

Optical design of the time-resolved ARPES beamline of the new material spectroscopy experimental station for the update of CAEP THz-FEL facility

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INSTRUMENTATION AND MEASUREMENT

Optical design of the time-resolved ARPES beamline of the new material spectroscopy experimental station for the update of CAEP THz-FEL facility

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The Chinese Academy of Engineering Physics Terahertz Free Electron Laser Facility (CAEP THz FEL, CTFEL) is the only high-average power free electron laser terahertz source based on superconducting accelerators in China. The update of the CTFEL is now undergoing and will expand the frequency range from 0.1–4.2 THz to 0.1–125 THz. Two experimental stations for material spectroscopy and biomedicine will be built. A high harmonic generation (HHG) lightsource based beamline at the material spectroscopy experimental station for time-resolved angle-resolved photoemission spectroscopy (ARPES) research will be constructed and the optical design is presented. The HHG lightsource covers the extreme ultraviolet (XUV) photon energy range of 20–50 eV. A Czerny–Turner monochromator with two plane gratings worked in conical diffraction configuration is employed to maintain the transmission efficiency and preserve the pulse time duration. The calculated beamline transmission efficiency is better than 5% in the whole photon energy range. To our knowledge, this is the first time in China to combine THz-infrared FEL with HHG light source, and this experimental station will be a powerful and effective instrument that will give new research opportunities in the future for users doing research on the dynamic evolution of the excited electron band structure of a material's surface.

Keywords: high harmonic generation (HHG), femtosecond extreme ultraviolet pulse, conical diffraction, grating monochromator, transient, spectral experiment

PACS: 42.65.Ky, 42.65.Re, 32.80.Rm, 32.80.Wr **DOI:** 10.1088/1674-1056/ad73b1

1. Introduction

Free electron lasers (FELs) are one of the most powerful tools as a terahertz lightsource and have many advantages, such as high average power, full coherence, linear polarization, continuously tunable frequency, and so on.[1] A lot of FEL facilities, such as FELIX in Holland, ELBE in Germany and Novo FEL in Russia, have played important roles in the THz sciences.[2–4] The Chinese Academy of Engineering Physics Terahertz Free Electron Laser Facility (CTFEL) is the first high average power terahertz FEL facility based on superconducting accelerators in China, covering the frequency range of 0.1–4.2 THz. The highest repetition rate of CTFEL is 54.17 MHz. The first lasing of CTFEL was achieved in August 29, 2017. Since the opening for users in 2018, more than 40 experiments have been done, covering the research fields of material property analysis, terahertz spectrum, terahertz devices, terahertz biological effects, electron beam application, flash radiotherapy, and so on. In order to meet more science applications, CTFEL will be updated to cover a much wider frequency range of 0.1–125 THz.[5]

In recent decades, ARPES has gained a unique ability to study the binding energy and the momentum of the electrons in materials. The extension of time resolved ARPES (trARPES) provides invaluable insights into the nonequilibrium state of matter that cannot be observed in steady state.[6–9] The probe lightsource used in trARPES can be generated by nonlinear optical effect (NOE) or high harmonic generation (HHG). HHG can generate extreme ultraviolet (XUV) source (> 20 eV), while NOE is typically smaller than 7 eV.[10–16] In most of the existing trARPES instruments, the lasers that generate the HHG source are also used for pumping, limiting the research fields to weakly correlated systems.[17] Strong fields such as strong THz fields for driving surface states are needed for research of strongly correlated systems. Some experiments that drive surface states with THz fields have been done and outstanding results have been achieved.[8] However, the driving THz fields were also generated based on the lasers that generate the HHG sources and the THz fields are limited to several limited frequencies in these works.

Two experimental stations for material spectroscopy and biomedicine will be built in the updated CTFEL project. The material spectroscopy experimental station will be a time-resolved comprehensive research platform that can be used for multi-mode transient characterization of electronic band structure, superconducting energy gap, transient conductivity, and so on. A HHG based trARPES beamline will be constructed in the new material spectroscopy experimental station. Both the laser that generates the HHG source and the THz/IR FEL can be chosen for driving the surface states. The continuously tunable frequency of CTFEL provides more choices for the design of physical experiments. To our knowledge, this is the

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first to combine THz/IR FEL with HHG based trARPES in China. This new experimental station will give new opportunities for research on the dynamic evolution of the excited electron band structure of a material's surface.[7] The optical design of the beamline is described in the following section.

2. Beamline overview

Figure 1 shows an overview of the optical design of the trARPES beamline, which consists of three major sections: (1) HHG lightsource, (2) plane grating monochromator, and (3) experimental chamber. At the HHG lightsource section, a Ti:sapphire laser amplifier with a central wavelength of 800 nm (i.e., 1.55 eV), a pulse duration of 40 fs, and a max pulse energy of 13 mJ at 1 kHz repetition rate is used to drive a HHG process and produce coherent XUV laser pulses. A Czerny–Turner monochromator with two plane gratings worked in conical diffraction configuration, and an adjustable exit slit is used to select the required harmonic and further narrow the energy resolution. A gold-coated plane mirror mounted on a motorized linear stage and placed in front of the slit will reflect the focused harmonics to the XUV CCD detector when inserted into the beam. An XUV photodiode is used to detect the selected XUV laser pulse energy and a phosphor screen is used for position detection. Then, the selected XUV pulse will be focused to the experimental chamber by the gold coated toroidal mirror 3 operating at an incidence angle of 85°. The light from the Ti:sapphire laser amplifier and the THz/IR FEL pulse will also be transferred to the ARPES experimental chamber for pumping. When the THz/IR FEL is chosen, the frequency of the THz/IR FEL will be adjusted to be consistent with the Ti:sapphire laser amplifier. A signal produced by the Ti:sapphire laser amplifier will be sent to the FEL accelerator for synchronization and the synchronization accuracy can reach picosecond order. The resulting setup of the HHG based beamline will achieve a typical operating performance at a photon energy range of 20–50 eV, a photon flux well than 1×10^9 photons/s and a time resolution of better than 500 fs. Below, we describe the HHG lightsource and the optical design of the monochromator in more detail.

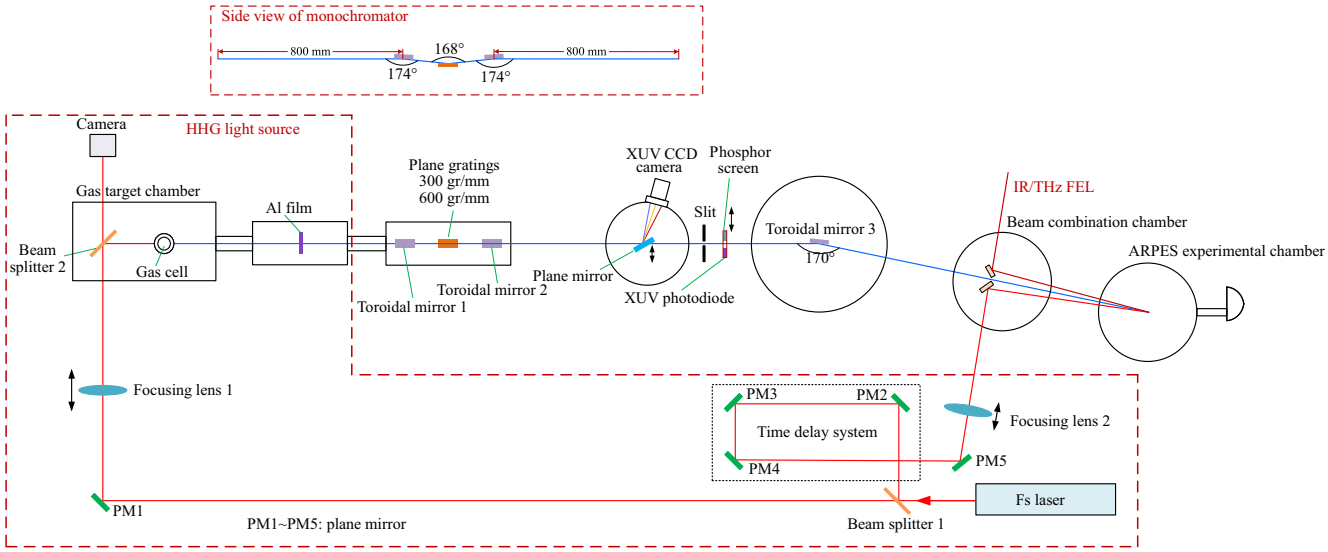


Fig. 1. Layout of the optical system.

3. HHG lightsource

HHG is a nonlinear process in which high order odd harmonics of the driving fundamental frequency pulses are coherently generated, typically in the XUV region of 10–100 eV. In our setup, as shown in Fig. 1, a beam splitter with a reflection/transmission ratio of 90/10 is used to separate the incident laser into two beams. The reflection beam is focused to the ARPES experimental chamber for pumping through a time delay system and a focusing lens. The transmission beam then propagates through a plane mirror, a focusing lens, a beam splitter with a reflection/transmission ratio of 90/10 and finally focuses in the cell which is located in the gas target chamber for generating high harmonics. A camera located at the equivalent position of the focal point of the transmission laser is used for focal beam diagnosis. After the gas target chamber, a film with a thickness of 200 nm Al is used to filter out the fundamental frequency light. The transmission efficiency is shown in Fig. 2.

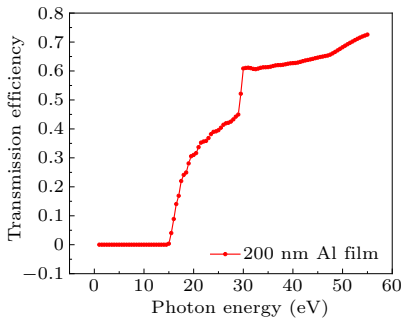


Fig. 2. Transmission efficiency of 200 nm Al film.

4. Conical diffraction monochromator

Since the photon energy of the laser amplifier is 1.55 eV (i.e., 800 nm), the monochromator photon energy resolution should be better than 3.0 eV to separate the different harmonics, while ensuring short pulse duration and high flux throughput. As depicted in Figs. 1 and 3, inspired by the time-preserving single-grating concept of Luca Poletto's group,[18,19] in our setup, a Czerny–Turner type monochromator with a pair of gold-coated toroidal mirrors $1/2$ and two plane gratings operated in conical diffraction is chosen. During the operation, the toroidal mirrors $1/2$ with a focal length $f = 800$ mm, working at an grazing incident angle of 3°, can collimate the incident light from the HHG source and focus the diffracted light after grating on the exit slit. The mirrors are operated at equal angles and unity magnification to minimize aberrations at the output. To select the photon energy, the grating is rotated around an axis that is tangent to the surface, parallel to the grooves, and passes through the grating center.

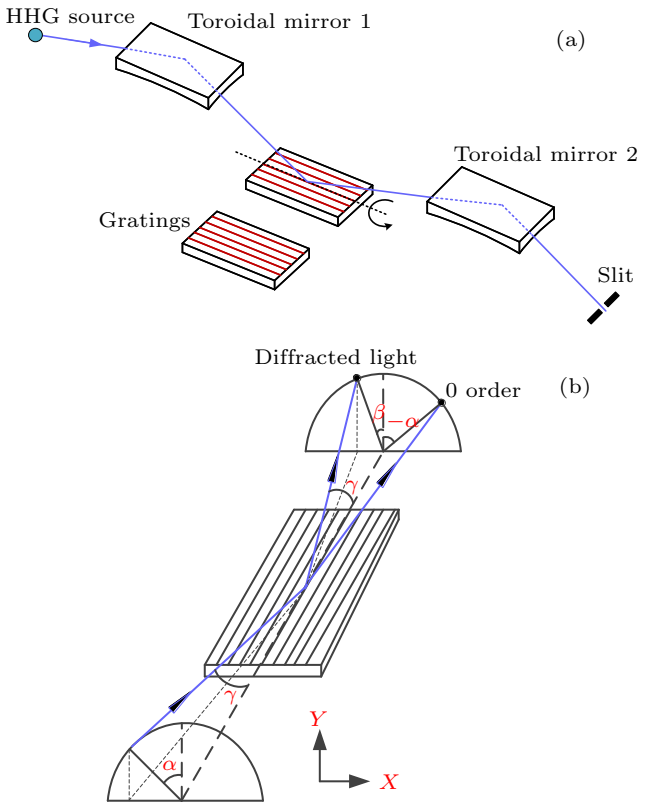


Fig. 3. Layout of the conical diffraction monochromator: (a) optical layout of monochromator; (b) light diffracted by a conical diffraction mounted grating.

As shown in Fig. 3(b), in the conical diffraction configuration, the direction of the incident ray is defined by the altitude angle γ (the angle between the direction of the incident ray and the direction of the grooves) and the azimuth angle α, which is zero if they lie in the plane perpendicular to the grating surface and parallel to the rulings. Let β define the azimuth of the diffracted light at wavelength λ and diffraction order m, the grating equation is written as

$$\sin\gamma(\sin\alpha + \sin\beta) = mn\lambda, \tag{1}$$

where n is the groove density. In our setup, $\alpha = \beta$, and the gratings operate at $+1$ diffraction order, the grating equation then is written as

$$2\sin\gamma\sin\alpha = n\lambda. \tag{2}$$

Two commercial Au coated blazed gratings with groove densities of 1200 gr/mm and 600 gr/mm respectively are chosen for the monochromator to cover the photon energy range of 20–50 eV, considering the efficiency, the energy separating ability, and the cost. The altitude angle γ of the gratings is set to be 6°. Optical elements of the monochromator are summarized in Table 1.

Table 1. Parameters of the optical elements of the monochromator.

Spectral region	20–50 eV	
Toroidal mirror 1/2	coating material	Au
	long radius R (mm)	30571.72
	short radius ρ (mm)	83.74
	angle of incidence (°)	87
Grating 1	coating material	Au
	photon energy region (eV)	30–50
	groove density (gr/mm)	1200
	blazed angle (°)	7.9
Grating 2	coating material	Au
	photon energy region (eV)	20–40
	groove density (gr/mm)	600
	blazed angle (°)	13.9

The main advantages of the conical diffraction mount of the grating are that it preserves time for pulsed duration and has high diffraction efficiency. According to the previous studies, the diffraction efficiency of the grating with the conical diffraction mount is close to the reflectivity of the grating's coating, which is much higher than the classical grating mount in the extreme ultraviolet photon energy region.[20,21] The calculated reflectivity of the mirrors and the diffraction efficiency of the gratings are shown in Figs. 4 and 5, respectively. As shown, the reflectivity of the toroidal mirror $1/2$ is better than 80% and the toroidal mirror 3 is better than 70% in the whole photon energy range. The peak diffraction efficiency of the gratings is better than 60% close to the Au coated mirrors working in 6° grazing incidence angle. The calculated total transmission efficiency of the system from source to sample (including the Al filter, three toroidal mirrors and a grating) is better than 5% in the designed photon energy range. The calculated result is shown in Fig. 6.

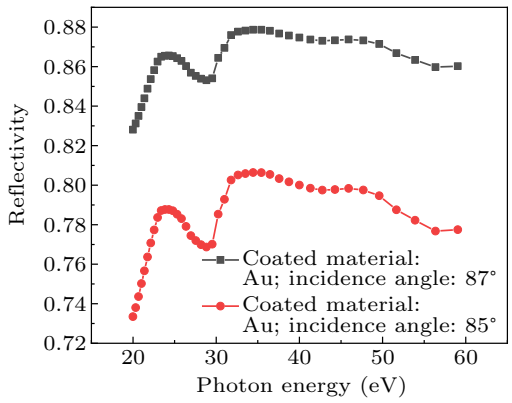


Fig. 4. Calculated reflectivity of the mirrors.

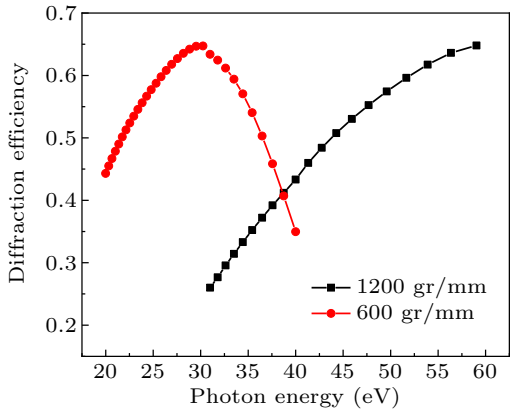


Fig. 5. Calculated diffraction efficiency of the gratings.

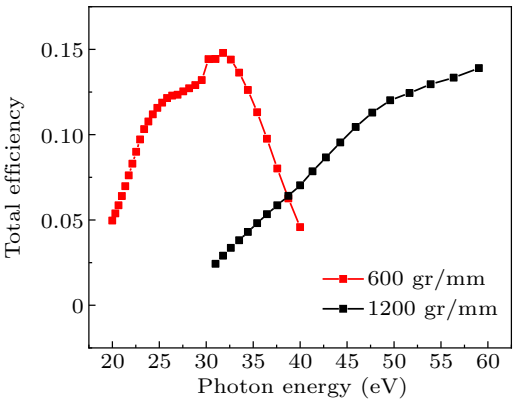


Fig. 6. Calculated total efficiency of the beamline.

The pulse temporal half-width caused by grating diffraction is expressed as

$$\Delta t \cong \frac{1/2Nm\lambda}{c} = \frac{p\cdot\Delta\theta\cdot n}{2\cos\alpha}\cdot\frac{m\lambda}{c}, \tag{3}$$

where N is the number of illuminated grooves and p is the incident arm length of the toroidal mirror 1, which is 800 mm in this setup. $\Delta\theta$ is the divergence angle of the HHG source, which is set to be 10 mrad in this design. The angle α is usually larger than 80° in a classical diffraction mount, which makes the pulse temporal broadening much larger than in conical diffraction mount, in which the angle α is only a few degrees. The calculated time broadening caused by grating diffraction is shown in Fig. 7 and the peak time broadening is less than 500 fs.

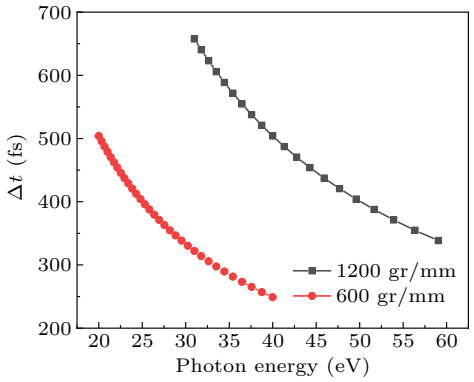


Fig. 7. Calculated time broadening caused by grating diffraction.

From grating aberration theory, the major contributions to the energy broadening are from source size, optical aberrations of toroidal mirrors, exit slit width, slope error of the optical elements, and the diffraction limit. In this designed beamline, the source size and exit slit width have the greatest impact and are considered. In this design, the source size S_1 is set to be 0.1 mm and the slit width S_2 is equal because of the symmetrical configuration. The slope errors of the three optical elements of the monochromator are designed to be RMS 1.0″. The calculated resolving power of the monochromator is shown in Fig. 8, and is better than 50 in the whole photon energy range, meeting the requirement for separating the harmonics.

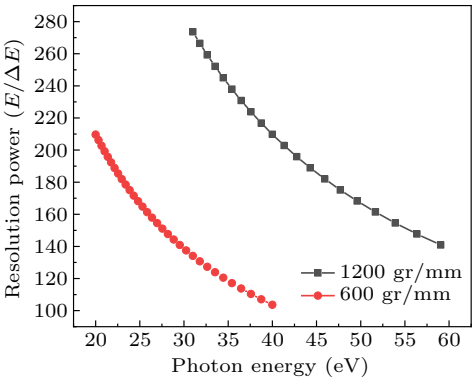


Fig. 8. Calculated spectral resolution power of the monochromator.

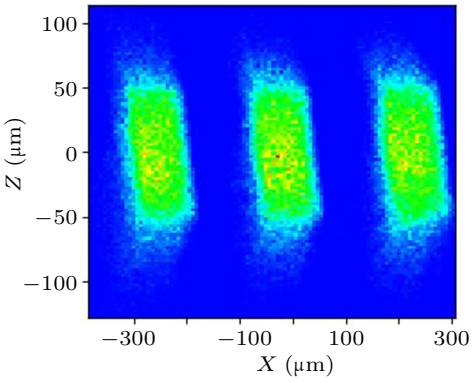


Fig. 9. Ray tracing simulation result (50±0.5 eV, 1200 gr/mm).

The performance simulation of the beamline is done with the simulation software OASYS[22] and the typical result is shown in Fig. 8. We can see that a resolution power of 100@50 eV can be obtained.

5. ARPES experimental chamber

The ARPES experimental chamber consists of six main parts: a UV lamp, a sample transfer system, a cryogenic sample stage, a hemispherical electron analyzer, a vacuum chamber, a hemispherical electron analyzer, and some auxiliary equipment. The UV lamp covers a photon energy range of 8.4 eV–40.8 eV, and will be used for calibration of the system and static ARPES experiments. The cryogenic sample stage has a translation accuracy better than 0.05 mm and a lowest temperature lower than 10 K. The temperature of the sample stage can be controlled continuously with an accuracy better than ± 0.1 K. The vacuum chamber will be equipped with two groups of molecular pumps, vacuum measurement, and residual gas analysis systems, getting an ultimate vacuum better than 5×10^{-9} mbar. The hemispherical electron analyzer is the key equipment and the energy resolution is set to be better than 5 meV.

6. Conclusion and perspectives

The optical design of the HHG based trARPES beamline at the new material spectroscopy experimental station for the update of CAEP THz-FEL facility is described in detail and the ARPES experimental chamber is briefly introduced. This beamline covers an energy range of 20–50 eV and a Czerny–Turner monochromator operated in conical diffraction is adopted. The beamline can be expanded to wider energy range by adding another grating with different groove densities. The overall efficiency of the beamline from source to sample is better than 5%. Combined with the THz/IR FEL, this beamline can be useful for further studies in the ultrafast dynamic evolution of the excited electron band structure of a material's surface.

Acknowledgement

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