PROCEEDINGS OF SPIE

Next-Generation Spectroscopic Technologies VI

Mark A. Druy Richard A. Crocombe Editors

29–30 April 2013 Baltimore, Maryland, United States

Sponsored and Published by SPIE

Volume 8726

Proceedings of SPIE 0277-786X, V. 8726

SPIE is an international society advancing an interdisciplinary approach to the science and application of light.

Next-Generation Spectroscopic Technologies VI, edited by Mark A. Druy, Richard A. Crocombe, Proc. of SPIE Vol. 8726, 872601 · © 2013 SPIE CCC code: 0277-786X/13/\$18 · doi: 10.1117/12.2031968

Proc. of SPIE Vol. 8726 872601-1

The papers included in this volume were part of the technical conference cited on the cover and title page. Papers were selected and subject to review by the editors and conference program committee. Some conference presentations may not be available for publication. The papers published in these proceedings reflect the work and thoughts of the authors and are published herein as submitted. The publisher is not responsible for the validity of the information or for any outcomes resulting from reliance thereon.

Please use the following format to cite material from this book: Author(s), "Title of Paper," in Next-Generation Spectroscopic Technologies VI, edited by Mark A. Druy, Richard A. Crocombe, Proceedings of SPIE Vol. 8726 (SPIE, Bellingham, WA, 2013) Article CID Number.

ISSN: 0277-786X ISBN: 9780819495174

Published by **SPIE** P.O. Box 10, Bellingham, Washington 98227-0010 USA Telephone +1 360 676 3290 (Pacific Time) · Fax +1 360 647 1445 SPIE.org

Copyright © 2013, Society of Photo-Optical Instrumentation Engineers.

Copying of material in this book for internal or personal use, or for the internal or personal use of specific clients, beyond the fair use provisions granted by the U.S. Copyright Law is authorized by SPIE subject to payment of copying fees. The Transactional Reporting Service base fee for this volume is \$18.00 per article (or portion thereof), which should be paid directly to the Copyright Clearance Center (CCC), 222 Rosewood Drive, Danvers, MA 01923. Payment may also be made electronically through CCC Online at copyright.com. Other copying for republication, resale, advertising or promotion, or any form of systematic or multiple reproduction of any material in this book is prohibited except with permission in writing from the publisher. The CCC fee code is 0277-786X/13/\$18.00.

Printed in the United States of America.

Publication of record for individual papers is online in the SPIE Digital Library.



Paper Numbering: Proceedings of SPIE follow an e-First publication model, with papers published first online and then in print and on CD-ROM. Papers are published as they are submitted and meet publication criteria. A unique, consistent, permanent citation identifier (CID) number is assigned to each article at the time of the first publication. Utilization of CIDs allows articles to be fully citable as soon as they are published online, and connects the same identifier to all online, print, and electronic versions of the publication. SPIE uses a six-digit CID article numbering system in which:

- The first four digits correspond to the SPIE volume number.
- The last two digits indicate publication order within the volume using a Base 36 numbering
- system employing both numerals and letters. These two-number sets start with 00, 01, 02, 03, 04, 05, 06, 07, 08, 09, 0A, 0B ... 0Z, followed by 10-1Z, 20-2Z, etc.

The CID Number appears on each page of the manuscript. The complete citation is used on the first page, and an abbreviated version on subsequent pages. Numbers in the index correspond to the last two digits of the six-digit CID Number.

Contents

- vii Conference Committee
- ix Introduction

SESSION 1 HYPERSPECTRAL IMAGING SPECTROMETERS AND APPLICATIONS

- 8726 04 High-performance hyperspectral imaging using virtual slit optics [8726-3]
 B. B. Behr, Tornado Spectral Systems (United States); J. T. Meade, A. R. Hajian, A. T. Cenko, Tornado Spectral Systems (Canada)
- 8726 05 Development of a handheld widefield hyperspectral imaging (HSI) sensor for standoff detection of explosive, chemical, and narcotic residues [8726-4]
 M. P. Nelson, A. Basta, R. Patil, O. Klueva, P. J. Treado, ChemImage Corp. (United States)

SESSION 2 MEMS- AND MOEMS-BASED SPECTROMETERS

- 8726 08 Hydrocarbon gas detection with microelectromechanical Fabry-Perot interferometer [8726-8]
 R. Mannila, M. Tuohiniemi, J. Mäkynen, I. Näkki, J. Antila, VTT Technical Research Ctr. of Finland (Finland)
- 8726 09 First application close measurements applying the new hybrid integrated MEMS spectrometer [8726-9]
 H. Grüger, T. Pügner, J. Knobbe, H. Schenk, Fraunhofer-Institut für Photonische Mikrosysteme (Germany)

SESSION 3 QUANTUM CASCADE AND TUNABLE DIODE LASERS

Tunable picosecond spectroscopy for detection of nitric oxide [8726-11]
 C. Tanjaroon, C. J. Lue, S. W. Reeve, J. B. Johnson, Arkansas State Univ. (United States);
 S. D. Allen, Embry-Riddle Aeronautical Univ. (United States)

8726 OC Low-cost lightweight airborne laser-based sensors for pipeline leak detection and reporting [8726-12]
 M. B. Frish, R. T. Wainner, M. C. Laderer, M. G. Allen, Physical Sciences Inc. (United States); J. Rutherford, P. Wehnert, Heath Consultants Inc. (United States); S. Dey, J. Gilchrist, R. Corbi, New Era Technology, Inc. (United States); D. Picciaia, TEA Sistemi S.p.A. (Italy); P. Andreussi, Univ. degli Studi di Pisa (Italy); D. Furry, Leak Surveys Inc. (United States)

8726 0D Trace-gas sensing using the compliance voltage of an external cavity quantum cascade laser [8726-13]

M. C. Phillips, M. S. Taubman, Pacific Northwest National Lab. (United States)

8726 OE **Mid-infrared microspectroscopic imaging with a quantum cascade laser** [8726-14] K. Yeh, M. Schulmerich, R. Bhargava, Univ. of Illinois at Urbana-Champaign (United States)

SESSION 4 DATA ANALYSIS TECHNIQUES AND APPLICATIONS

- 8726 OF Performance characterization of a combined material identification and screening algorithm [8726-15]
 R. L. Green, M. D. Hargreaves, C. M. Gardner, Thermo Fisher Scientific Inc. (United States)
- 8726 OH **Discrimination methodologies using femtosecond LIBS and correlation techniques** [8726-17] S. Sunku, E. Nageswara Rao, G. Manoj Kumar, S. P. Tewari, S. Venugopal Rao, Univ. of Hyderabad (India)

SESSION 5 LIBS, RAMAN, AND TERAHERTZ

- 8726 01 Portable sub-terahertz resonance spectrometer combined with microfluidic sample cell [8726-18]
 J. P. Ferrance, Vibratess, LLC (United States), J²F Engineering (United States), and Univ. of Virginia (United States); A. Khromov, Vibratess, LLC (United States) and Univ. of Virginia (United States); A. Moyer, T. Khromova, Vibratess, LLC (United States); B. Gelmont, Univ. of Virginia (United States); I. Sizov, Vibratess, LLC (United States); T. Globus, Vibratess, LLC (United States) and Univ. of Virginia (United States) and Univ. of Virginia (United States) and Univ. of Virginia (United States); I. Sizov, Vibratess, LLC (United States); T. Globus, Vibratess, LLC (United States) and Univ. of Virginia (United States)
- 8726 0J THz-Raman: accessing molecular structure with Raman spectroscopy for enhanced chemical identification, analysis, and monitoring [8726-19]
 R. A. Heyler, J. T. A. Carriere, F. Havermeyer, Ondax, Inc. (United States)
- 8726 OK **Design and industrial testing of ultra-fast multi-gas Raman spectrometer** [8726-20] M. P. Buric, J. Mullen, S. D. Woodruff, B. Chorpening, National Energy Technology Lab. (United States)
- 8726 OL High-throughput spectrometer designs in a compact form-factor: principles and applications [8726-21]
 S. M. Norton, Wasatch Photonics, Inc. (United States)
- A novel laser-based approach for cleaning contaminated metallic surfaces coupled with rapid residue analysis [8726-23]
 R. V. Fox, L. Roberts, Idaho National Lab. (United States); F. C. DeLucia Jr., A. W. Miziolek, U.S. Army Research Lab. (United States); A. I. Whitehouse, Applied Photonics Ltd. (United Kingdom)
- 8726 00 Effects of incomplete light extinction in frequency-agile, rapid scanning spectroscopy
 [8726-25]
 D. A. Long, National Institute of Standards and Technology (United States); S. Wójtewicz,
 National Institute of Standards and Technology (United States) and Nicolaus Copernicus
 Univ. (Poland); J. T. Hodges, National Institute of Standards and Technology (United States)

- 8726 OP **The evaluation of a new technology for gunshot residue (GSR) analysis in the field** [8726-26] E. Hondrogiannis, D. Andersen, Towson Univ. (United States); A. W. Miziolek, U.S. Army Research Lab. (United States)
- 8726 0Q Spectroscopy methods for identifying the country of origin [8726-27]
 E. Hondrogiannis, E. Ehrlinger, Towson Univ. (United States); A. W. Miziolek, U.S. Army Research Lab. (United States)

SESSION 6 PORTABLE AND NOVEL DESIGNS I

- 8726 OR Handheld spectrometers: the state of the art [8726-28] R. A. Crocombe, Thermo Fisher Scientific Inc. (United States)
- 8726 0S A microfabricated, low dark current a-Se detector for measurement of microplasma optical emission in the UV for possible use on-site [8726-29]
 S. Abbaszadeh, K. S. Karim, V. Karanassios, Univ. of Waterloo (Canada)
- A handheld FTIR spectrometer with swappable modules for chemical vapor identification and surface swab analysis [8726-30]
 W. J. Doherty III, B. Falvey, G. Vander Rhodes, L. Krasnobaev, K. Vachon, Thermo Fisher Scientific Inc. (United States)
- 8726 0U Advanced sampling techniques for hand-held FT-IR instrumentation [8726-31] J. Arnó, M. Frunzi, C. Weber, D. Levy, Smiths Detection (United States)
- 8726 0V **Tapered air-core Bragg waveguide spectrometers for lab-on-a-chip applications** [8726-32] B. A. Drobot, A. D. Melnyk, T. W. Allen, R. G. DeCorby, Univ. of Alberta (Canada)

SESSION 7 PORTABLE AND NOVEL DESIGNS II

- 8726 0W Feasibility study of birefringent electro-optic NIR FTS imaging systems [8726-33] V. Finnemeyer, P. Bos, Kent State Univ. (United States)
- 8726 0X Continuous-wave near-photon counting spectral imaging detector in the mid-infrared by upconversion [8726-34] J. S. Dam, P. Tidemand-Lichtenberg, C. Pedersen, Technical Univ. of Denmark (Denmark)
- 8726 0Y Tunable up-conversion detector for single photon and bi-photon infrared spectroscopic applications [8726-35]
 O. Slattery, L. Ma, P. Kuo, Y.-S. Kim, X. Tang, National Institute of Standards and Technology (United States)
- Fourier transform infrared phase shift cavity ring down spectrometer [8726-36]
 E. Schundler, D. J. Mansur, R. Vaillancourt, R. Benedict-Gill, S. P. Newbry, J. R. Engel, J. Rentz Dupuis, OPTRA, Inc. (United States)

POSTER SESSION

8726 10 Broadband absorption and emission millimeter-wave spectroscopy between 220 and 325 GHz [8726-37]

M. Szymkiewicz, Fraunhofer-Institut für Angewandte Festkörperphysik (Germany) and Karlsruher Institut für Technologie (Germany); A. Hülsmann, A. Tessmann, M. Schlechtweg, A. Leuther, Fraunhofer-Institut für Angewandte Festkörperphysik (Germany); O. Ambacher, Fraunhofer-Institut für Angewandte Festkörperphysik (Germany) and Univ. of Freiburg (Germany); S. Koch, M. Riedel, Sony Deutschland GmbH (Germany); I. Kallfass, Fraunhofer-Institut für Angewandte Festkörperphysik (Germany) and Karlsruher Institut für Technologie (Germany)

Author Index

Conference Committee

Symposium Chair

Kenneth R. Israel, Major General (USAF Retired) (United States)

Symposium Cochair

David A. Whelan, Boeing Defense, Space, and Security (United States)

Conference Chairs

Mark A. Druy, Physical Sciences Inc. (United States) Richard A. Crocombe, Thermo Fisher Scientific Inc. (United States)

Conference Program Committee

Leigh J. Bromley, Daylight Solutions (United States) John M. Dell, The University of Western Australia (Australia) Richard D. Driver, Headwall Photonics Inc. (United States) Michael B. Frish, Physical Sciences Inc. (United States) Fredrick G. Haibach, Block Engineering, LLC (United States) Martin Kraft, Carinthian Tech Research AG (Austria) Jouko O. Malinen, VTT Technical Research Center of Finland (Finland) Curtis A. Marcott, Light Light Solutions, LLC (United States) Ellen V. Miseo, Analytical Answers, Inc. (United States) David W. Schiering, Smiths Detection (United States) John Seelenbinder, Agilent Technologies (United States)

Session Chairs

- Hyperspectral Imaging Spectrometers and Applications
 Richard A. Crocombe, Thermo Fisher Scientific Inc. (United States)
- 2 MEMS- and MOEMS-Based Spectrometers **Michael B. Frish**, Physical Sciences Inc. (United States)
- 3 Quantum Cascade and Tunable Diode Lasers Mark A. Druy, Physical Sciences Inc. (United States)
- 4 Data Analysis Techniques and Applications **Richard A. Crocombe**, Thermo Fisher Scientific Inc. (United States)
- 5 LIBS, Raman, and Terahertz Leigh J. Bromley, Daylight Solutions (United States)

- Portable and Novel Designs I
 Mark A. Druy, Physical Sciences Inc. (United States)
- 7 Portable and Novel Designs II **Richard A. Crocombe**, Thermo Fisher Scientific Inc. (United States)

Introduction

The past twenty-five years have seen a massive investment in photonics, electronics and MEMS, aimed at developing new telecommunications capabilities and innovative consumer products. These investments have led to advances in miniature optics, light sources, tunable filters, array detectors, fiber optic sensors, and a range of other photonic devices, across the whole electromagnetic spectrum, along with technologies for their mass production. These and related advances are increasingly being exploited in new spectroscopic instruments. In recent years, there have been remarkable developments in handheld consumer electronics, especially cell phones and portable audio/video players. These devices contain advances in RF technology, processors, operating systems, user interfaces, memory, Bluetooth, WiFi, cameras, accelerometers, etc., and are now poised to be the basis of next-generation handheld scientific instruments.

Portable and handheld instruments are being developed that are often more sensitive and selective, smaller, cheaper, and more robust than their laboratory predecessors. Concurrent improvements in analytical theory, data analysis methods, algorithms and portable processors enable these spectroscopic devices to give specific actionable answers to their non-specialist operators. Spectroscopy-based systems are now making critical judgments in environments and applications that were unreachable twenty years ago, from hazardous materials to the operating theater, and from field geologists to customs and border personnel.

Advances in array detectors (CCD, CID, InGaAs, InSb, MCT, CMOS, etc.) are enabling a new generation of faster imaging spectrometers, with both laboratory and field applications. Lower-cost infrared arrays have been developed, employing MEMS techniques. New laser sources, particularly in the mid-infrared, are being used in combination with advances in detector technology to create new spectroscopic platforms.

The emphasis in this conference is on advanced technologies for spectroscopic instrumentation, particularly the infrared, near-infrared, and Raman molecular techniques, but also including advances enabling miniature and portable spectrometers across the electromagnetic spectrum, including x-ray fluorescence, laser induced fluorescence, Terahertz, nuclear magnetic resonance and mass spectrometry.

This conference premiered at Optics East 2007 in Boston, MA and is now part of the Defense Sensing & Security Symposium. In 2013, the conference spanned two days, and was divided into sessions focusing on: Hyperspectral Imaging Spectrometers and Applications; MEMS- and MOEMS-Based Spectrometers; Quantum Cascade and Tunable Diode Lasers; Data Analysis Techniques and Applications; LIBS, Raman and Terahertz Spectroscopies, and Portable and Novel Designs. In all, 35 papers were presented, and we are pleased to be able to bring you 28 of them in these proceedings.

On behalf of our program committee members, we hope that we can count on your participation in a future Next-Generation Spectroscopic Technologies conference.

Mark A. Druy Richard A. Crocombe