	Email	Institution
Baldwin	David	dbaldwin@ameslab.gov	Ames
Lewis	Laurence	lewis105@llnl.gov	Berkeley
Moses	Lance	mosesman11@gmail.com	BYU
Jones	Sarah	smharri@g.clemson.edu	Clemson
Locklair	David	wlockla@clemson.edu	Clemson
Mannion	Joseph	jmannio@clemson.edu	Clemson
Hague	Bob	robert.hague@inl.gov	INL
Horkley	Jared	jared.horkley@inl.gov	INL
Houghton	Tracy	tracy.houghton@inl.gov	INL
Olson	John	john.olson@inl.gov	INL
Watrous	Matt	matthew.watrous@inl.gov	INL
Zarzana	Chris	christopher.zarzana@inl.gov	INL
Byerly	Benjamin	byerly@lanl.gov	LANL
Jarvinen	Gordon	gjarvinen@lanl.gov	LANL
Meyers	Lisa	lmeyers@lanl.gov	LANL
Spencer	Khalil	spencerk@lanl.gov	LANL
Stanley	Floyd	floyd@lanl.gov	LANL
Steiner	Robert	steiner@lanl.gov	LANL
Russo	Rick	rerusso@lbl.gov	Lawrence Berkeley
Robel	Martin	robel1@llnl.gov	LLNL
Weber	Peter	weber21@llnl.gov	LLNL
Ramon	Erick	Ramon1@llnl.gov	LLNL
Cunningham	Heather	hcunningham@mccrone.com	McCrone
Ingeneri	Kristofor	kingeneri@mccrone.com	McCrone
Brown	Kenneth	brownkl3@miamioh.edu	Miami-Ohio
Conte	Elise	conteer@miamioh.edu	Miami-Ohio
Daly	George	dalyge@miamioh.edu	Miami-Ohio
Kuentz	David	kuentz@miamioh.edu	Miami-Ohio
McHugh	Kelly	mchughkc@miamioh.edu	Miami-Ohio
Widom	Elisabeth	widome@MiamiOH.edu	Miami-Ohio
Glover	Sam	seg3@cdc.gov	NIOSH
Szakal	Christopher	christopher.szakal@nist.gov	NIST
Dixon	Eleanor	eleanor.dixon@nnsa.doe.gov	NNSA

Manard	Manuel	manardmj@nv.doe.gov	NSTec
Plionis	Alexander	plioniaa@nv.doe.gov	NSTec
Hexel	Cole	Hexelcr@ornl.gov	ORNL
Ticknor	Brian	ticknorbw@ornl.gov	ORNL
Barinaga	Charles	Charles.barinaga@pnnl.gob	PNNL
Carman	April	april.carman@pnnl.gov	PNNL
Duckworth	Doug	douglas.duckworth@pnnl.gov	PNNL
Duffin	Andrew	andrew.duffin@pnnl.gov	PNNL
Eiden	Greg	greg.eiden@pnnl.gov	PNNL
Hart	Garret	garret.hart@pnnl.gov	PNNL
Liezers	Martin	martin.liezers@pnnl.gov	PNNL
Springer	Kellen	kellen.springer@pnnl.gov	PNNL
Hubbard	Josh	jahubba@sandia.gov	Sandia
Spahn	Olga	oblum@sandia.gov	Sandia
Smith	Julie	julie.smith@schafercorp.com	Schafer
Shick	Charles	charles.shick@srnl.doe.gov	SRNL
Patin	Joshua	joshua.patin@schafercorp.com	SVL
Sams	David	david.sams@schafercorp.com	SVL
Lavelle	Kevin	lavellkb@mail.uc.edu	U Cincinnati
Denton	Bonner	mbdenton@email.arizona.edu	University of Arizona
Bertoia	Julie	juliea@unlv.nevada.edu	UNLV
Fitzgerald	Marc	fitzgerald22@llnl.gov	UNLV
Gallardo	Athena	gallar14@unlv.nevada.edu	UNLV
Nell	Julia	nell@unlv.nevada.edu	UNLV
Burns	David	david.burns.30@us.af.mil	US Air Force
Hofstetter	Theresa	theresa.hofstetter@us.af.mil	US Air Force
Rybicki	George	george.rybicki@us.af.mil	US Air Force
Watson	Larry	larry.watson@us.af.mil	US Air Force
Brewer	Aaron	aaronbrewer5@gmail.com	UW
Gu	Haiou	haiougu@uw.edu	UW
Kuehner	Scott	kuehner@u.washington.edu	UW
Teng	Fangzhen	fteng@u.washington.edu	UW
Wang	Shuijiong	sxw057@gmail.com	UW
Sun	Weidong	weidongsun@gig.ac.cn	UW
Bryce	Keith	brycekc@vcu.edu	Virginia Commonwealth University
Williams	Ammon	williamsan25@vcu.edu	Virginia Commonwealth University

Rod	Kenton	kenton.rod@gmail.com	WSU

Table 4: Closed Session Attendees

Last Name	First Name	Email	Faculty	Govt	Other	Institution
Baldwin	David	dbaldwin@ameslab.gov		X		Ames
Hague	Bob	robert.hague@inl.gov		X		INL
Olson	John	john.olson@inl.gov		X		INL
Watrous	Matt	matthew.watroud@inl.gov		X		INL
Zarzana	Chris	christopher.zarzana@inl.gov		X		INL
Jarvinen	Gordon	gjarvinen@lanl.gov		X		LANL
Spencer	Khalil	spencerk@lanl.gov		X		LANL
Stanley	Floyd	floyd@lanl.gov		X		LANL
Steiner	Robert	steiner@lanl.gov		X		LANL
Russo	Rick	rerusso@lbl.gov		X		LBNL
Weber	Peter	weber21@llnl.gov		X		LLNL
Cunningham	Heather	hcunningham@mccrone.com			X	McCrone
Ingeneri	Kristofor	kingeneri@mccrone.com			X	McCrone
Glover	Sam	seg3@cdc.gov	X			NIOSH
Szakal	Christopher	christopher.szakal@nist.gov		X		NIST
Dixon	Eleanor	eleanor.dixon@nnsa.doe.gov		X		NNSA
Hexel	Cole	Hexelcr@ornl.gov		X		ORNL
Ticknor	Brian	ticknorbw@ornl.gov		X		ORNL
Sylvester	Diane	dianems@ucia.gov		X		Other
Barinaga	Charles	charles.barinaga@pnnl.gov		X		PNNL
Bowyer	Ted	ted.bowyer@pnnl.gov		X		PNNL
Carman	April	april.carman@pnnl.gov		X		PNNL
Duckworth	Doug	douglas.duckworth@pnnl.gov		X		PNNL
Duffin	Andrew	andrew.duffin@pnnl.gov		X		PNNL
Eiden	Greg	gregory.eiden@pnnl.gov		X		PNNL
Hart	Garret	garret.hart@pnnl.gov		X		PNNL
Naes	Benjamin	benjamin.naes@pnnl.gov		X		PNNL
Springer	Kellen	kellen.springer@pnnl.gov		X		PNNL
Wacker	John	john.wacker@pnnl.gov		X		PNNL
Willingham	David	david.willingham@pnnl.gov		X		PNNL
Wunschel	Dave	david.wunschel@pnnl.gov				PNNL
Hubbard	Josh	jahubba@sandia.gov		X		Sandia
Spahn	Olga	oblum@sandia.gov		X		Sandia
Smith	Julie	julie.smith@schafercorp.com			X	Schafer
Patin	Joshua	joshua.patin@schafercorp.com		X		SVL

Sams	David	david.sams@schafercorp.com		X	SVL
Bonner	Denton	mbdenton@email.arizona.edu	X		U Arizona
Burns	David	david.burns.30@us.af.mil		X	US Air Force
Hofstetter	Theresa	theresa.hofstetter@us.af.mil		X	US Air Force
Rybicki	George	george.rybicki@us.af.mil		X	US Air Force
Watson	Larry	larry.watson@us.af.mil		X	US Air Force

Table 5: Student and Stipend Award List. Note that the yellow highlighted students were foreign nationals and therefore not eligible for stipend.

Last Name	First Name	Email	Institution	Stipend
Lewis	Laurence	lewis105@llnl.gov	Berkeley	YES
Moses	Lance	mosesman11@gmail.com	BYU	YES
Jones	Sarah	smharri@clemson.edu	Clemson	NO (At PNNL)
Locklair	David	wlockla@clemson.edu	Clemson	YES
Mannion	Joseph	jmannio@clemson.edu	Clemson	YES
Brown	Kenneth	brownkl3@miamioh.edu	Miami-Ohio	YES
Conte	Elise	conteer@miamioh.edu	Miami-Ohio	YES
Daly	George	dalyge@miamioh.edu	Miami-Ohio	YES
McHugh	Kelly	mchughkc@miamioh.edu	Miami-Ohio	YES
Lavelle	Kevin	lavellkb@mail.uc.edu	U Cincinnati	YES
Fitzgerald	Marc	fitzgerald22@llnl.gov	UNLV	YES
Gallardo	Athena	gallar14@unlv.nevada.edu	UNLV	YES
Nell	Julia	nell@unlv.nevada.edu	UNLV	YES
Brewer	Aaron	aaronbrewer5@gmail.com	UW	
Gu	Haiou	haiougu@uw.edu	UW	NO
Bryce	Keith	brycekc@vcu.edu	VA Commonwealth U	NO
Yoon	Dalsung	yoond2@vcu.edu	VA Commonwealth U	NO
				12

2.0 Registration Information

Two registration sheets were used to register and track attendees. One version was used for the open two day short course and the other version was used to track attendees for the closed session.

- Figure 1: Registration Sheet for the open two day short course. This information is also found in the separate document "2014_MassSpecRegistration.pdf"

- Figure 2: Registration Sheet for the closed one day working group. This information is also found in the separate document "2014_MassSpecRegistration_v2.pdf"

Figure 1: Registration Sheet for the open two day short course.

2014 Mass Spectroscopy Workshop

JUNE 17-18 | PACIFIC NORTHWEST NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

NNSA

Registration

2014 Mass Spectroscopy Workshop (MSW) – Mass Spectroscopy (MS) Short Course

Pacific Northwest National Laboratory
Richland, WA

June 17-18, 2014

Name: _____

Address: _____

_____

Email: _____

Phone Number: _____

Citizenship: _____

Institution: _____

Role/Research focus at Institution: _____

I would like to attend (check all that apply):

No host group dinner on Tuesday, June 17 (cost and location TBD): _____
PNNL laboratory tours: _____
Hanford B Reactor tour (one tour will be scheduled based on participants' preference)
Monday afternoon, June 16: _____
Thursday morning, June 19: _____

To request additional information or return completed forms, contact

Angie Springer (PNNL), angela.springer@pnnl.gov, (509) 375-3901
April Carman (PNNL), april.carman@pnnl.gov, (509) 372-6587
Or fax 509-375-2946

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Figure 2: Registration Sheet for the closed one day working group.

2014 Mass Spectroscopy Workshop

JUNE 17-19 | PACIFIC NORTHWEST NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

NNSA

Registration

2014 Mass Spectroscopy Workshop (MSW) – Mass Spectroscopy (MS) Short Course

Pacific Northwest National Laboratory | Richland, WA

June 17-19, 2014

Name: _____

Address: _____

_____

Email: _____

Phone Number: _____

Citizenship: _____

Institution: _____

Role/Research focus at Institution: _____

I would like to attend (check all that apply):

Workshop Days: June 17, 18 _____ and/or June 19 _____

NOTE: SECRET level clearance is required for June 19. Details for passing clearances will be provided upon confirmed registration.

No host group dinner on Tuesday, June 17 (cost and location TBD): _____

PNNL laboratory tours: _____

Hanford B Reactor tour (one tour will be scheduled based on participants' preference)

Monday afternoon, June 16: _____

Thursday morning, June 19: _____

To request additional information or return completed forms, contact

Angie Springer (PNNL), angela.springer@pnnl.gov, (509) 375-3901

April Carman (PNNL), april.carman@pnnl.gov, (509) 372-6587

Or fax 509-375-2946

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3.0 Poster Presentation

The ICP-MS Workshop was advertised at the 2014 MPD Review at Oak Ridge National Laboratory in April 2014. A poster presentation was given on the topic and a flyer was available for distribution.

- Figure 3: The poster that was presented at the 2014 MPD Review is shown.. This information is also found in the separate document "MS Workshop 2014 Poster.pdf"

- Figure 4: The flyer that was distributed at the 2014 MPD is shown here. This information is also found in the separate document "MassSpec_workshop2.jpg"

Figure 3: The poster that was presented at the 2014 MPD Review is shown.

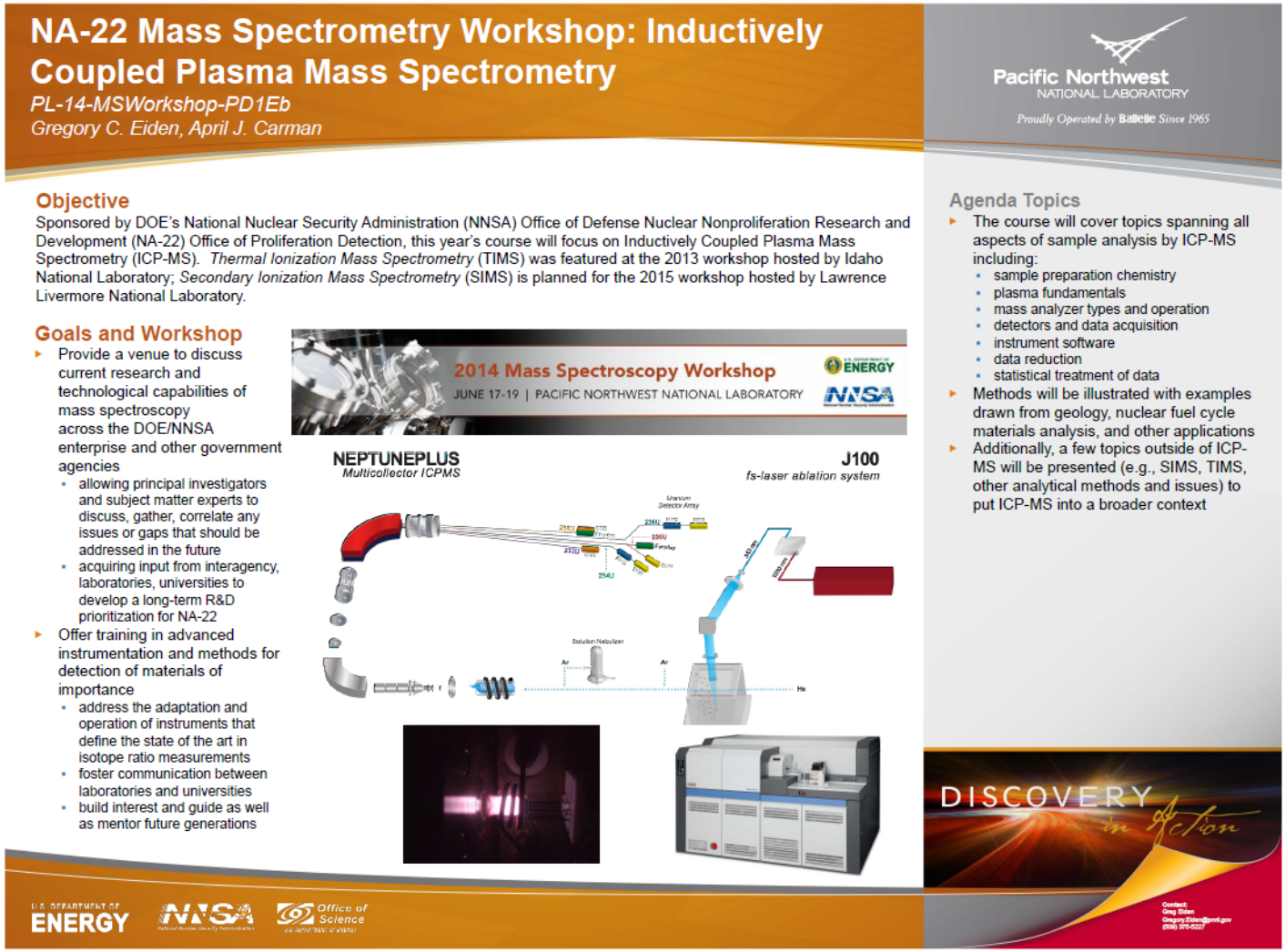

Figure 4: The flyer that was distributed at the 2014 MPD is shown here.

4.0 Presenter's Biosketches

Biosketches about each of the presenters at the ICP-MS Workshop were available in the Final materials distributed electronically to participants of the two day short course. The biosketches are reproduced here for convenience but are also found in the file "ICP-MS Workshop FinalVol1.pdf."

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Charles Barinaga is a Senior Research Scientist in the Advanced Radioanalytical Chemistry Group of the National Security Directorate at Pacific Northwest National Laboratory. He specializes in research and development of analytical instrumentation, particularly for atomic mass spectrometry in general and ICP-MS in particular. Dr. Barinaga has contributed to several successful projects at PNNL funded by the DOE including Ion Trap ICP/MS (gas phase ion/molecule reactions to reduce polyatomic interferences in ICP-MS) and "All the Signal, All the Time" (successful development of a multichannel-array ion detector). The gas phase ion/molecule work became a component of Collision Reaction Cell (CRC) technology that is a part of nearly every quadrupole ICP-MS sold today. For these and other work Dr. Barinaga has received several national awards, been granted several patents, and wrote several publications and delivered presentations. He received his Ph.D. in Analytical Chemistry from the University of Idaho in 1988.

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Douglas Duckworth is a Senior Scientist specializing in nuclear materials analysis at Pacific Northwest National Laboratory. He joined PNNL in 2006 and serves as a Program Manager in the National Security Administration Sector, supporting projects in the DOE's National Nuclear Administration's Office of Nonproliferation and Verification Research and Development (NA-22). He holds a Ph.D. in Analytical Chemistry from Clemson University and began his career at Oak Ridge National Laboratory developing, executing, and managing research programs in isotopic and elemental analysis.

Dr. Duckworth's primary expertise is in mass spectrometry and its application to elemental and isotopic analysis in radiological, nuclear, biological, and chemical analyses. His background includes investigations of fundamental gas-phase chemistry; instrument development and applications for advancing chemical separations and analysis; development and management of research programs in isotopic and elemental analysis; technical support for elemental and isotopic analysis of nuclear, environmental, materials; and development of light and heavy isotope isotopic signatures.
Dr. Duckworth's expertise has been recognized with collaborative research and/or funding from the

DOE's Office of Basic Energy Sciences, U.S. Department of Homeland Security, National Institutes of Justice, and the National Nuclear Security Administration. He is the Chair-elect for the Analytical Division of the American Chemical Society.

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Andrew Duffin received his Ph.D. in Physical Chemistry from the University of California, Berkeley in 2010. Since then, he has worked at PNNL as a post-doctoral researcher and now as a staff scientist. His research at PNNL involves the application of fs-laser ablation coupled to multi-collector ICP-MS into a method for rapid, precise, and spatially resolved uranium analysis. In addition to fs-laser ablation, Dr. Duffin works on projects using advanced synchrotron analysis techniques for uranium analysis.

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Gregory Eiden is a Chief Scientist at Pacific Northwest National Laboratory with 25 years' experience in the development of mass spectrometry methods including nearly every type of mass analyzer (time-of-flight, Paul traps, multi-sector field, quadrupole) and ion source (plasma, laser, electron impact) in common use. While at PNNL, Dr. Eiden has focused on how such methods can address applications in national security. He is a co-inventor of "chemical resolution" mass spectrometry, an approach that is now recognized worldwide as a new paradigm in addressing spectral interferences in ICPMS. This approach earned an R&D 100 Award in 1996, a Federal Laboratory Consortium (FLC) Award in 1997, and the 2004 FLC Award for Excellence in Technology Transfer. His other interests include optical spectroscopic methods (especially resonant photo excitation/ionization-based spectroscopies), the chemistry of gas phase cations, plasma processing etch and deposition for semiconductor fabrication, and surface analysis. Dr. Eiden is the author or co-author of 34 peer-reviewed publications, 80 conference presentations, numerous book chapters, and U. S. and international patents. He has taught short courses in mass spectrometry at key international meetings. Dr. Eiden received his Ph.D. in Physical Chemistry, from the University of Wisconsin-Madison.

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Garret Hart is a Staff Scientist in the Nuclear Materials Analysis Group within the National Security Directorate at Pacific Northwest National Laboratory. Dr. Hart has also worked as a Research Faculty in Isotope Geochemistry at Washington State University where was a member of the GeoAnalytical Laboratory for six years. Along with his background in Geology, Dr. Hart has expertise in thermal and plasma source multi-collector mass spectrometry, elemental and isotopic sample characterization by laser ablation, and clean room chemistry procedures. Dr. Hart is working on integrating his experience with mid- to high-mass elements (U, Fe, Cu, Sr, Hf, and Pb) into existing and new research projects and goals. He is the author or co-author of 18 publications and many conference presentations. He received his Ph.D. in Geology from the University of Wisconsin-Madison in 2002.

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Martin Liezers joined the PNNL Radiochemistry group as a Staff Scientist specializing in elemental-isotopic analysis by ICP-MS techniques. Over the past few years he has had opportunity to work on some interesting projects:

- Detection of femtogram levels of ^{135}Cs and ^{137}Cs in groundwater by ICP-MS
- Electrochemical separation/preconcentration of U and Pu using glassy carbon (Pu-239 DL <3 attograms = <7,500 atoms!) by ICP-MS
- Development of Ultrahigh resolution ICP-MS (300,000 res) sufficient to resolve ^{87}Rb from ^{87}Sr (proton versus neutron mass difference)
- Production of surrogate nuclear explosion debris using high power techniques that include the ICP, exploding wires and high power lasers.

Dr. Liezers received his Ph.D from the Department of Instrumentation and Analytical Science (DIAS) at the University of Manchester Institute of Science and Technology (UMIST), England. Before joining PNNL in 2006, he was a post-doctoral fellow at UMIST for 3 years based at the Atomic Energy Research Establishment (AERE), Harwell, England. He spent two years as a Higher Scientific Officer at AERE looking at actinide speciation using laser spectroscopy. He joined VG Elemental Ltd, Winsford, England in 1990 as a research scientist working on alternate plasmas to the ICP for Mass Spectrometry applications and improving ICP-MS sensitivity (S-option, Cool Plasma!). During this time he travelled extensively performing installations, service, method development and customer training on VG ICP-MS instruments, along with presenting numerous conference presentations and authoring scientific

publications. Dr. Liezers contributed sections on plasma sampling and ion optics to two ICP-MS books, *Inductively Coupled Plasma Mass Spectrometry Handbook* (Simon Nelms, ed.) and *The Encyclopedia of Mass Spectrometry, Volume 5, Elemental and Isotope Ratio Mass Spectrometry* (by Diane Beauchemin and Dwight Matthews).

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Richard Russo is the founder and scientific director of the laser material interactions group at the Lawrence Berkeley National Laboratory. His group pioneered laser ablation for chemical analysis, with over 30 years' contribution to fundamental and applied research. Dr. Russo has an international scientific reputation in chemistry and physics related to nanosecond and femtosecond laser-material-interactions (laser ablation), is co-inventor of the nanowire laser, and developer of a real-time standoff laser ultrasonic sensor, which earned an R&D 100 Award in 2006. He also is co-inventor of a patented process for nano-texturing (ITEX process) thin-films, lead-inventor of the patented ion-assisted pulsed laser deposition (IBAD process), which produced a world record critical current for HTSC materials, and a pioneer in elucidating fundamental laser heating and laser ablation processes for chemical analysis. His research group achieved world record 450nm spatial resolution and a detection limit of 220 attograms using a single femtosecond laser pulse for laser induced breakdown spectroscopy (LIBS) measurements. By pioneering near-field scanning optical microscopy (NSOM) with laser ablation, his group achieved 25nm diameter spatial resolution for sampling and analysis. Most recently, his Berkeley research group, with the assistance of Applied Spectra staff, demonstrated and patented the use of laser plasmas for real-time measurement of isotopes. The new technology has been named LAMIS (Laser Ablation Molecular Isotopic Spectroscopy), which won an R&D100 Award in 2012. Dr. Russo has over 250 scientific publications; 45 refereed proceedings; 320 (226 invited) presentations-lectures, 10 book chapters and 15 patents. Fourteen students have received their PhD degree under his direction at the University of California, Berkeley. Dr Russo received his Ph.D. in Chemistry, Laser Spectroscopy from Indiana University, Bloomington in 1981.

Dr. Russo also is founder and president of Applied Spectra, Inc. (ASI). Russo founded ASI with the assistance of several of his Ph.D. students from Berkeley. Together, they are the world experts in laser ablation chemical analysis using LIBS and Laser Ablation with ICP-OES and ICP-MS. Company core expertise is research, development and manufacture of laser ablation chemical analysis instrumentation, and analytical measurement services

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Dr. Christina Sorensen is a scientist in the National Security Directorate at PNNL. She received a Ph.D. in Inorganic Chemistry from the University of Wyoming where she specialized in mass spectrometry with

an emphasis on inorganic and bioanalytical characterization. She did her post-doctoral work in Dick Smith's group at PNNL, focusing on multivariate analysis of metabolomics data.

At PNNL, Dr. Sorensen has a number of areas of research including characterization and identification of metals, small compounds, biofuel compounds, oligomers, organometallic compounds and proteins. She has provided and developed separation and purification methods for a variety of different compounds in different matrices. In addition, she has applied multivariate statistical analysis for metabolic profiles and fuel analysis. She has used mass spectrometry for characterization of compounds of interest for many multifaceted applications in a variety of different groups across the laboratory. One of her specializations has been method development for projects where trace detection of different compounds requires research and development of a standard operating procedure. She has had the opportunity to apply her chemistry knowledge to a wide range of projects in national defense, forensic marker characterization, diabetes markers, peptide and protein markers, small molecule analysis including characterization of synthesis products. Dr. Sorensen has used a broad range of instrumental techniques with different applications for evaluation of characterization methods.

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Kellen Springer is a scientist in the Radiochemical Analysis Group at the Pacific Northwest National Laboratory. Mr. Springer joined PNNL after earning an M.S. in Geology from the University of Houston in 2010 where he studied isotope geochemistry. His thesis research focused on the timing of the Alpine orogenic event as recorded in high-pressure, low-temperature metamorphic assemblages. From these metamorphic assemblages, and associated garnets, Sm-Nd and Lu-Hf geochronometers were used to estimate the duration of the metamorphic event, as recorded in the pro-grade garnet growth. At PNNL Mr. Springer has applied his previous academic experience in clean-room chemistry and trace isotopic analysis to nuclear forensic and nuclear nonproliferation arenas in support of a number of U.S. Government agencies.

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Chris Zarzana received his Ph.D. in Chemistry from the University of Arizona in 2011, under the direction of Professor M. Bonner Denton. His thesis work involved the development and characterization of advanced array ion detectors and their application to dispersive mass spectrometry instrumentation. He was a postdoc at the University of Arizona, where he continued work on using advanced charge amplifier arrays as detectors for mass spectrometers. Dr. Zarzana has been a postdoc at Idaho National Laboratory since 2013, conducting research on electrospray ionization mass spectrometry, with an emphasis on ion formation chemistry.

5.0 Presentation Abstracts

The presentations were all summarized in abstracts to provide context for the overall short course. The biosketches are reproduced here for convenience but are also found in the file "ICP-MS Workshop FinalVol1.pdf."

Introduction and Overview of Inductively Coupled Plasma Mass Spectrometric Techniques

Greg Eiden, Pacific Northwest National Laboratory

This short course is the second in a series of courses sponsored by the U.S. Department of Energy (DOE). DOE seeks to offer training in advanced instrumentation and methods for detection of materials of importance. This training is designed to address the adaptation and operation of instruments that define the state of the art in isotope ratio measurements and to foster communication between laboratories and universities. It is hoped that these short courses will build interest and guide/mentor future generations of mass spectroscopy researchers. The course in 2014 is focused on inductively coupled plasma mass spectrometry (ICP-MS). In 2013, Idaho National Laboratory hosted a meeting and short course focused on thermal ionization mass spectrometry (TIMS) and in 2015, Lawrence Livermore National Laboratory will host a meeting focused on secondary ion mass spectrometry (SIMS).

Plasma and Ion Sampling Fundamentals in ICP-MS

Martin Liezers, Pacific Northwest National Laboratory

In ICP-MS "plasma and ion sampling" can be summarized as: How to form ions and then lose most of them! The ICP is a very effective ion source for elemental/isotopic analysis as can be gauged by the numbers of optical emission and mass spectrometry instruments in use. Much of the explosive development of ICP-MS, which has gone from "a wild idea" in the 1970s to an everyday lab instrument today, has been centered on what goes on in the plasma and the ion sampling interface, which still remains the region where most ions are lost. In spite of the low ion numbers that are actually transmitted into the mass spectrometer, ICP-MS remains one of the most sensitive techniques for elemental and isotopic analysis. Plasma and ion sampling covers the characteristics of the ICP that make it a good ion source, hot-cold plasmas, ion sampling from the plasma, enhanced interface pumping to improve ion transmission, ion energy with mass, and ion acceleration for magnetic sector ICP-MS.

Mass Separation

Greg Eiden, Pacific Northwest National Laboratory

The ICP ion source has been coupled to almost every conceivable kind of mass separator and ion detector, however the most common instruments utilize either a quadrupole mass filter or a magnetic sector field to perform mass-based separation of the ions prior to detection. This talk will provide an overview of the hardware components of these two key mass separators as well as a brief introduction to the physics basis for separation. A few analytical performance metrics of interest such as resolution and sensitivity will also be described.

Sample Introduction Techniques

Charles Barinaga, Pacific Northwest National Laboratory

You've got a sample. You've got an ICP-MS instrument. Now what? All the various types of analytical instrumentation have particular techniques and requirements regarding how a sample is presented to the instrument in order for it to be able to produce meaningful data related to the sample. The two more common sample introduction techniques for ICP-MS, liquid nebulization and laser ablation of solids, will be introduced and briefly discussed. In addition, some alternative sample introduction techniques for different sample types (solids, liquids, and gases) will be presented.

Overview of Inductively Coupled Plasma Mass Spectrometry for Elemental Analysis

Chris Sorensen, Pacific Northwest National Laboratory

Applications of elemental analysis are far reaching, including trace elemental detection in medicine, geology, archeology, semi-conductors, and nuclear energy. Elemental analysis using inductively coupled mass spectrometry can be highly informative even when complex mixtures are analyzed. However, careful experimental design, use of the appropriate standards, and reference materials also need to be considered, prior to data interpretation. These slides highlight important experimental considerations and briefly describe some aspects of calibration and correction of signals from ICP-MS. Highlights from recent publications will be made to illustrate how elemental analysis information can be applied.

Sample Preparation and Protocols

Kellen Springer, Pacific Northwest National Laboratory

Experimental design, sample preparation and interpretation of isotope ratio measurements are presented through an example from isotope geochemistry.

Multi-collector Methods and Examples

Garret Hart, Pacific Northwest National Laboratory

The multi-collector (magnetic sector) inductively coupled plasma mass spectrometer (MC-ICP-MS) provides a powerful tool for the isotopic (and elemental) analysis of many of the elements across the periodic table. The MC-ICP-MS is ideal for high-precision isotope ratio spectrometry because of its flat top peaks, its efficient ion transmission, and its simultaneous detection of the ion beam on either faraday cups or ion counters. In this presentation Dr. Hart will focus on one example of the MC-ICP-MS—the Neptune Plus by Thermo Scientific. He will discuss some key characteristics of this instrument first, including the high-efficiency front-end, the interface pump, the ion energy filters, and the unique collector array designed specifically for U and Pu applications. Second, he will discuss some important parameters used to establish and evaluate the state-of-health of the instrument, including sensitivity, beam coincidence, peak shape, mass calibration, backgrounds, stability, and abundance sensitivity. Finally, Dr. Hart will provide a few example data sets generated with a MC-ICP-MS from his work in geosciences and from work at the lab.

Mass Spectrometry at the National Laboratories: An Overview

Erick Ramon, Lawrence Livermore National Laboratory

The results of a survey of national laboratory mass spectrometry capabilities are presented.

Laser Ablation ICP/MS Topics

Part 1. Laser Ablation – Chemical Analysis

Rick Russo, Lawrence Berkeley National Laboratory

Laser ablation (LA) with mass ICP-MS detection is an excellent technology for direct sample (solid, liquid, or gas) analysis. Benefits of laser ablation include no sample preparation, no consumables, every sample, real-time analysis, standoff (LIBS) measurements, and more. Although the concept of laser ablation sampling is relatively straightforward—a high-power pulsed laser beam on a sample removes a small portion of mass for analysis—the fundamental processes are relatively complex and interdependent. Knowledge of ablation processes, reliable system components, and development of methods has led to excellent performance metrics (accuracy and precision) of this technology for routine chemical analysis. In general, LA-ICP-MS provides ppb elemental analysis and isotopic ratios with per-mil precision. New research shows the ability to perform isotope measurements in the laser plasma at atmospheric pressure to complement ICP-MS measurements. This talk will present a general overview of the governing mechanisms for laser ablation, attributes of LA-ICP-MS, and the ability to simultaneously measure mass and optical emission providing a complete toolbox for rapid elemental and isotopic chemical analysis.

Part 2. Laser Ablation

Andrew Duffin, Pacific Northwest National Laboratory

Laser ablation coupled to inductively coupled plasma mass spectroscopy (LA-ICP-MS) is a versatile and powerful technique for direct elemental and isotopic analysis of solid samples. Advantages of LA-ICP-MS include atmospheric pressure sampling, no dissolutions and therefore no reagent blanks, and no chemical separations. Moreover, LA-ICP-MS can efficiently analyze (high percentage of atoms ablated reach the detectors) materials with micron scale spatial resolution, leading to applications in elemental and isotopic mapping. Of course, the simple sample preparation can also be a disadvantage when the matrix presents isobaric interferences. One of the main drawbacks of LA-ICP-MS is the necessity of dealing with transient signals. These slides give a brief overview of nuances to be aware of during LA-ICP-MS analysis, discuss strategies to deal with transient signals, and present examples of elemental and isotopic analysis.

ICP-MS Instrument Specializations

Charles Barinaga, Pacific Northwest National Laboratory

This presentation is primarily concerned with isobaric interferences in ICP-MS. An isobar is an ion that has the same mass-to-charge (m/z) ratio as an analyte ion. If a mass spectrometer cannot separate it from the analyte, it becomes an interferent in the analysis, i.e., making the intensity of the response at that m/z appear to be greater than would be expected from the analyte alone. The nature and sources of atomic and polyatomic isobaric interferences will be discussed, as will the problems they create. Various techniques (high mass resolution, collision/reaction cell technology, and kinetic energy discrimination) for removing or lessening the effect of these interferences will be presented, including current, commercially available instrumentation that incorporate these techniques. Lastly, two alternative mass separation techniques, time-of-flight (TOF) and distance-of-flight (DOF) will be briefly presented.

Ion Optics Modeling

Chris Zarzana, Idaho National Laboratory

SIMION is an ion optics simulation computer program used to design and analyze charged particle optical systems, from simple electrostatic lenses to complex mass spectrometry instrumentation. The program solves for the electric and magnetic fields produced by a collection of electrodes, and can compute ion trajectories due to those fields. This course presents a broad overview of SIMION, with emphasis on how to perform common tasks. Additionally, features in the newer versions of SIMION are highlighted.

Advanced Detector Technology, Revolutionizing Science Through Better Detection

M. Bonner Denton, University of Arizona

Array detectors have revolutionized many areas of optical spectroscopy. However, until recently the limited array detector technology suitable for the detection of ions has suffered from a variety of problems and limitations. This presentation will present the evolution as well as the current state of the art of a new family of array ion detectors capable of providing high sensitivity, high-stability detection of ions over large dynamic ranges. When coupled with mass analyzers capable of dispersing ions on a spatial focal plane, these detectors provide simultaneous analysis of large mass ranges.

Modes of operation including nondestructive readout, random access integration, and individual pixel gain control and addressing, will be described. Performance, figures of merit including detection capabilities, dynamic range, read noise and dark current will all be presented. Additionally, current and future design considerations will be considered.

Alternative Ion Sources for Trace Inorganic Mass Spectrometry

Doug Duckworth, Pacific Northwest National Laboratory

Why choose one ion source over another for inorganic MS? While the main MS methods considered in this series of short courses (TIMS, ICP-MS, and SIMS) are the workhorses of elemental and (inorganic) isotopic analysis, many other methods are also in widespread use or the subject of ongoing research. Ion source selection is based on many factors including sample size and type, whether the instrument is to be used in a fixed laboratory or is to be portable, and perhaps most importantly, performance trades: sample utilization efficiency (SUE), ionization specificity, and production of background and interfering species. The methods presented and discussed with respect to these performance trades include TIMS, Spark Source MS (SSMS), Glow Discharge MS (GDMS), pulsed glow discharge and RF glow discharge MS, atmospheric sampling glow discharge MS, laser ionization MS, and secondary ion and sputtered neutral MS.

6.0 Agenda

The agendas for each of the days can be found in Volumes one and two (respectively for Day 1 and Day2) of the Presentation Booklet "ICP-MS Workshop FINALVol.1.pdf" and "ICP-MS Workshop FINALVol.2.pdf"

- Table 6: Agenda for Day One, June 17, 2014 of the ICP-MS Workshop
- Table 7: Agenda for Day Two, June 18, 2014 of the ICP-MS Workshop

Table 6: Agenda for Day One, June 17, 2014 of the ICP-MS Workshop

TIME	Presentation	Speaker
7:45 a.m.	Morning Hospitality	
8:00 a.m.	Welcome to PNNL	Randy Hansen
8:10 a.m.	Introduction and Overview of Inductively Coupled Plasma Mass Spectrometric Techniques	Greg Eiden
8:30 a.m.	Plasma and Ion Sampling Fundamentals in ICP-MS	Martin Liezers
9:30 a.m.	Break	
10:00 a.m.	Mass Separation	Greg Eiden
10:45 a.m.	Sample Introduction Techniques	Charles Barinaga
11:30 a.m.	Overview of Inductively Coupled Plasma Mass Spectrometry for Elemental Analysis	Chris Sorensen
12:15 p.m.	Lunch	
12:55 p.m.	Move to CSF/BSF Lobby	
1:10 p.m.	Poster Session	
2:00 p.m.	Move to EMSL	
2:15 p.m.	Sample Preparation and Protocols	Kellen Springer
3:00 p.m.	Break	
3:15 p.m.	Sample Preparation and Protocols (cont'd)	Kellen Springer
4:00 p.m.	Multi-collector Methods and Examples	Garret Hart
4:45 p.m.	Adjourn	
6:30 p.m.	No Host Dinner at Bookwalter Winery, Richland	

Table 7: Agenda for Day Two, June 18, 2014 of the ICP-MS Workshop

TIME	Presentation	Speaker
7:45 a.m.	Morning Hospitality	
8:00 a.m.	Welcome to Day Two	Greg Eiden
8:15 a.m.	Mass Spectrometry in the DOE Complex	Erick Ramon
9:00 a.m.	LA-ICPMS Topics - Laser Ablation – Chemical Analysis - Laser Ablation-Multi-Collector ICPMS	Rick Russo Andrew Duffin
10:00 a.m.	Break	
10:30 a.m.	ICP-MS Instrument Specializations	Charles Barinaga
11:30 am.	Lunch	
11:45 a.m.	Student Opportunities at PNNL	Marisela Linares-Mendoza
12:30 p.m.	Ion Optics Modeling	Chris Zarzana, Idaho National Laboratory
1:15 p.m.	Advanced Detector Technology	Bonner Denton, University of Arizona
2:00 p.m.	Break	
2:30 p.m.	Alternative Plasma Sources for Trace Inorganic Mass Spectrometry	Doug Duckworth
3:30 p.m.	Wrap Up	
4:00 p.m.	Adjourn	

7.0 Presentation Files

All of the presentations for the ICP-MS Workshop were collected as two documents each covering one of the two days. The team opted to make these available only electronically to reserve resources for student travel stipends. The Presentation booklet was substantial in size and the expense to print it up and logistics to get 80 copies to the venue would have been significant. Instead the team opted to make the materials available on the website to enable the participants to either use personal electronic device (laptop or tablet) to access the materials in the short course, or to opt to print up the materials themselves.

Workshop Website:

http://events.pnnl.gov/default.aspx?topic=2014_Mass_Spectrometry%20Workshop

Presentation Downloading:

http://events.pnnl.gov/Reports.aspx?topic=2014_Mass_Spectrometry_Workshop&rpttype=Presentations

The presentation files are included in this packet:

- Volume 1 – Day 1: "ICP-MS Workshop FINALVol.1.pdf"
- Volume 2 – Day 2: "ICP-MS Workshop FINALVol.2.pdf"

8.0 Conclusions

The participation in this workshop demonstrates strong interest at the graduate student level as well as by USG agencies in mass spectrometry. In spite of the maturity of ICPMS, senior scientists, as well as newcomers and grad students, from universities, industrial labs, and government labs attended. Interest came not just from those wishing to apply a mature technique to their problem, but from instrument and method developers as well. This broad interest is understandable in that continued improvements in analytical methods, not just mass spectrometry, are central to the advancement of scientific inquiry in the physical sciences. Without continued improvements in analytical methods such as mass spectrometry, the advancement represented by "Moore's Law" (the growth over time in device density in integrated circuits) and related metrics in other fields, stops!

If PNNL can be of any assistance in the preparation for the 2015 TIMS course at LLNL, please don't hesitate to contact us. We look forward to attending.

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