Spectral Characteristics of Dual-Period Elliptically Polarized Undulators

Authors: Zou Ying, Zhenhua Chen, Junqin Li, Huang Yaobo, Yong Wang, Zhang Wei, Zhou Qiaogen, Ding Hong, Tai Renzhong

Date: 2025-04-30T16:28:01+00:00

Abstract

Angle-resolved photoemission spectroscopy (ARPES) is a direct experimental method for studying the electronic structure of materials. ARPES based on synchrotron radiation enables three-dimensional electronic structure analysis and investigation of the electronic structure of material surfaces ($_{20}$200 eV) or bulk phases (~>200 eV) through tuning of the incident photon energy. However, due to limitations in magnetic field period and strength, single-period undulators cannot cover the aforementioned required photon energy range. The Shanghai Synchrotron Radiation Facility pioneered the dual-period juxtaposed out-of-vacuum hybrid undulator—the Dual-period Elliptically Polarized Undulator (DEPU). This paper presents the measured relationship between magnetic gap and energy region, as well as the application results, for the DEPU commissioned at the SSRF beamline BL09U ("Dreamline").

Full Text

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Vol. 36, No. 1
January 2013

NUCLEAR TECHNIQUES Vol. 36, No. 1 January 2013

The Energy Spectral Performance of a Double Elliptically Polarized Undulator

ZOU Ying[1], CHEN Zhenhua[1], LI Junqin[1], HUANG Yaobo[1], *WANG Yong*[1], *ZHANG Wei*[1], *ZHOU Qiaogen*[1], *DING Hong*[2], *TAI Renzhong*[1]
[1](Shanghai Advanced Research Institute, Chinese Academy of Science, Shanghai

201204, China)
[2](Shanghai Jiaotong University, Shanghai 201800, China)

Abstract

Angle-resolved photoemission spectroscopy (ARPES) is a direct experimental method for studying the electronic structure of materials. ARPES based on synchrotron radiation can perform three-dimensional electronic structure analysis and investigate the electronic structure of material surfaces (~20–200 eV) or bulk phases (~>200 eV) by tuning the incident photon energy. However, due to limitations in magnetic field period and intensity, a single-period undulator cannot cover the required photon energy ranges mentioned above. The Shanghai Synchrotron Radiation Facility (SSRF) pioneered the development of a double-period elliptically polarized undulator (DEPU)—a vacuum-external hybrid undulator with two periods arranged in parallel. This paper presents the measured relationship between magnetic gap and energy domain for the DEPU deployed at the SSRF beamline BL09U (Dreamline), along with its application performance.

Keywords: Undulator, Gap, ARPES, Photon energy
CLC: TL50, TL99

Angle-resolved photoemission spectroscopy (ARPES) is an experimental technique based on the photoelectric effect, involving photon injection and electron emission. ARPES can directly probe electronic band structures in momentum space and is an indispensable tool for studying complex systems such as high-temperature superconductors [1-2], spintronic materials [3], topological quantum materials [4-5], and dilute magnetic semiconductors [6]. In the widely used deep ultraviolet (EUV) and soft X-ray energy ranges (e.g., 10–200 eV), the photoelectron escape depth in solids is only a few angstroms [7], meaning ARPES experiments in this energy range possess high surface sensitivity. To probe material interiors, longer-wavelength radiation or soft X-ray excitation must be used, both of which offer greater escape depths. While high energy resolution is easily achieved at longer wavelengths, the momentum space detection range is limited due to lower photon energies (typically smaller than the Brillouin zone of representative materials). Soft X-ray photons in the ~1000 eV range enable bulk-sensitive measurements covering multiple Brillouin zones while simultaneously providing high momentum resolution perpendicular to the sample surface, thus offering greater advantages.

Third-generation synchrotron radiation insertion devices, particularly in-vacuum undulators, have become important sources for VUV and soft X-ray synchrotron radiation. However, a single undulator cannot cover both energy ranges: simulations using SPECTRA [8] show that undulators with periods above 100 mm cover fundamental energies below 200 eV, while those with ~50 mm periods cover fundamental energies around 1000 eV. Using two undulators with different periods arranged in parallel and switching between them horizontally represents an effective method for expanding the energy range. BESSY II in Germany employed this parallel double-period configuration for in-vacuum undulators, extending X-ray energy coverage to 70 eV–15 keV [9].

To meet the research demands of frontier condensed matter physics for studying both surface and bulk electronic structures, the Shanghai Synchrotron Radiation Facility (SSRF) [10] first implemented a vacuum-external double-period parallel undulator (DEPU) in the soft X-ray beamline BL09U (also known as Dreamline), as shown in [Figure 1: see original paper]. The low-energy insertion device (LEID) with a period length of 148 mm generates low-energy photons (h $<$ 250 eV), while the high-energy insertion device (HEID) with a period length of 58 mm generates high-energy photons (h $>$ 250 eV). Both undulators have approximately the same magnet array length of about 5 meters, share a common support structure, and can be moved transversely (perpendicular to the accelerator electron beam direction). The two undulators are positioned side-by-side in the straight section, allowing easy switching without obstructing the electron beam.

The magnetic design, specific mechanical structure, and magnetic field characteristics of both undulators have been reported in previous studies [11-12]. [Figure 2: see original paper] shows the theoretical simulation of flux versus photon energy from the two insertion devices at a beam current of 300 mA, after the white slit. The white slit aperture uses typical experimental settings (3000 m × 1000 m) with a bandwidth of 10^{-4}. The flux for both insertion devices in circular polarization state is higher than that in horizontal linear polarization state.

This study utilizes the operational SSRF BL09U beamline and experimental station located downstream of the parallel undulator to measure the spectral characteristics of the undulator, compare them with theoretical expectations, and demonstrate the effectiveness of using both low- and high-energy photons in user experiments.

1 Test Equipment and Scheme

The layout of beamline BL09U used to test the DEPU spectral characteristics is shown in [Figure 3: see original paper] [13]. Synchrotron radiation from the double-period undulator (DEPU) passes through the crenellated wall, then through a white slit with adjustable aperture size. After pre-reflection by a plane mirror (M1) that deflects the beam horizontally by 1.2°, absorbs heat load, and suppresses higher-order harmonics, the radiation enters a plane grating monochromator (PGM). This monochromator features an internally cooled plane mirror plus four variable-line-spacing gratings for dispersing the white synchrotron radiation. The central line densities of each grating are 400 L/mm (LEG), 800 L/mm (MEG), 1200 L/mm (HEG), and 3600 L/mm (VEG). The LEG/MEG gratings are used for low-energy photon monochromatization, while

HEG/VEG gratings are used for high-energy photon monochromatization. The monochromatized beam passes through a downstream deflection mirror (M2) into different experimental station branches, each equipped with a monochromatic slit (Mono Slit) to select appropriate bandwidth in conjunction with the upstream grating monochromator. Following the monochromatic slit is the key apparatus for measuring spectral characteristics—the ionization chamber, which contains a microchannel plate for photon energy calibration via measurement of ionization excitation (absorption) spectra of high-purity characteristic gases. The ionization chamber also houses a photodiode that can be inserted into the beam path for photon flux measurement. The structure and testing method of the ionization chamber are described in [14]. Downstream of the ionization chamber on each branch, a set of post-focus mirrors focuses the beam onto the sample position at the respective experimental station.

As shown in [Figure 4: see original paper], based on the above beamline layout, the total transmission efficiency from the beamline to the sample point (ARPES) is presented, combining the efficiencies of M1, the grating monochromator, and the two post-focus mirrors. In the plane mirror efficiency calculation, the grazing incidence angles of M1 and the two post-focus mirrors are set to 1.2°, 1.5°, and 1.25°, respectively. For the grating monochromator diffraction efficiency calculation, the incidence angles of the plane mirror and grating are set according to the variable included angle method, with the LEG grating selected for the LEID energy range and the HEG grating selected for the HEID energy range. The figure shows that transmission efficiency in the low-energy region is on the order of 10%, while in the high-energy region it drops to ~1% due to the high line-density HEG grating.

2 Energy Calibration

To characterize both low- and high-energy domains, this study measured the double ionization excitation spectrum of argon 3s3p6np, argon 2p ionization excitation, nitrogen 1s ionization excitation, and neon 1s ionization excitation spectra, comparing them with reported spectral peak energy values from literature [15-18].

2.1 Low-Energy Undulator Calibration

The expected energy range of the low-energy undulator (LEID) is 20–250 eV. In this range, the low-energy end can be calibrated using argon 3s3p6np double ionization excitation lines near 29 eV, while the high-energy end can be calibrated using argon 2p level ionization excitation lines near 245 eV [15].

As shown in [Figure 5: see original paper], using the low-energy undulator at GAP = 30.5 mm with a 400-line grating, white slit aperture of 1200 m × 2400 m, and monochromatic slit aperture of 30 m, the measured argon double ionization excitation spectrum shows the entire double ionization excitation series resolved up to n = 23 high-order transitions. Comparing the energy position of the n = 10 high-order transition peak with literature yields a measured value of 28.903 eV versus a literature value [15] of 29.043 eV, giving an energy deviation of Δ = -0.14 eV.

[Figure 6: see original paper] shows the argon 2p level ionization excitation spectrum measured using the low-energy undulator at GAP = 80.2 mm with a 400-line grating, white slit aperture of 700 m × 2050 m, and monochromatic slit aperture of 20 m. This spectrum includes transitions from spin configurations $2\mathrm{p}_3/_2$, $2\mathrm{p}_1/_2$ to the 4s level, as well as transitions to Rydberg states. The $2\mathrm{p}_3/_2$\$→\$4s excitation peak appears at 243.1 eV, compared to the literature value [15] of 244.3 eV, giving Δ = -1.2 eV.

These two test results demonstrate that the LEID undulator, within its operating gap range, provides fundamental wave energy that well covers the photon energy interval of 29–244 eV.

2.2 High-Energy Calibration

The expected energy range of the high-energy undulator (HEID) is 200–2000 eV. In this range, the low-energy end can be calibrated using nitrogen 1s level ionization excitation lines near 400 eV [16,18], while the high-energy end can be calibrated using neon 1s level ionization excitation lines near 867 eV [17,18].

As shown in [Figure 7: see original paper], using the high-energy undulator at GAP = 24.3 mm with a 1200-line grating, white slit aperture of 200 m × 1460 m, and monochromatic slit aperture of 30 m, the measured nitrogen 1s level ionization excitation spectrum shows multiple vibrational-rotational level peaks characteristic of nitrogen-edge excitation. The first peak appears at 398.6 eV, compared to literature values [16,18] of 400.8 eV, giving Δ = -2.2 eV.

[Figure 8: see original paper] shows the neon 1s ionization excitation to Rydberg states np measured using the high-energy undulator at GAP = 34.45 mm with a 1200-line grating, white slit aperture of 150 m × 350 m, and monochromatic slit aperture of 10 m. The first peak appears at 861.8 eV, compared to literature values [17,18] of 867.1 eV, giving Δ = -5.3 eV.

These results demonstrate that the HEID undulator, within its operating gap range, provides fundamental wave energy covering the photon energy interval of 400–870 eV. Broader photon energy coverage will be presented below in combination with gap-fundamental (third harmonic) energy position relationships and flux variations.

3 Gap-Energy Correspondence

After energy calibration, the undulator gap can be gradually adjusted while scanning the monochromator (energy). A photodiode in the ionization chamber downstream of the monochromatic slit measures the energy position of the fundamental main peak's maximum intensity, thereby determining the actual gap-energy correspondence. Using the photodiode photocurrent under this main peak irradiation, the photon flux at the corresponding energy can be obtained via the following formula [19]:

$$\text{Flux} = \frac{I \times e}{E_p \times I_{BC} \times 66.3}$$

where I is the photocurrent recorded by the photodiode (A), e is the elementary charge 1.6$×10^{-19}$ C, E is the energy position of the main peak (eV), and *I_{BC}* is the actual beam current during measurement (mA).

Since the emission angle of the fundamental wave changes with undulator gap adjustment, the white slit size must be correspondingly adjusted to maintain a 4σ aperture. [Figure 9: see original paper] shows the horizontal (X) and vertical (Y) 4σ emission angles of the fundamental waves from both LEID/HEID undulators and the corresponding aperture sizes at the downstream white slit. The figure shows that LEID's 4σ emission angle continuously changes throughout its entire energy range (~20–250 eV). For HEID, the 4σ emission angle changes dramatically below 400 eV but stabilizes above 400 eV.

LEID Gap-Energy Relationship

As shown in [Figure 10: see original paper], scanning GAP from 22–80 mm for the low-energy undulator using a 400-line grating, the relationship between each gap value and the corresponding fundamental main peak energy position was measured using a photodiode. The dashed line represents the relationship simulated from the undulator magnet array [12]. The measured correspondence follows theoretical expectations, showing that the fundamental energy interval provided by this undulator's gap variation well covers 22–250 eV, satisfying low-energy undulator requirements.

[Figure 11: see original paper] shows the flux variation with main peak energy for the low-energy undulator using LEG/MEG gratings. Below 100 eV, the LEG (300-line) grating flux is below 10^{12} ph/s; above 100 eV, this grating's flux gradually falls below 10^{12} ph/s, while the MEG (800-line) grating maintains flux well above 10^{12} ph/s.

HEID Gap-Energy Relationship

As shown in [Figure 12: see original paper], scanning GAP from 22–58 mm for the high-energy undulator using a 1200-line grating, the relationship between each gap value and the corresponding fundamental and third harmonic energy positions was measured using a photodiode. The dashed line represents the relationship simulated from the undulator magnet array [12]. The measured correspondence follows theoretical expectations, showing that the fundamental energy interval effectively covers 250–1700 eV; for energies between 1700–2000 eV, the third harmonic must be used to better meet requirements.

[Figure 13: see original paper] shows the flux variation with main peak energy for the high-energy undulator using HEG/VEG gratings. Using the HEG grating, flux above 10^{12} ph/s can be obtained below 800 eV. For energies above 1400 eV, the fundamental provides less flux than the third harmonic, so experiments in this higher energy range should utilize the third harmonic for better performance.

4 ARPES Results Demonstration

The SSRF BL09U (Dreamline) passed technical acceptance in October 2014 and began trial operation. The advantages of the double-period undulator in providing photon energies from EUV to soft X-ray (20–2000 eV) for probing both surface and bulk electronic states were subsequently validated in user research. For example, a team from the Institute of Physics, Chinese Academy of Sciences, used ARPES based on Dreamline with 30–60 eV EUV light (LEID) to resolve the theoretically predicted surface-state Fermi arcs characteristic of Weyl fermions in the solid material tantalum arsenide [20], becoming one of the first teams internationally to discover this novel fermionic state. Additionally, using 300–1000 eV soft X-rays (HEID), the team detected bulk electronic structures with triple-degeneracy characteristics in topological semimetals molybdenum phosphide and silicon carbide [21-22]. In studies of unconventional chiral fermion materials like cobalt silicide [23], the team used UV light below 30–110 eV from LEID to resolve surface Fermi arcs while simultaneously using 300–600 eV soft X-rays from HEID to probe bulk chiral electronic structures, successfully discovering this exotic electronic structure for the first time internationally. A series of similar studies [5] have demonstrated that the double-period undulator achieves its intended performance.

The double-period undulator achieves coverage of low-energy (20–200 eV) and high-energy (>200 eV) photons from the EUV to soft X-ray energy domain. The measured flux agrees in magnitude with theoretical simulations, and combined with ARPES and other techniques, enables depth-resolved electronic structure studies of materials.

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