Accepted: 23 November 2022

DOI: 10.1002/xrs.3319

News Article

X-RAY SPECTROMETRY WILEY

Kenji Sakurai, News Editor

Correspondence
Email: kenji.sakurai@sakuraixlab.com

Denver X-ray conference award (August 3, 2022)

During the 71st Annual Denver X-Ray Conference, which finally returned as an in-person event after two virtual conferences due to the COVID-19 pandemic, the following award were presented. The Birks Award, given biennially to recognize outstanding contributions to the field of X-ray spectrometry, was presented to Professor Kouichi Tsuji (Osaka Metropolitan University, Japan) for his contributions to the development and applications in the field of X-ray fluorescence spectrometry including depth profiling using confocal XRF, full field WDXRF imaging, micro XRF, TXRF; and for his commitment to his students and to the international XRF community. For further information, visit the Web page, http://www.dxcicdd.com/.

How to cite this article: K. Sakurai, *X-Ray Spectrom* **2023**, *52*(1), 46. https://doi.org/10.1002/xrs.3319

Accepted: 19 January 2023
DOI: 10.1002/xrs.3332

News Article

X-RAY SPECTROMETRY WILEY

Kenji Sakurai, News Editor

Correspondence
Email: kenji.sakurai@sakuraixlab.com

X-ray laser pioneer receives Isaac Newton Medal and Prize (October 25, 2022)

The Isaac Newton Medal and Prize for 2022 was given to Professor Margaret Murnane (University of Colorado, Boulder, USA) for pioneering and sustained contributions to the development of ultrafast lasers and coherent X-ray sources and the use of such sources to understand the quantum nature of materials. Nowadays, it is well known that ultrashort pulses and coherent light in the soft and hard X-ray regions can be obtained by using high-order harmonics of infrared laser source. The research group led by Professor Murnane is a pioneer in the development of such advanced tabletop X-ray laser and the new research. One of the most impressive reports for many X-ray users is the laboratory XAFS with 10^9 counts/s (1% bandwidth) intensity at around C-K, Fe-LIII, and Sc-LIII absorption edges in the soft X-ray region (0.2–1.6 keV) (D. Popmintchev et al., "Near- and Extended-Edge X-Ray-Absorption Fine-Structure Spectroscopy Using Ultrafast Coherent High-Order Harmonic Supercontinua," *Phys. Rev. Lett.* 120, 093002 (2018). https://doi.org/10.1103/PhysRevLett.120.093002). Some of the recent stimulating progresses is advanced ptychographic imaging such as linear dichroism imaging of molecular orientation in nanodomains (see, for example, Yuan Hung Lo et al., "X-ray linear dichroic ptychography," *Proceedings of the National Academy of Sciences* 118, e2019068118 (2021). https://doi.org/10.1073/pnas.2019068118; Arjun Rana et al., "Direct observation of 3D topological spin textures and their interactions using soft x-ray vector ptychography," submitted. https://doi.org/10.48550/arXiv.2104.12933). For further information on the Isaac Newton Medal and Prize, visit the Web page, https://www.iop.org/about/awards/isaac-newton-medal-and-prize/isaac-newton-medal-and-prize-recipients.

How to cite this article: K. Sakurai, *X-Ray Spectrom* **2023**, *52*(2), 102. https://doi.org/10.1002/xrs.3332

Accepted: 21 March 2023
DOI: 10.1002/xrs.3346

News Article

X-RAY SPECTROMETRY WILEY

Kenji Sakurai, News Editor

Correspondence
Email: kenji.sakurai@sakuraixlab.com

Possible impacts of Large Language Models on X-ray spectroscopy (March 17, 2023).

Recent announcement of releasing OpenAI's Generative Pretrained Transformer 4 (GPT-4) could mark the beginning of a new era of the practical application of artificial intelligence. Compared with the previous versions of OpenAI's Large Language Models (LLM), its function in handling the images even in the text-based chat system is surprising. In the presentation, which has been archived as a Youtube video (https://www.youtube.com/live/outcGtbnMuQ?feature=share), the chat system can handle a screenshot image of a handwriting note with some sketch, and can instantly transform it into an html code. Then one can create a new Web page. In addition, the reasoning ability has been upgraded considerably from the previous version, which had not been very good; previous ChatGPT seems to give the correct answer only to 26% of the junior high school level mathematics problems (see, for example, Simon Frieder et al., "Mathematical Capabilities of ChatGPT", https://arxiv.org/abs/2301.13867). The new version seems to be much better and is now quite good at the tax calculation and the bar exam problem. Generally, the ability of text-based job has become further better than ever. The number of characters that can be handled has increased, and overall processing has become higher quality. One of the recent interesting discussions on the application of artificial intelligence to spectroscopy has been described in the article, by Jerome Workman, Jr., and Howard Mark, "Artificial Intelligence in Analytical Spectroscopy, Part I: Basic Concepts and Discussion", Spectroscopy, 38, (2), 13–22 (2023). https://doi.org/10.56530/spectroscopy.og4284z8. Some of the related contents have been also discussed in the podcast, Analytically Speaking Podcast Episode 9, "Automating Advanced Chemometric Methods for Data Processing" (https://www.spectroscopyonline.com/view/ep-9-automating-advanced-chemometric-methods-for-data-processing). As the present artificial intelligence is more powerful in handling billions of images, for a while, image-based scientific applications could be preceding (see, for example, Lei Zhang and Shaofeng Shao, "Image-based machine learning for materials science", Journal of Applied Physics 132, 100701 (2022). https://doi.org/10.1063/5.0087381; Samantha Phan and Christine K. Luscombe, "Recent trends in marine microplastic modeling and machine learning tools: Potential for long-term microplastic monitoring", Journal of Applied Physics 133, 020701 (2023). https://doi.org/10.1063/5.0126358). On the same day of the announcement of GPT-4, Anthropic Inc, which is a rival company founded by former Open AI employees, released Claude. It has been tested in private systems on systems such as Notion, Quora, and DuckDuckGo, and has been very well received. The LLM and its application such as chatbots will be used more frequently than before. On the other hand, the system is like a black box, and therefore we will need to be careful when considering some real use (see, for example, Noah Giansiracusa, "Three Easy Ways to Make AI Chatbots Safer", Scientific American, March 17, 2023, https://www.scientificamerican.com/article/three-easy-ways-to-make-ai-chatbots-safer/).

How to cite this article: K. Sakurai, *X-Ray Spectrom* **2023**, *52*(3), 151. https://doi.org/10.1002/xrs.3346

Accepted: 19 May 2023

DOI: 10.1002/xrs.3372

News Article

X-RAY SPECTROMETRY WILEY

Kenji Sakurai, News Editor

Correspondence
Email: kenji.sakurai@sakuraixlab.com

Book, "X-Ray Spectroscopy for Chemical State Analysis" (Jun Kawai, Springer, 2023)

Professor Jun Kawai (Kyoto University, Japan) has published an interesting and useful book on materials characterization methods using X-ray emission, absorption, and photoelectron spectroscopies. Readers will be able to learn about basic X-ray physics topics such as "Particle and Wave Duality of X-rays" (Chapter 1), "Profile Change of X-Ray Spectra" (Chapter 2), and "Chemical Effects of Multiply Ionized Satellites" (Chapter 3). They can also gain some practical knowledge on instrumentation, including "Pyroelectric X-Ray Emission" (Chapter 4), "Small-Size and Low-Power X-Ray Instruments" (Chapter 5), "Synchrotron Radiation Experiments" (Chapter 6), and "Quantitative Analysis Using XRF and SEM" (Chapter 7). The book includes some interesting historical episodes, such as Professor Yoneda's discovery of enhanced diffuse scattering at the total reflection critical angle (now often called the Yoneda peak or Yoneda wing in grazing-incidence small angle X-ray scattering) and TXRF. The author also describes his own experience - how he has achieved novel experiments. The book consists of 243 pages. Overall, this book seems to provide a good overview of X-ray spectroscopy methods and their applications. The inclusion of historical context and the author's experiences helps to give readers insight into how these techniques were developed and applied in practice. For further information of the book, see the following page, https://doi.org/10.1007/978-981-19-7361-1

How to cite this article: K. Sakurai, *X-Ray Spectrom* **2023**, *52*(4), 197. https://doi.org/10.1002/xrs.3372

DOI: 10.1002/xrs.3393

News Article

X-RAY SPECTROMETRY WILEY

Kenji Sakurai, News Editor

Correspondence
Email: kenji.sakurai@sakuraixlab.com

Detection of single atom using soft X-ray spectroscopy (May 31, 2023)

A research group at Argonne National Laboratory's APS synchrotron radiation facility has reported the detection of single atoms using synchrotron radiation X-rays (Tolulope M. Ajayi, Nozomi Shirato, Tomas Rojas, Sarah Wieghold, Xinyue Cheng, Kyaw Zin Latt, Daniel J. Trainer, Naveen K. Dandu, Yiming Li, Sineth Premarathna, Sanjoy Sarkar, Daniel Rosenmann, Yuzi Liu, Nathalie Kyritsakas, Shaoze Wang, Eric Masson, Volker Rose, Xiaopeng Li, Anh T. Ngo and Saw-Wai Hla, "Characterization of just one atom using synchrotron X-rays," Nature, 618, 69–73 (2023) https://doi.org/10.1038/s41586-023-06011-w). This research was performed at XTIP21, a beamline equipped with an STM probe in an ultrahigh vacuum chamber that can simultaneously perform STM imaging and soft X-ray spectroscopy experiments. The research sample is a supramolecular assembly with a ring structure consisting of seven terpyridine-metal-terpyridine bridges, with six ruthenium atoms and one iron atom on the metal. First, the sample was imaged by STM, and then, under the same conditions, the X-ray energy near the $L_{2,3}$ absorption edge of iron was scanned with a monochromator, and the excitation current was measured by the probe. The electric current changed at the absorption edge, indicating that a single atom could be detected. Since the X-ray signal was detected only when the probe was placed extremely close to the atom, X-ray excitation resonance tunneling is dominant, confirming the detection of atom localization in the tunneling region. Another sample in this study, a terbium complex, was also measured. In this complex, the terbium is firmly anchored by three brominated pyridine-2,6-dicarboxamide ligands. As with the previous sample, STM imaging was performed and the synchrotron radiation energy was varied near the $M_{4,5}$ absorption edge of terbium under the same conditions and a single atom was detected. Some readers may ask whether such a measurement can be achieved with X-ray fluorescence. It would depend on the sample conditions. The analysis of very small numbers of atoms by X-ray fluorescence spectroscopy is mainly limited by the background. If a sample has almost no background, in contrast to conventional X-ray analysis, it would theoretically be possible to detect a single atom. For example, if we have a sample in which only one atom is trapped in a fullerene, and the fullerene is placed in a carbon nanotube, it is possible to detect characteristic X-rays excited by electron beams with a semiconductor detector while observing the single atom with a transmission electron microscope. This was reported more than 10 years ago. For more details, see T. C. Lovejoy, Q. M. Ramasse, M. Falke, A. Kaeppel, R. Terborg, R. Zan, N. Dellby, and O. L. Krivanek, "Single atom identification by energy dispersive x- ray spectroscopy," Appl. Phys. Lett. 100, 154101 (2012). https://doi.org/10.1063/1.3701598, and Kazu Suenaga, Toshiya Okazaki, Eiji Okunishi, and Syo Matsumura, "Detection of photons emitted from single erbium atoms in energy dispersive x-ray spectroscopy," Nature Photonics 6, 545–548 (2012). https://doi.org/10.1038/nphoton.2012.148.

How to cite this article: K. Sakurai, *X-Ray Spectrom* **2023**, *52*(5), 269. https://doi.org/10.1002/xrs.3393

Accepted: 20 September 2023
DOI: 10.1002/xrs.3410

News Article

X-RAY SPECTROMETRY WILEY

Kenji Sakurai, News Editor

Correspondence
Email: kenji.sakurai@sakuraixlab.com

Advances in Cryogenic Radiation Detectors (September 7, 2023).

Cryogenic radiation detectors are attractive because of their extremely high energy resolution, typically on the order of eV for X-rays in the keV range. One of their applications is in astrophysics. Recently, the Japan Aerospace Exploration Agency (JAXA) launched the XRISM (X-Ray Imaging and Spectroscopy Mission) satellite in collaboration with NASA and ESA (for more details, see Daniel Clery, "Revolutionary x-ray sensor to probe workings of black holes and supernovae", Science, 381, 720–721 (2023). https://doi.org/10.1126/science.adk3474). The X-ray telescope is equipped with a high-energy resolution microcalorimeter detector called Resolve, which is expected to reveal more details about exploding stars, the matter orbiting supermassive black holes, and the merging of galaxy clusters. The detectors appear to be useful not only in such astrophysics, but also in X-ray spectrometry. One of the most important research projects is the precise determination of the fundamental X-ray parameters for many L lines in the soft X-ray region. The research team at NIST in Boulder, Colorado, USA has published a number of papers since 2017 (see, for example, J. W. Fowler et al., "A reassessment of the absolute energies of the x-ray L lines of lanthanide metals", Metrologia 54, 494 (2017). https://doi.org/10.1088/1681-7575/aa722f, "Absolute energies and emission line shapes of the L x-ray transitions of lanthanide metals", Metrologia 58, 015016 (2021). https://doi.org/10.1088/1681-7575/abd28a, "Energy Calibration of Nonlinear Microcalorimeters with Uncertainty Estimates from Gaussian Process Regression", Journal of Low Temperature Physics 209, 1047–1054 (2022). https://doi.org/10.1007/s10909-022-02740-w, "The potential of microcalorimeter X-ray spectrometers for measurement of relative fluorescence-line intensities", Radiation Physics and Chemistry, 202, 110,487 (2023). https://doi.org/10.1016/j.radphyschem.2022.110487). For more information on recent advances in cryogenic radiation detectors and their applications, see some review articles such as J. Ullom and D. Bennett, "Review of superconducting transition-edge sensors for x-ray and gamma-ray spectroscopy", Superconducting Science and Technology, 28, 084003 (2015). https://doi.org/10.1088/0953-2048/28/8/084003 and M. Ohkubo, "Advances in superconductor quantum and thermal detectors for analytical instruments", Journal of Applied Physics. 134, 081101 (2023). https://doi.org/10.1063/5.0151581

How to cite this article: K. Sakurai, *X-Ray Spectrom* **2023**, *52*(6), 486. https://doi.org/10.1002/xrs.3410