FEMTO-SECONDS ELECTRON BEAM DIFFRACTION USING PHOTOCATHODE RF GUN*

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Abstract

One of the 21st century scientific frontiers is to explore the molecule structure transition in the femto-second time scale. X-ray free electron laser (XFEL) is one of the tools now under development for investigating femto-second structure transition. We are proposing an alternative technique – femto-second electron diffraction based on the photocathode RF gun. We will present a design of a kHz femto-seconds electron diffraction system based on the photocathode RF gun. Our simulation shows that, photocathode RF gun can produce 100 fs (FWHM) electron bunch with millions electrons at about 2 MeV. This is at least one order of magnitude reduction in bunch length, and two orders of magnitude increase in number of electrons comparing to present DC electron diffraction system. We will also discuss various issues and limitations related to MeV electron diffraction.

INTRODUCTION

X-ray and electron are two most powerful tools for characterizing atomic and molecular structures. The recent development of electron storage ring based X-ray source and electron microscope made it possible to observe the ultra-small world with Å resolution [1,2]. On the other hand, development of the laser technologies, especially picosecond (10^{-12} s) and femtosecond (10^{-15}) lasers, made it possible of observing the ultra-fast process [3].

Directly observation of structure transition and molecular dynamics process, such as chemical bond breaking, is one of the fundamental issues in nano-science, chemistry, biology and many other scientific endeavours. Such capability demands the marriage of ultra-small technologies, such as X-ray and electron diffraction, and ultra-fast technolgies. X-ray free electron laser (FEL) now being developed in US and Germany [4,5] is one of the examples of such marriage. Ultra-fast electron diffraction (UED) [3, 6] has been developed to investigate the ultra-fast structure transition.

X-ray and Electron diffraction are two complementary technologies. For example, X-ray diffraction is better suit for large angle diffraction; while electron diffraction is the choice for small angle diffraction. The Thompson scattering cross section is dominating contributing factor for X-ray diffraction while it is the Rutherford scattering cross section for electron diffraction. The difference between x-ray and electron scattering arises from the scattering operator L:[7]

$$\text{X-ray diffraction:} \quad L_x = \sum_i e^{i\mathbf{s}\mathbf{r}_i}$$

$$\text{Electron diffraction:} \quad L_e = \sum_j Z_j e^{i\mathbf{s}\mathbf{R}_j} - \sum_i e^{i\mathbf{s}\mathbf{r}_i}$$

The sums in these formulas stretch over all particles of a molecule. Where s is the magnitude of the momentum transfer vector, Z_j is the nuclear charge of atom j, and the distances R_j and r_i are over the nuclei j and electrons i, respectively. It can be seen that the x-ray diffraction signal is the Fourier transform of the electron density distribution within a molecule. The electron diffraction signal is the Fourier transform of nuclear and electronic charge distributions. For gas molecule and charge density distribution characterization, electron diffraction is widely used because of large interaction cross section. Electron diffraction is also relative compact and less harmful to bio-molecules.

Using a streak camera tube, 100 ps time resolution was realized in the initial UED setup [6] (Fig.1). A single laser is used for both electron beam generation and pump the sample under investigation. Most advances in UED are due to the progress of the laser technologies in the last twenty years. The state of art UED has time resolution on the order of several ps with 10^4 electrons [8]. Since molecular structure transition and chemical bond breaking take place on the time scale of 100 fs or less [3], femtosecond electron diffraction is desired for femtochemistry and other ultra-fast studies. We propose to develop a femtosecond electron diffraction facility using photocathode RF gun technology [9].

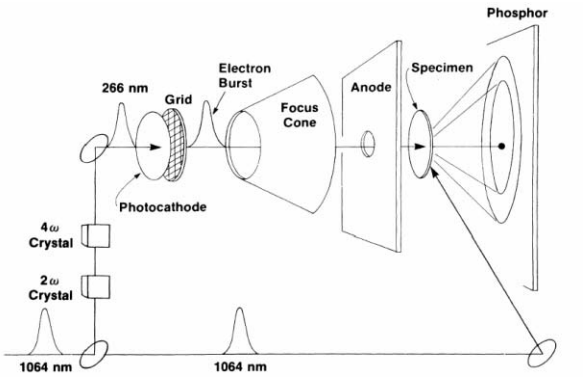

Figure 1: Schematic of UED setup from ref.[6].

The birth of photocathode RF gun can be traced to UED, it is a marriage of laser and high power RF technologies. Laser is used to generate electron beam, and control both the temporal and spatial distribution of

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electron beam. The photoelectron generated by the laser is rapidly accelerated to high energy. The higher electron beam energy, and flexibility of electron beam control made it possible to generate 100 fs electron in the photocathode RF gun. In the following section, a brief discussion on the time resolution of electron diffraction is presented. Then we will present the femtosecond electron beam generation using photocathode RF gun, and concluded with the discussion on the possible issues of femtosecond electron diffraction using photocathode RF gun.

CHALLENGES IN FEMTOSECONDS ELECTRON DIFFRACTION

For a typical electron diffraction based pump-probe experiment depicted in figure 1, the total time resolution can be expressed as following [10],

$$\Delta t^2 = \Delta t^2 la + \Delta t^2 VM + \Delta t^2 eb + \Delta t^2 jit \quad (1)$$

where is Δt_{la} is the laser pulse length, which is limited to 4.5 fs. Δt_{VM} is so called velocity mismatch between the laser and electron beam in the interaction region. It depends on the geometry of the interaction and dimension of the sample or molecule beam. It can be reduce with higher energy electron beam or geometric optimization. For the laser and electron beam parallel configuration and molecule beam size on the order of a couple hundred microns, Δt_{VM} will be less than 100 fs if electron beam energy more than one MeV. Δt_{jit} is the jitter between the pump laser and electron beam. For DC gun based electron diffraction system, it is negligible. To break the picosecond time barrier and reach 100 fs time resolution, femtosecond electron beam is the key.

Femtosecond electron beam generation for electron diffraction was studied extensively recently [11-12] for electron beam energy around 50 keV. The large energy spread and bunch lengthening due to space charge effect prevents it from reaching below ps. Space charge effects play a fundamental role in generation and preservation of femtosecond electron beam. To generate and preserve femtoseconds electron beam, longitudinal space charge effect must be carefully considered since it is much more sensitive to the beam energy than transverse space charge effect (fifth power vs third power). The bunch lengthening due to space charge effect can be estimated in a drift space by [13]:

$$\Delta \ell = \frac{2 QcL}{I_a R \ell \gamma^4}^2 \quad (2)$$

where Q is the charge in the bunch, c is the speed of the light, L is the drift distance, Ia =17 kA, R is the bunch radius, ℓ is the bunch length and γ is the beam energy. The strong dependency of the bunch lengthening on the energy is the major barrier to produce and preserve femtosecond electron beam. As beam energy increases, it becomes more rigid and difficult to control (focusing) longitudinally. Balancing between space charge effects and bunching (focusing) demands that, bunching should be accompanied by the acceleration simultaneously. Photocathode RF gun is the technology capable of producing femtosecond electron beam with reasonable number of electrons [14].

FEMTOSECONDS ELECTRON BEAM GENERATION BY RF GUN

Higher electric field and beam energy from RF gun will lead to significant reduction in space charge effect. Another important advantage of using photocathode RF gun to produce femtoseconds electron beam is its capability of compressing the electron beam as it is being accelerated in the time dependent RF field [14]. This allows us to use longer laser pulse and reduce space charge effect further near the cathode region. Figure 2 shows photo-electron beam energy as function of the RF gun phase and field gradient on the cathode. By choosing proper field gradient and RF gun phase, the electron beam energy spread can be minimized. The photocathode RF gun considered here is 1.6 cell BNL S-band RF gun. The electron bunch length at both the RF gun exit and the target station (1 m down stream) is plotted as RF gun phase in figure 3 for the field gradient 50 MV/m. The number of electrons for this simulation is about 10^6, and laser pulse length is about 500 fs. If the number of electron is reduce to 10^5, simulation shows that, electron bunch length at the target station will be less than 100 fs. Table 1 summarize the expected performance of the photocathode RF gun at the field gradient 50 MV/m. For the purpose of comparison, typical DC gun is also listed there.

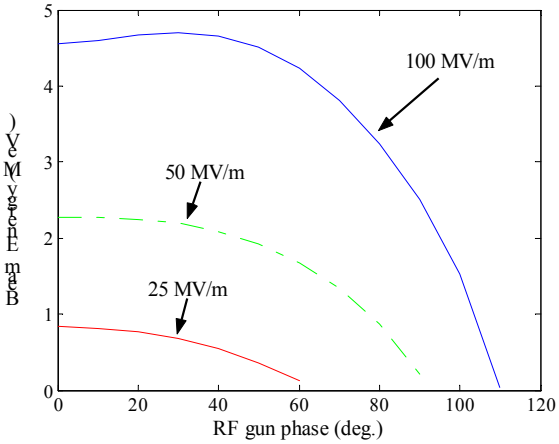

Figure 2: photo-electron beam energy vs. RF gun phase for three field gradients.

Several new issues arise from using photocathode RF gun, energy spread and timing jitter between the RF field and laser are two prominent examples. As we pointed out earlier, by proper selecting the field gradient (50 MV/m) and RF gun phase, energy spread as low as 0.01% can realized, which is comparable to DC gun.

Our studies show timing jitter can be easily controlled to below 100 fs even with couple hundreds fs jitter between

the laser and RF systems [15]. For pump-probe experiment, one laser system will be used for both pumping the sample and generating electron beam, so the jitter is the arrive time between the laser and electron beam. This jitter is dominated by the electron beam energy jitter because of the flatness of energy beam energy as function of the RF gun phase [15].

The success of femtoseconds electron diffraction depends on the electron beam quality. We propose to perform a proof of principle experiment at the BNL DUV-FEL facility to answer one of the key questions, that is, whether electron diffraction is measurable with MeV electron beam produced by the photocathode RF gun. We propose initial diffraction experiment will performed using thin metal film, such as Al. This can also be used to optimize electron beam for diffraction in the later stage. We will consider using gas sample, such as CCl4 or CF3I, or single crystal.

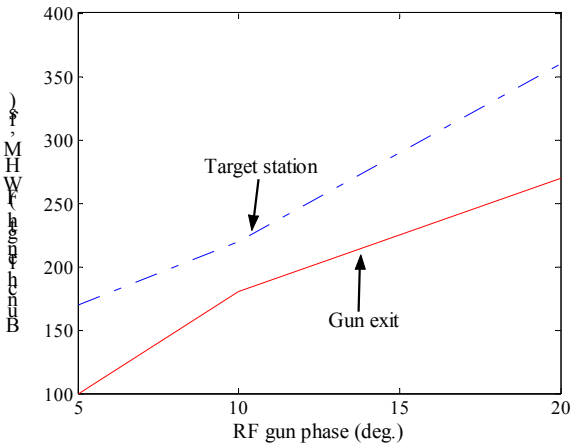

Figure 3: photo-electron beam bunch length vs. RF gun phase at gun exit and target station.

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Table 1: Summary of femtoseconds electron beam properties for RF and DC guns.

	RF gun	DC Gun
Field on the cathode (MV/m)	50 – 100	10
Beam energy (MeV)	1.5 -4	0.03
No. of electrons	10^5 - 10^6	10^4
Bunch length (FWHM, fs)	100 - 200	4000
Energy spread (%)	0.01 – 0.005	0.01

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