REIMEI Workshop: Positron Diffraction Studies on 2D Materials and Related Novel Surface Analysis Techniques

30th March 2026, 13:30 – 17:20 (JST), Online

Scope: In recent years, research on material surfaces and two-dimensional (2D) materials using positrons — the antiparticles of electrons — has advanced markedly. Synergistic studies that combine positron techniques with photoelectron spectroscopy and first-principles calculations are also progressing rapidly. At the same time, novel surface-analysis methods based on positrons are being developed. This workshop will bring together leading researchers who are at the forefront of such synergistic positron-based investigations and of new methodological development. We will discuss the current state of positron-based surface science and explore future directions for the field.

Program

Chair: Y. Fukaya

13:30 - 13:35 Opening remarks

13:35 - 14:00 **T. Hyodo** (KEK)

Positron Diffraction

14:00 - 14:25 **Y. Yamada-Takamura** (JAIST)

Structural Details of Epitaxial Xenes Revealed by Total-Reflection High-Energy Positron Diffraction

14:25 - 14:50 **Y. Tsujikawa** (Keio Univ.)

Structural Identification Using Positron Diffraction and Insights into Electronic Properties of Cu Boride Surfaces

14:50 - 15:00 Break

Chair: Y. Yamada-Takamura

15:00 - 15:25 **F. Matsui** (IMS)

Comprehensive Valence Band Characterization by Multi-Beam Photoelectron Momentum Microscopy

15:25 - 15:50 **K. Wada** (KEK)

Development of a LINAC-Based LEPD System and Current Status of its SATLEED-Based Analysis Code

15:50 - 16:15 **I. Mochizuki** (KEK)

Detection of Hydrogen Atoms Adsorbed on a Ceria Surface Using Total-Reflection High-Energy Positron Diffraction (TRHEPD)

16:15 - 16:25 Break

Chair: F. Matsui

16:25 - 16:50 **R. Ahmed** (KEK)

Quantitative Surface Structure Determination Using LEPD and Multiprobe Studies at the Slow Positron Facility, KEK

16:50 - 17:15 **Y. Nagata** (TUS)

Experimental Study of Positronium Diffraction Using Graphene

17:15 - 17:20 Closing remarks

Organizers: Y. Yamada-Takamura (JAIST), Y. Fukaya (JAEA), F. Matsui (IMS)

Abstract

13:35 - 14:00

Positron Diffraction

Toshio Hyodo, Slow Positron Facility, Institute for Materials Surface Science, High Energy Accelerator Research Organization (KEK)

Positron diffraction is the positron counterpart of electron diffraction. This includes TRHEPD, the positron version of RHEED, and LEPD, the positron version of LEED. Despite requiring larger equipment than electron diffraction, there are sufficient reasons for performing positron diffraction. TRHEPD directs positrons of approximately 10 keV on a sample surface at a small glancing angle. It exhibits total reflection not observed in RHEED, enabling precise determination of the atomic arrangements of outermost surface layers. In LEPD, since there is no exchange interaction between the positron and the electrons in the sample, the intensity of the diffraction spots is calculated with exceedingly high reliability and remarkably good agreement with experimental values. At Slow Positron Facility, KEK, a space of about 300 m2 accommodates a dedicated electron linac, positron production units, and the TRHEPD and LEPD stations. A klystron for the linac, located in a separate room, occupies an area of less than 10 m2. This presentation will introduce the facility and provide a basic overview of positron diffraction, including how to generate slow positrons.

14:00 - 14:25

Structural Details of Epitaxial Xenes Revealed by Total-Reflection High-Energy Positron Diffraction

Yukiko Yamada-Takamura, School of Materials Science, Japan Advanced Institute of Science and Technology (JAIST)

Post-graphene mono-elemental two-dimensional materials called “Xenes” are often synthesized on single crystal substrates through epitaxial growth due to the lack of layered mother crystals. The crystal and electronic structures of such epitaxial Xenes can be different from those predicted for the freestanding ones, so applying multiple, complementary characterization methods as well as first-principles calculations is necessary to clarify their structures. Total-reflection high-energy positron diffraction (TRHEPD) demonstrate strengths in the structural analysis of such materials owing to its extremely high surface sensitivity. In this talk, I will introduce our recent work on a two-dimensional lattice made of Ge atoms, which TRHEPD has contributed significantly to reveal its mysterious structure.

14:25 - 14:50

Structural Identification Using Positron Diffraction and Insights into Electronic Properties of Cu Boride Surfaces

Yuki Tsujikawa, Department of Chemistry, Keio University

Accurate structural analysis is crucial for understanding materials in solid state physics. However, determining the structure of solid surfaces, which are only a few atomic layers thick, remains challenging because they are difficult to observe directly. Diffraction methods, which analyze periodic structures produced by translational symmetry, are widely used for structural analysis.

Here we introduce a highly surface-sensitive structural analysis technique based on a diffraction method that employs positrons, known as total-reflection high-energy positron diffraction. By this method a structural analysis of the surface formed by depositing boron onto a copper substrate was conducted. Two structural models had been debated for this surface: a single atomic layer of boron (borophene) and a compound structure of boron and copper (Cu-boride). Positron diffraction resolved this debate, identifying Cu-boride as the correct structure. Furthermore, this finding revealed boron configurations and electronic states unique to Cu-boride, attracting attention to this new class of compounds.

15:00 - 15:25

Comprehensive Valence Band Characterization by Multi-Beam Photoelectron Momentum Microscopy

Fumihiko Matsui, Institute for Molecular Science, UVSOR Synchrotron Facility

The photoelectron momentum microscope (PMM) is a cutting-edge hybrid system integrating a PEEM, an energy analyzer, and a 2D projection detector. This instrumentation represents a paradigm shift in materials characterization by enabling the simultaneous acquisition of constant-energy photoelectron intensity distributions. It provides high-resolution, real-space imaging with elemental and chemical selectivity while concurrently mapping reciprocal-space structures—such as Fermi surfaces and valence band dispersions—from micro-scale localized regions. A transformative advantage of PMM is the "snapshot" acquisition of spin-polarized distributions, facilitated by the seamless integration of a spin filter. Originally developed in Germany, this technology has gained global traction, with several Japanese institutions now spearheading unique research programs. In this presentation, we review the current state of spin-resolved measurements and outline future challenges for this advanced instrumentation. We highlight recent developments at the UVSOR Synchrotron Facility, where PMM has been optimized for sub-GeV light sources via a grazing-incidence SX beamline (BL6U) and a new VUV branch (BL7U). The latter features a normal-incidence geometry designed for full-hemisphere photoemission spectroscopy. We present valence band studies using various polarizations and discuss how PMM is expanding the frontiers of photoemission spectroscopy at compact synchrotron facilities.

15:25 - 15:50

Development of a LINAC-Based LEPD System and Current Status of its SATLEED-Based Analysis Code

Ken Wada, Institute of Materials Structure Science, High-Energy Accelerator Research Organization (KEK).

A practical low-energy positron diffraction (LEPD) station for precise determination of surface atomic arrangements has been developed at the Slow Positron Facility (SPF), KEK. LEPD is the positron counterpart of low-energy electron diffraction (LEED) and enables experiments at normal incidence to the sample surface. This geometry is advantageous for future studies targeting small crystalline domains with a narrow beam.

Owing to the absence of electron-exchange terms, LEPD yields smoothly varying positron–atom scattering factors resembling those in X-ray diffraction. Forward shadowing, rather than LEED-like forward focusing, suppresses multiple scattering along atomic chains and enhances sensitivity to the topmost atomic layers.

This presentation will summarize the development of the current LEPD station and describe positron diffraction calculations based on the standard Barbieri/Van Hove symmetrized automated LEED (SATLEED) package, with the charge sign reversed and the exchange term removed.

15:50 - 16:15

Detection of Hydrogen Atoms Adsorbed on a Ceria Surface Using Total-Reflection High-Energy Positron Diffraction (TRHEPD)

Izumi Mochizuki, The Slow-Positron Facility (SPF), Institute of Materials Structure Science, High-Energy Accelerator Research Organization (KEK).

Total-reflection high-energy positron diffraction (TRHEPD) is the positron counterpart of reflection high-energy electron diffraction (RHEED), which provides a technique for precisely determining the topmost atomic-layer structure assembled on various crystalline surfaces. The TRHEPD station at the Slow-Positron Facility (SPF) is publicly available under the framework of collaborative research programs for shared use of KEK-PF (including SPF). In this presentation, we show that the TRHEPD exhibits an exceedingly high sensitivity to the position of the atoms existing on the topmost surface, capable of detecting even hydrogen (H) atoms precisely. We have successfully determined the three-dimensional coordinates of the location of the H atoms adsorbed on a ceria (CeO_2) surface through the TRHEPD rocking-curve analysis. This will provide a key method for locating H atoms adsorbed on materials surfaces, supplying essential information for understanding a variety of functional properties associated with H adsorption.

16:25 - 16:50

Quantitative Surface Structure Determination Using LEPD and Multiprobe Studies at the Slow Positron Facility, KEK

Rezwan Ahmed, Synchrotron Radiation Science Division I, Institute of Materials Structure Science, High-Energy Accelerator Research Organization, (KEK).

A practical Low-Energy Positron Diffraction (LEPD) system has been developed at the Slow Positron Facility (SPF), enabling precise determination of surface atomic structures. Using a high-intensity LINAC-based slow-positron beam with a newly developed experimental station, more than 100 LEPD patterns can be recorded within a few hours by scanning the incident energy. From these patterns, intensities of inequivalent diffraction spots are extracted as a function of energy to construct LEPD I-V datasets for quantitative structure analysis. LEPD I-V analyses on metal surfaces including Cu(001), Cu(111), Ni(111), Ag(111), Pt(111), and Pd(111) show markedly improved agreement between experiment and dynamical diffraction calculations compared with conventional LEED I-V studies. In addition, multiprobe studies combining LEPD and ARPES have been initiated using the same sample transferred under ultra-high vacuum from SPF to the Photon Factory at the KEK Tsukuba campus. These efforts provide a pathway toward an integrated LEPD-DFT-ARPES methodology for comprehensive surface characterization.

16:50 - 17:15

Experimental Study of Positronium Diffraction Using Graphene

Yugo Nagata, Riki Mikami, Yasuyuki Nagashima, Department of Physics, Tokyo University of Science.

Positronium (Ps), a bound state of an electron and a positron, has a small mass and is electrically neutral. If the Ps could be applied to surface crystal diffraction like positron diffraction experiments, it might enable structure analysis of insulator and magnetic surfaces. However, there have been no attempts of Ps diffraction experiments so far because it was technically difficult to produce fast and coherent Ps beams.

In recent years, a high-quality energy-tunable Ps beam has been developed in Tokyo University of Science. The energy spread is around 2% and the angular divergence is less than 0.3 degrees. The beam energy lies in the keV region and is suitable for applying on the crystal diffraction. We used a self-standing graphene target and succeeded in observing transmission diffraction patterns of the Ps passing through the graphene. We present details of the experiment and the Ps diffraction patterns.