The Development of High-Energy X-ray Total Scattering Method at Beijing Synchrotron Radiation Facility

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Abstract

As a powerful probe for local structure analysis, high energy X-ray total scattering method has been widely used in condensed matter physics, materials science and other fields. With a super-conducting wiggler (SCW) and sagittal focusing monochromator, a high energy X-ray total scattering apparatus has been developed at 3W1 beamline of Beijing Synchrotron Radiation Facility, BSRF, a first-generation synchrotron source. The total scattering apparatus mainly consists of a large two-dimensional flat-panel detector and high-energy X-rays of 50-70 keV, enabling total scattering measurements to be carried out for pair distribution function (PDF) analysis with a Q range of 0.5-25 A-1. Based on this apparatus, a series of in-situ devices were developed, data with good signal-to-noise ratio were obtained and analyzed. Demonstration results for the observation of perovskite oxides with various A-site doping and bioactive glasses upon annealing were introduced. Notably, the PDF method can provide detailed local structural information of amorphous materials, liquids and structural disorder in crystalline materials. This work offers a guideline for people who consider developing and using total scattering methods at other synchrotron facilities.

Full Text

Preamble

The development of a high-energy X-ray total scattering method at the Beijing Synchrotron Radiation Facility∗

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As a powerful probe for local structure analysis, the high-energy X-ray total scattering method has been widely used in condensed matter physics, materials science, and other fields. With a superconducting wiggler (SCW) and sagittal focusing monochromator, a high-energy X-ray total scattering apparatus has been developed at the 3W1 beamline of the Beijing Synchrotron Radiation Facility (BSRF), a first-generation synchrotron source. The total scattering apparatus mainly consists of a large two-dimensional flat-panel detector and high-energy X-rays of 50–70 keV, enabling total scattering measurements for pair distribution function (PDF) analysis with a Q range of 0.5–25 $Å^{-1}$. Based on this apparatus, a series of in-situ devices were developed, and data with good signal-to-noise ratio were obtained and analyzed. Demonstration results for the observation of perovskite oxides with various A-site doping and bioactive glasses upon annealing are presented. Notably, the PDF method can provide detailed local structural information of amorphous materials, liquids, and structural disorder in crystalline materials. This work offers a guideline for people considering developing and using total scattering methods at other synchrotron facilities.

Keywords: High energy X-ray, Total scattering, Beijing Synchrotron Radiation Facility, Pair distribution function

Introduction

Bragg diffraction provides a powerful experimental approach to probe atomic-scale structures. This technique reveals the average long-range order in crystalline materials by leveraging the fundamental principle of lattice periodicity. However, relying solely on long-range structural information is insufficient for comprehensive material characterization. On one hand, almost all crystals are imperfect, meaning various inevitable defects exist, such as point defects, dislocations, and chemical inhomogeneity [1]. Many properties of crystalline materials are strongly dependent on the local disorder structure. On the other hand, materials with amorphous nature preclude Bragg diffraction and necessitate alternative approaches to understanding their local structure [2, 3].

There are several local structure probes, such as extended X-ray absorption fine structure (EXAFS) [4], nuclear magnetic resonance (NMR), Raman spectroscopy [5, 6], and so on. Of all the local structure detection techniques, pair distribution function (PDF) based on high-energy X-ray total scattering has gained much more attention because of its in-situ device capabilities and good signal-to-noise ratio. Total scattering technique is the measurement of the complete diffraction pattern, including both Bragg and diffuse components, using synchrotron high-energy X-rays throughout reciprocal space and covering a wide range of momentum transfer (Q). The weighted probability that atoms might be found at certain distances from other atoms, named PDF, can be obtained

from total scattering measurements.

The resolution of the PDF method is determined by the maximum Q value, Qmax (Δr 2π/Qmax). Qmax is limited by the wavelength of X-ray (λ), the area of the detector, and the distance from sample to detector, since Q = 4π sin /λ, where 2 is the scattering angle. It is essential to decrease λ to obtain larger Qmax. In addition to the wavelength of incident X-ray, high flux is needed to detect weak signals at high Q due to the rapid decrease of scattering length with increasing Q value. Meanwhile, lower background is required, so a well-collimated light source and a thin container with easily removed signal are necessary.

The advent of synchrotron-based radiation sources provides X-rays with high intensity and short wavelength, making accurate and reliable PDF data available. Up to now, a series of beamlines with total scattering capability have been built, e.g., beamline I15-1 at Diamond Light Source (DLS) [7], beamline Powder Diffraction (PD) at the Australian Synchrotron [8], beamline 28-ID-1 at National Synchrotron Light Source II (NSLS-II) [9], beamline BL04B2 at Super Photon ring-8 (SPring-8) [10], and ID11 and ID15A of European Synchrotron Radiation Facility (ESRF) [11, 12].

It is worth mentioning that ESRF completed its Extremely Brilliant Source (EBS) upgrade in 2022, which represents a new generation of synchrotron. In the last few decades, the total scattering method has been widely utilized in the structural study of liquids (including melts) [13–16], amorphous materials [13, 17], disordered crystalline materials [18, 19], and so on. It is worth pointing out that PDF has played a key role in understanding local structure, which is fundamentally important for amorphous and disordered systems.

The Beijing Synchrotron Radiation Facility (BSRF) is a first-generation synchrotron source with electron energy in the storage ring of 2.5 GeV in dedicated mode. BSRF operates in two modes: dedicated mode and parasitic mode. To utilize the parasitic mode, the original biological macromolecule crystallography station was moved to the 1W2 straight section, and 3W1 was transformed into a high-energy beamline station. In 2019, a superconducting wiggler (SCW) was successfully installed in the 3W1 beamline of BSRF, replacing the original permanent magnetic wiggler and offering a wider energy range from 40 keV to 80 keV with sufficiently high flux. These upgrades have prompted us to develop a high-energy X-ray total scattering apparatus at the 3W1 beamline.

The aim of this study was to report the optimization process of this device and benchmark total scattering measurements carried out at this beamline, demonstrating what can be offered to our user community.

Theoretical Basis

[Figure 1: see original paper]. Scattering triangle of wavevectors of a typical total scattering experiment [20].

The scattering triangle of wavevectors in a typical total scattering experiment is shown in fig.1, where **k** and **k**f represent the momentum before scattering and after scattering, respectively. The scattering intensity includes both elastic scattering and inelastic scattering, but elastic scattering plays a major role and determines the diffraction pattern. Here we assume that there was no energy exchange between the incident quantum and sample, such that $|\mathbf{k}| = |\mathbf{kf}| = 2\pi/\lambda$. **Q** is the scattering vector, **Q** = **k** - **k**f. For isotropic samples, $|\mathbf{Q}| =$ Q. As such, the scattering vector Q is related to the incident wavelength λ and scattering angle 2 via: $Q = 2|\mathbf{k}| \sin = 4\pi \sin /\lambda$.

In a scattering experiment, the structure factor, S(Q), is related to the measured differential scattering cross section, I(Q) [21]:

$$S(Q) - 1 = \frac{I(Q) - \langle \sum_i c_i f_i^2(Q) \rangle - C(Q)}{\langle \sum_i c_i f_i(Q) \rangle^2}$$

where c is the atomic fraction of element i, f (Q) the X-ray atomic form factor, and C(Q) the inelastic (Compton) scattering contribution. The pair distribution function G(r) can be calculated by Fourier transformation of S(Q) via:

$$G(r) - 1 = \frac{1}{2\pi^2 r\rho} \int_{Q_{\min}}^{Q_{\max}} Q[S(Q) - 1] \sin(Qr) dQ$$

where Qmin and Qmax represent the finite range in reciprocal space used during Fourier Transform, which is limited by the Q range of the instrument, and is the atomic number density in $Å^{-3}$ [22]. Except for G(r), the total density function D(r) and total correlation function T(r) are often used in publications [21], where D(r) = 4 r[G(r) - 1] and T(r) = 4 rG(r). Peaks in T(r) indicate the existence of atoms with a density exceeding the average number density at a distance r, whereas a valley suggests the absence of atoms.

Light Source Parameters

The total scattering method was designed and developed at the 3W1 beamline of BSRF. Currently, 3W1 is the only beamline that can provide high-energy (E > 50 keV) X-ray flux at BSRF, equipped with a 2.3 T superconducting wiggler. A sagittal focusing monochromator with a Si (111) crystal was placed 32 meters away from the source. With horizontal focusing of the monochromator, the beam size before the beam-defining slit (slit 1 in fig.3) is 1.7(H) mm × 2.9(V) mm. The photon energy is in the range of 50–70 keV and the energy resolution is better than 0.65%. The beam is optimized by adjusting the bending radius of the second crystal before the total scattering experiment. Calculated photon flux and Q-space resolution of the 3W1 beamline are shown in fig.2. From fig.2(b), subtle differences for $\Delta Q/Q$ at three energies and a value of 0.3% at high Q region can meet the requirement of PDF experiments in many cases.

[Figure 2: see original paper]. (a) Calculated photon flux of BSRF 3W1 beamline (blue dashed line); (b) Measured (symbol lines) and calculated (lines) FWHM of selected peaks from the 50 keV, 60 keV and 70 keV total scattering data shown as ΔQ/Q.

Apparatus Optimization Process

A. Experimental Setup

High-energy X-ray total scattering experiments were designed and conducted in the range 50–70 keV (wavelengths from 0.247–0.178 Å). Obtaining a clean background is quite important before a total scattering experiment, as the background signal needs to be reliably subtracted during data processing. Weak background signal is crucial for weak signal samples, e.g., thin films, nano-materials, and other disordered systems. Here we utilized several pairs of slits and an evacuated stainless-steel tube with Kapton windows to decrease parasitic scattering and air scattering. Before the experiment, all optics were carefully aligned.

The first set of slits (labeled A in fig.3) close to the incoming beam was used to define the beam size and shape. The beam-defining slit was composed of four tungsten blades with a thickness of 2 mm, and the blade positions could be adjusted by high-precision slides, thus defining the beam size to 0.5–0.8 mm. Parasitic scattering produced by the beam-defining slit was unavoidable, so a clean-up slit (C in fig.3) was designed to eliminate the parasitic scattering from slit 1. In the meantime, two lead shields with a thickness of 3 mm were installed just after slit 1 and slit 2 to reduce background radiation. An evacuated stainless-steel tube with a pressure of 10 Torr was designed to reduce background from air scatter. Another clean-up slit (F in fig.3) and a large lead shield were placed just in front of the sample to remove scatter or diffraction generated by upstream devices.

At the beginning of the total scattering apparatus design and construction, a Mar345 detector was utilized and placed 180 mm downstream of the sample. To increase experimental efficiency and obtain a larger Qmax value, we upgraded the detector to Mercu 1717HS, which is a high-speed large two-dimensional flat-panel detector that combines a pixelated detector with a CsI sensor and features 139 μm pitch pixels, 3072 × 3048-pixel submodule arrangement, generating a large effective area of 17 × 17 inches. With Mercu 1717HS, a sample-to-detector distance of 180 mm and an energy of 60 keV, a Qmax of 25 $Å^{-1}$ could be obtained.

It is worth mentioning that, benefiting from the high frame rate of Mercu 1717HS (30 fps), it is possible to collect total scattering and diffraction data on subsecond timescales, although the data quality might not be sufficient due to the low photon flux. XRD patterns of 304 stainless steel during remelting process were collected with a temporal resolution of 0.1 s.

B. Determination of Incident X-Ray Energy

The most important parameter in PDF experiments, Qmax, is limited by the instrument and affected by the energy of the light source. The higher the energy, the larger Qmax value that can be achieved, while the scattering factor of X-ray decreases rapidly with increasing Q value. To obtain large Qmax and detect weak signals at high Q region, high energy and high flux are usually required. As shown in fig.2a, there is still high flux at energies $>$ 50 keV, though the photon flux decreases with increasing energy. Therefore, the data quality at 50 keV was first tested, then gradually increased to 60 keV and 70 keV. The selection of energy points was determined by comparing comprehensive data quality.

Energy calibration was achieved using a 'two distances method' : (1) adjusting the sagittal monochromator to the target energy; (2) using a standard LaB_6 sample and the distance between detector and sample to calibrate the energy preliminarily; (3) moving the sample station by motor with a known distance; (4) calculating scattering angle 2 according to the geometrical relation of two positions of LaB_6, and the exact energy using Bragg' s equation.

[Figure 3: see original paper]. Schematic layout and photographs of a typical high-energy scattering setup at 3W1 beamline of BSRF. A: beam-defining slit (slit 1); B: lead shield 1; C: clean-up slit (slit 2); D: lead shield 2; E: evacuated stainless steel tube with mylar windows; F: clean-up slit (slit 3); G: lead shield 3; H: sample station; I: beamstop; J: detector

[Figure 4: see original paper]. (a) The X-ray total structure factors S(Q) and (b) pair distribution functions G(r) of CeO_2 at 50 keV, 60 keV and 70 keV with an exposure time of 60 s using a mar345 detector. Note that the same Qmax of 22 $Å^{-1}$ was used during the Fourier Transform and the peak intensity amplitudes of the three datasets were normalized.

Diffraction patterns of CeO_2 at three energy points were collected with an exposure time of 60 s using a Mar345 detector. The X-ray total structure factor S(Q) and pair distribution functions G(r) are displayed in fig.4. The maximum Q value of the instrument at 50 keV, 60 keV and 70 keV is 25, 27 and 32 $Å^{-1}$, respectively. From the perspective of Qmax, 70 keV is a good choice. However, in the high Q range, the oscillation of 70 keV S(Q) is more severe than at 50 keV and 60 keV as the flux is lower. From the perspectives of both signal-to-noise ratio and Qmax, and considering the small fluctuation of low r region (fig.4b), 60 keV was selected as the target energy for total scattering experiments. If necessary, the energy can be adjusted in the range of 50–70 keV.

Benchmark Results

A. Ex-Situ Total Scattering Experiment of High-Entropy Perovskite Oxides

For ex-situ experiments, samples were collected with Kapton tapes and glued to an aluminum alloy frame with an aluminum-tungsten-aluminum 'sandwich' configuration to suppress stray light. The sample station repeatability is controlled at an accuracy of 0.1 mm by changing samples with a magnetic base. The Mercu 1717HS detector was placed 200 mm downstream of the sample. The setup was calibrated using the diffraction pattern of polycrystalline CeO_2 powder. The measurement procedure was controlled by iDetector software and an exposure time of 20 s was set. Background patterns were collected with the same setup and exposure time. The raw diffraction data were reduced from two-dimensional images and corrected for the effects of polarization and geometry using the program Fit2D [23]. The absorption, geometry, detector effect, and normalization procedure were carried out using PDFgetX3 [24].

As a typical perovskite thermoelectric oxide, $SrTiO_3$ displays relatively good electrical properties [25]. The total scattering method was utilized to interpret the structure-property relationship of $SrTiO_3$-based oxides with different A-site doping (La, Ba, Ca, and Pb). The X-ray total structure factors S(Q) and pair distribution functions G(r) of $SrTiO_3$-based oxides with various A-site doping are shown in fig.5. To explore more detailed structural information, 3D structural models were derived using RMC simulation [26]. The starting configuration consisting of 5000 atoms was created. Several types of constraints were added: atom-atom approaches, Ti-O connectivity (all titanium atoms were coordinated to a certain number of oxygen atoms up to 2.5 Å). The choice of these constraints was determined to avoid physically unrealistic structures. Structural information is derived from counting the atomic configurations generated by RMC simulations.

From the total scattering experiment and RMC simulation results, A-O and Ti-O bond lengths for $SrTiO_3$-based perovskite oxides (ABO_3) of different entropies designed at A sites were extracted to calculate the tolerance factor t via equation $t = \text{length(A-O)}/[\sqrt{2} \times \text{length(B-O)}]$. The tolerance factor is a key parameter in perovskites to reflect the correlation between the relative size relationship of elements and structural symmetry, and the extent of the t value deviating from 1 describes the extent of symmetry breaking [27]. In this work, with t approaching 1, the mobility recovered, meaning that the tolerance factor helps explain why A-site entropy engineering could enhance the weighted mobility and decouple the carrier-phonon transport by only tuning the average element sizes to tailor the symmetry and Ti displacement, revealing the structural origin of mobility recovery. This work was published in Nature Communications, in cooperation with Tsinghua University [28].

[Figure 5: see original paper]. (a) The X-ray total structure factors S(Q) and (b) pair distribution functions G(r) for $SrTiO_3$-based perovskite oxides with various

A-site doping collected at 3W1 beamline of BSRF.

B. In-Situ Heating High-Energy Total Scattering Experiments

High-temperature experiments are among the most common and important for condensed matter physics and materials structure research. For example, the structural response of glasses to temperature and/or pressure is closely pertinent to ionic transport properties, relaxation, and glass-forming transition. PDF is one of the most effective means to characterize the local order and connectivity of glass, so in-situ heating PDF experiments were used to study the response of different glass structures to temperature. As shown in fig.6a, coupled with high-energy synchrotron radiation, a high-temperature and high-pressure device was designed with a large exit angle 2 $>$ 40°, with temperature up to 873 K and pressure to 40 atm (BEIJING OPERANDO TECHNOLOGY CO., LTD).

[Figure 6: see original paper]. (a) Photography of the high-temperature and high-pressure device installed at 3W1 beamline, (b) X-ray total structure factors S(Q) and (c) pair distribution functions G(r) of bioactive glasses at different temperatures.

Bioactive glasses are extensively utilized in orthopedics and dentistry. The structural rearrangement upon heating is a key factor in determining its processability. Here, in cooperation with Shanghai Jiao Tong University, we tracked the structural changes of Hench' s composition glass [29] using in-situ high-energy X-ray total scattering, and the results are presented in fig.6b and 6c. As shown in fig.6b, the first sharp diffraction peak (FSDP) exhibits minimal variation upon heating, indicating that the medium-range order Si-O-Si rings/chains maintain approximate rigidity and cannot be depolymerized by heating below Tg. This subtle change of FSDP is also observed in real-space structural correlations (as depicted by the G(r) plot in panel (c)). The shoulder peak around 3.2 Å remains almost constant, implying that the Si-Si packing is intact, thereby suggesting that these large Si-O-Si rings or chains are rigid. In contrast to the FSDP, the second peak in S(Q) patterns undergoes considerable change with increasing temperature, indicating nonnegligible rearrangement of short-range order (SRO) local structures upon heating. The changes of the SRO structures can be intuitively visualized in G(r) patterns, as the intensities of peaks at 2.4 Å and 3.6 Å decrease markedly at high-temperature conditions, elucidating that the modifier-oxygen and modifier-cation interactions will be much weakened upon heating.

C. Total Scattering Coupled with Raman Spectra and Acoustic Levitator

X-ray total scattering can realize atomic-scale observation, and Raman spectroscopy is sensitive to chemical species in solution. To obtain chemical species information and local atomic structural evolution of solutions under low gravity conditions, a multi-modal platform integrating an acoustic levitator, portable

Raman spectrometer, and high-energy X-ray total scattering was constructed to study the structure of levitated aqueous solution droplets. The schematic of the multi-modal platform is shown in fig.7a. During the experiment, solutions were injected as 0.5 mm^3-2 mm^3 droplets, and the X-ray beam and Raman spectrometer were focused on the same droplet simultaneously. Several colored droplets are shown in the inset of fig.7b for visual clarity, although the detected solutions are colorless. The scattering and Raman spectra data of aqueous M_2SO_4 (M = Li, Na, K) solutions are shown in fig.7b and 7c, respectively.

This method is expected to be used in the study of precious samples (1.0 L) and in-situ observation of chemical reactions in solution. It is noteworthy that, combined with laser heating and temperature-controlled systems, the levitation device is applicable for detecting the microstructure of high-temperature melts in a container-free environment, eliminating heterogeneous nucleation at the melt-container interface and increasing the propensity for supercooling. A humidity control system is also available, demonstrating the potential for in-situ studies on the evaporation and crystallization processes of aqueous droplets. The levitation platform was established in cooperation with Qinghai Institute of Salt Lakes, Chinese Academy of Sciences. More research work is referred to in publications by Yongquan Zhou et al. [30–32].

[Figure 7: see original paper]. (a) Schematic of the main components of an acoustic levitator; (b) total scattering patterns with an exposure time of 30 s and (c) Raman spectrum of 2 mol/L Li_2SO_4 aqueous solution droplet, the inset shows several levitated droplets.

D. In-Situ Tensile Testing of NiTi and Multi-Principal Element Alloys (MPEAs)

Apart from total scattering experiments, high-energy diffraction experiments coupled with an in-situ tensile frame were also conducted with a longer sample-to-detector distance of about 800 mm, an energy of 60.05 keV, and a beam size of 0.7 × 0.7 mm. A Gatan microtension tester equipped with a home-built tensile jig was used for tensile testing. The in-situ tensile tests were performed with a strain rate of 1×10^{-3} s^{-1}. The schematic of in-situ tensile testing and raw diffraction patterns of SLM-NiTi alloy during different loading conditions are shown in fig.8a. Two-dimensional diffraction patterns were converted into one-dimensional high-energy XRD diffraction spectra by caking and integrating over a $±$5° range along specified azimuth angles (fig.8b), and the diffraction peaks were fitted to a Gaussian distribution.

Utilizing the testing and diffraction methods mentioned above, we investigated the anisotropic phase transition, deformation behaviors, and orientation evolution of additively manufactured NiTi alloy during loading, in cooperation with Shanghai University. These results also help understand the competition between stress-induced phase transformation and dislocation slip in AMed NiTi alloys. We refer the reader to relevant publications [33–35], where Pengyue Gao

et al. explored the stress-induced phase transformation and lattice correspondence in NiTi shape memory alloy during deformation using in-situ high-energy synchrotron X-ray diffraction. In addition, the dislocation density of refractory multi-principal element alloys (MPEAs) under tension was determined according to the Williamson–Hall method, shedding light on the synergistic combination of ultrahigh strength and large tensile ductility in these advanced materials [36–39].

[Figure 8: see original paper]. (a) Schematic of in-situ tensile testing, diffraction patterns of SLM-NiTi alloy during loading with an exposure time of 3 s, and the integration area shown in blue; (b) diffraction patterns integrated along azimuth angle of 5° to -5°, peaks of martensite and austenite marked as short vertical blue and red lines, respectively.

Conclusions

The high-energy X-ray total scattering setups developed at the 3W1 beamline of BSRF are described in this paper. With an energy of 60 keV and a large-area detector, large amounts of high-quality data were obtained and utilized in related research. The apparatus is compatible with different environments, such as a magnetic field of 2 T, a self-designed heating furnace with a temperature range of 293–873 K and pressure of 40 atm, a tensile frame with a maximum tension of 2 kN and temperature of 823 K. This work demonstrates that the total scattering apparatus at 3W1 is able to collect PDF data with good signal-to-noise ratio for amorphous and disordered crystalline materials. It is worthwhile to mention that beamline scientists at BSRF are working on building a new synchrotron light source located in Huairou, Beijing, China.

Perspectives of Total Scattering Techniques at HEPS

The High Energy Photon Source (HEPS), the first fourth-generation synchrotron light source in Asia, will be completed by the end of 2025. HEPS will accelerate electrons up to energies of 6 GeV and produce high-energy beams that can probe samples at nanometer scales. Its time resolution will be 10,000 times better than that achieved by third-generation synchrotrons [40]. There are several beamlines providing total scattering capability at HEPS, e.g., Structural Dynamics, Engineering Materials, and High Pressure beamlines.

The Structural Dynamics Beamline (SDB) of HEPS is dedicated to elucidating the dynamic behavior and structural transformations of materials under varying conditions. SDB provides dual advantages of high energy (70 keV) and high flux (10^{15} ph/s), allowing for both typical PDF measurements and time-resolved PDF requirements, with a Qmax up to 25 $Å^{-1}$ and 18 $Å^{-1}$, respectively, by using a large-area detector and direct detector at MHz rates. Additionally, aerodynamic and ultrasound levitation techniques will be combined with the PDF method at SDB to study the structure of liquids, melts, and pharmaceutical drugs under containerless conditions.

The Engineering Materials Beamline (EMB) provides high-energy X-ray beams with an energy of 100 keV, which is suitable for conducting typical PDF experiments with larger Qmax and better spatial resolution. The High Pressure Beamline (HPB) is featured for high-pressure experiments, where the PDF method can be combined with high-pressure techniques to study the behavior of systems under extreme conditions at monochromatic beams between 20 and 75 keV with a flux of 10^{12} ph/s. It is worth mentioning that both the Engineering Materials and High Pressure Beamlines possess Eiger2 XE 16M detectors, which will help users collect diffraction data with better signal-to-noise ratio. At the High Pressure and Structural Dynamics Beamlines, X-ray beams will be focused to microscale, holding great promise for detecting solid-liquid interface structures during processes such as crystal growth, electro-catalysis, and so on. More information about HEPS beamlines can be found online at: https://www.ihep.ac.cn/dkxzz/HEPS/xmgk/HEPSjj/.

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Note: Figure translations are in progress. See original paper for figures.