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Design of a MeV ultra-fast electron diffraction experiment at Tsinghua university*

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Abstract Time-resolved MeV ultra-fast electron diffraction (UED) is a powerful tool for structure dynamics studies. In this paper, we present a design of a MeV UED facility based on a photocathode RF gun at Tsinghua University. Electron beam qualities are optimized with numerical simulations, indicating that resolutions of 250 fs and 0.01 Å, and bunch charge exceeding 10^5 electrons are expected with technically achievable machine parameters. Status of experiment preparation is also presented.

Key words ultra-fast electron diffraction, MeV, photocathode RF gun

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1 Introduction

Electron diffraction has long been a powerful tool for micro-structures studies, since Mark and Wierl[1] using electrons produced a diffraction pattern of gas-phase CCl_4 molecules in 1930. In 1980s, conventional electron diffraction was integrated with ultra-fast laser technologies. This combination, named ultra-fast electron diffraction (UED), opened the door to structures dynamics studies with time-resolved capacity on pico-second time scales. During the last two decades, several laboratories[2—4] further developed UED theories and technologies, and produced many exciting results of fundamental importance[5—8].

UED features several characteristics[9] compared with ultra-fast X-ray diffraction. First, the elastic scattering cross-section of electrons with molecules is some six orders of magnitude higher than that of X-ray photons[10]. This feature makes electrons well-suited for surface, thin samples, and gas-phase sample studies. Second, compared with ultra-fast, high brightness X-ray facilities such as the 3rd generation synchrotron light sources, free-electron lasers, and Thomson scattering sources, UED apparatuses are much more compact and affordable. Also, electrons are less damaging to samples than X-ray photons per useful (elastic) scattering event[11].

State-of-the-art UED apparatuses employ photocathde DC guns which generate ps (or shorter), tens of keV electron pulses. With these keV UED systems, it is routine to achieve 1 ps and 0.01 Åresolutions, while still challenging to reach a temporal resolution of 100 fs, the fundamental time scale of atomic motions. The limitation arises from space charge forces of electrons, which expand the pulse duration rather fast at the relatively low energy of tens of keV. Based on several apparatus performances[4, 5, 7], the number of electrons contained in a 100 fs, keV pulse are extrapolated to be less than 1000, indicating a long exposure time, a large amount of samples, and a stringent requirement of system stability.

To relieve the space charge induced limitation, Wang[12] proposed employing MeV high brightness electron pulses from a photo-cathode RF gun for UED experiments. By increasing the electron energy from keV to MeV, the space charge effects are dramatically

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reduced. A proof-of-principle MeV UED experiment was accomplished[13], and several groups, including NSLS SDL[14], UCLA[15], and Tsinghua, are building MeV UED systems with improved performances.

In this paper, we present the design and status of a time-resolved MeV UED system at the accelerator laboratory of Tsinghua University. Simulation studies indicate that resolutions of 250 fs and 0.01 Å, and bunch charge exceeding 10^5 electrons are expected with technically achievable machine parameters.

2 System layout and simulations

2.1 Facility overview

Layout of the Tsinghua MeV UED facility is shown in Fig. 1. An ultra-fast laser system generates short UV pulses for electrons production, and also IR pulses for samples pumping. An S-band BNL/SLAC/UCLA type photo-cathode RF gun is used to generate MeV, high quality electron pulses. The magnetic solenoid controls the emittance and spot-size of electron pulses along the beam-line, and normally sends a parallel beam into samples. Several chambers are placed downstream of the solenoid for UV laser incidence, electron pulses diagnostics, and samples holding. The sample is desired to be as close to photo-cathode as possible, allowing a minimum time for space charge induced pulses expanding. We also include an S-band RF deflecting cavity[16] to measure the pulse length and arriving time of electron pulses. After a distance of free drift after scattering, the diffracted electrons are detected by a high QE phosphor-CCD assembly, while the un-scatterd electrons pass through a hole in the center of the detector assembly and enter a spectrometer for energy and energy spread monitoring.

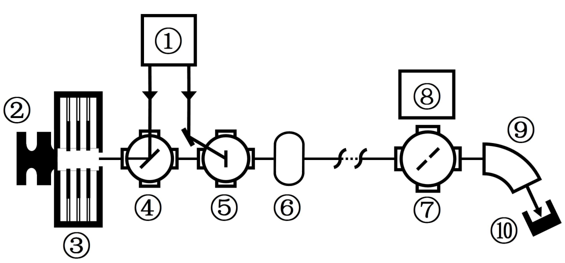

Fig. 1. Layout of the MeV UED facility at Tsinghua (not to scale). 1: ultra-fast laser system; 2: photocathode RF gun; 3: magnetic solenoid; 4: laser incidence chamber; 5: sample chamber; 6: RF deflecting cavity; 7: detector chamber; 8: detector; 9: spectrometer dipole; 10: electron beam dump. The RF power system and laser-RF timing system are not shown here.

2.2 Simulation and design parameters

The optimized electron pulses qualities and main machine parameters are listed in Table 1. We use the code PARMELA[17] to simulate the dynamics of electrons subject to RF field, magnetic field, and their self-fields, and the kinetic theory[18, 19] to model the scattering process of electrons on the sample (an aluminum foil of 100 nm thickness).

Table 1. Tsinghua MeV UED facility parameters.

physical dimension	
from gun cathode to sample	76 cm
from sample to detector	350 cm
initial electron pulses	
bunch length/(Gaussian, rms)	300 fs
bunch radius/(uniform, hard-edge)	0.2 mm
bunch charge	2×10^5 e$^-$
main machine parameters	
repetition rate	10 Hz
gun RF field amplitude	41 MV/m
electron pulse launching phase	5°
gun solenoid strength	968 Gauss
electron pulses parameters at sample	
electron kinetic energy	1.82 MeV
relative energy spread	6.7×10^{-4}
pulse duration (rms)	123 fs
spot-size (rms)	173 μm
divergence (rms)	45 μrad

Our strategy for system optimization is as follows: we first fix initial electron dimensions, then adjust the bunch charge, and other parameters, including RF amplitude, electron pulse launching phase, and solenoid strength, until an optimized diffraction pattern is obtained. Subsequently, we adjust the bunch charge, and then the initial spot-size. We repeat this iterative process many times, and achieve overall resolutions of 250 fs and 0.01 Å. Also, significance of each parameter to overall system performance is illustrated.

Initial electron pulse duration is chosen to be 300 fs rms, for this number is suited to achieve ~100 fs or shorter pulses at the sample due to bunch compression effect in a photo-cathode RF gun[20], and to contain as many electrons as possible. The choice of initial transverse spot-size is compromised between achieving a small spot-size at the sample and a higher bunch charge. In analogy to optics, finite source size leads to smearing of diffraction patterns, thus a small size at the sample is preferred.

As parameters listed in Table 1, we operate electron pulses in an ultra-short, ultra-low charge regime. According to theory[21] and our simulation results, the

RF induced emittance growth is negligible for ultra-short pulse length, and space charge induced emittance growth is negligible for ultra-low charge. Thus total emittance is dominated by the thermal value, obtained during the photoemission process.

In Fig. 2 we show the diffraction pattern and corresponding scattering intensity obtained with the parameters listed in Table 1. Angular position of each ring is given by Bragg's law as $\theta \propto \beta^{-1}\gamma^{-1}$, while the width of each ring is determined by the electron pulse spot-size and divergence, which changes slowly with γ. It is then evident that γ should be lowered to 'sharpen' diffraction rings, while kept high enough to relieve the space charge effects.

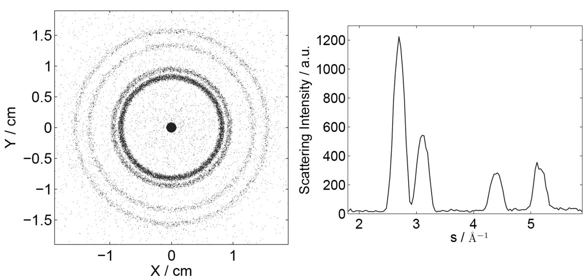

Fig. 2. Simulated diffraction pattern and corresponding scattering intensity with parameters listed in Table 1. In the diffraction pattern, un-scattered electrons form the bright spot in center, and multiple-scattered electrons contribute as smeared background.

Performances of a MeV UED system are summarized in terms of spatial and temporal resolutions. The precision of a diffraction ring position on detector is normally limited by the CCD pixel size, and corresponds to a precision of micro-structures of 0.01 Å. Regarding the temporal resolution $\tau = (\tau_l^2+\tau_e^2+\tau_{\rm jitter}^2+\tau_{\rm vm}^2)^{1/2}$, where τ_l and τ_l are the lengths of pump laser and probe electron pulses respectively, $\tau_{\rm jitter}$ is induced by the RF amplitude fluctuation and RF-laser timing jitter which are of 150 fs and 100 fs respectively with currently available techniques, and $\tau_{\rm vm}$[22] is negligible for thin foil and can be compensated by tilting laser pulses[23]. All these contributions sum to an overall temporal resolution of 250 fs.

3 Status of experiment preparation

A more detailed description of main subsystems can be found in Ref. [24]. The ultra-fast laser is now under commissioning. The RF power system, the photo-cathode RF gun, and the RF deflecting cavity are ready for RF conditioning. Beam-line components installation and alignments are to start soon at the time we prepare this paper. We foresee a MeV UED experiment later this year.

4 Summary

In this paper, we introduce the MeV UED and present a design of such a facility at Tsinghua. We optimize a MeV UED with numerical simulations, and achieve 250 fs, 0.01 Å resolutions with currently available machine parameters. We discuss considerations on the choices of some main electron pulses and machine parameters. Experiment preparation is in progress. We expect an experiment demonstration and comparison with simulations, and to further improve such a compact, powerful scientific tool.

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References

1 Mark H, Wierl R. Naturwissenschaften, 1930, **18**: 205
2 Zewail A H. Annu. Rev. Phys. Chem., 2006, **57**: 65 and references therein
3 Dwyer J R et al. Phil. Trans. R. Soc. A, 2006, **364**: 741 and references therein
4 CAO J et al. Appl. Phys. Lett., 2003, **83**: 1044
5 Ihee H et al. Science, 2001, **291**: 458
6 Baum P, YANG D S, Zewail A H. Science, 2007, **318**: 788
7 Siwick B J et al. Science, 2003, **302**: 1382
8 Nie S H et al. Phys. Rev. Lett., 2006, **96**: 025901
9 Srinivasan R et al. Helv. Chim. Acta, 2003, **86**: 1763 and references therein
10 Hargittai I. In: Stereochemical Applications of Gas-Phase Electron Diffraction, Part A: The Electron Diffraction Technique. eds. Hargittai I, Hargittai M. New York: VCH, 1988. 1
11 Henderson R. Q. Rev. Biophys., 1995, **28**: 171
12 WANG X J et al. J. Korean Phys. Soc., 2006, **48**: 390
13 Hastings J B et al. Appl. Phys. Lett., 2006, **89**: 184109
14 WANG X J. private communications
15 Musumeci P, Moody J T, Scoby C M. Ultramicroscopy, 2008, doi:10.1016/j.ultramic.2008.03.011
16 SHI J R et al. these proceedings
17 Young L. PARMELA Manual, LA-UR-96-1835, 1996
18 Salvat F. Phys. Rev. A, 1990, **43**: 578
19 LI X Z. Ultramicroscopy, 2004, **99**: 257
20 WANG X J, QIU X, Ben-Zvi I. Phys. Rev. E, 1996, **54**: R3121
21 Kim K J. Nucl. Instrum. Methods Phys. Res., Sect. A, 1989, **275**: 201
22 Williamson J C. Ph.D. Thesis, California Institute of Technology, 1998
23 Baum P, Zewail A H. Proc. Natl. Acad. Sci. USA, 2006, **103**: 16105
24 TANG C X et al. these proceedings