

ELECTRON DIFFRACTION ON VELA AT DARESBUURY

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Abstract

Accelerator based Ultrafast Electron Diffraction (UED) is a technique for static and dynamic structural studies in material and biological sciences. The recently commissioned VELA accelerator at the Daresbury Laboratory provides multi-MeV beams for science and industry and will provide a test bed for the UK electron diffraction community. We present the design of the diffractometer currently being installed on VELA which will allow capture of a single shot diffraction pattern with a 1 pC electron bunch and outline future options.

INTRODUCTION

X-ray diffraction has had a profound impact in chemistry, materials science and most especially structural biology and is the main science driver for the establishment of third generation synchrotron X-ray sources. There is, however, a wide class of materials which cannot be crystallised into sufficiently large samples (e.g. membrane proteins) and beam damage occurs before structural information can be obtained on these sources. A new generation of X-ray Free Electron Lasers (FELs) allow *Serial Femtosecond Crystallography* to obtain the structural information with a high intensity X-ray pulse before the molecules are damaged. Such sources also allow the study of structure evolution in pump probe experiments.

A complementary and proven technique for determining structure and measuring structural dynamics is offered by electron diffraction. Low energy (<150 eV) electron diffraction is used for surface structure determination and higher energy (typically up to 200 keV) for bulk structure. For studies of dynamics the duration of the probe electron pulse should not exceed ~100 fs, as it must be shorter than the time scale of the change being studied. Such short probe pulses cannot be generated at the lower non-relativistic energies used in apparatus for table-top ultrafast electron diffraction[1]. At these lower energies, Coulomb repulsion not only limits the pulse duration to ~0.5 ps but it also severely restricts the bunch charge to such an extent that single-shot imaging becomes impossible. Electron accelerators providing a few MeV beam energies allow short bunches with charge of ~1 pC with sub-100 fs bunch lengths. This charge is sufficient to obtain the diffraction pattern in a single shot for many materials.

Accelerator based electron diffraction is being pursued at DESY [2], along with labs in the USA [3], Japan [4]

and China [5]. It offers a number of advantages over X-ray diffraction with FELs as shown in Table 1.

Table 1: Advantages of Electron Diffraction

Scattering cross sections for electrons are 4-6 orders of magnitude higher than those for X-rays.

For the inelastic scattering events that do occur, electrons transfer three orders of magnitude less energy to the target molecules than do X-rays, resulting in much lower sample damage.

Smaller scale accelerators are required for UED, making it more cost effective.

The structural precision required is dependent on the particular system. It may be sufficient to simply monitor a loss in diffraction spots (e.g. to follow order-disorder transitions) or the appearance of additional spots (order-order phase transitions). On the other hand, extremely high spatial resolution is required to monitor the small change in bond length when diatomic molecules are photo excited. Continuous electron beam systems are capable of determining bond lengths to a precision of 0.001 Å. The spatial resolution of an electron diffraction instrument is dependent on the beam size and emittance, these parameters can be controlled easily in keV systems because the short distance between the source and detector minimizes these parameters.

We are now installing an electron diffraction facility on the VELA accelerator at the Daresbury Laboratory. In the current first phase of the programme our aim is to record single shot diffraction patterns with a 1 pC bunch of duration ~150 fs from a series of simple face centred cubic metals. We will then embark on a programme to improve the time resolution.

ELECTRON DIFFRACTION ON VELA

VELA consists of 2.5-cell S-band RF gun with a copper photocathode. The photo-injector laser and UV transport system has been described elsewhere [6]. Briefly, up to 2mJ of UV light at 266nm (76 fs rms pulse duration) is generated by frequency tripling the output of a Ti:Sapphire laser (4 W at 400 Hz). In normal (10 Hz) operation, 0.5 mJ is admitted into the UV transport, which is under vacuum, and focused onto the photocathode.

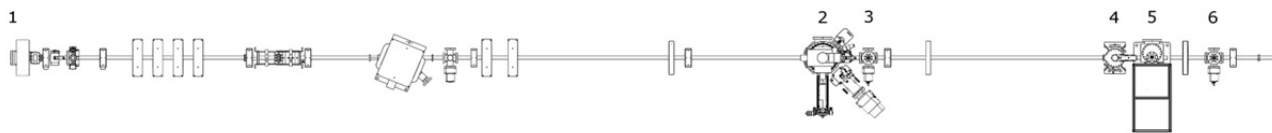


Figure 1: Layout showing {1} the photocathode, {2} the diffraction chamber {4} Faraday cup and {5} imaging system.

An attenuator consisting of a pair of Brewster polarisers and a half-wave plate give a factor of 20 attenuation of the UV beam and this is sufficient to control the electron bunch charge in the range ~10 to 250 pC. For the electron diffraction experiments, additional attenuation is required and is achieved by swapping (under remote control) one of the mirrors in the transport for an uncoated fused silica wedge that reflects ~4% of the incident radiation.

The layout of the electron diffraction system is shown in Fig.1. In the current configuration of VELA, which serves a variety of other research programmes, the sample chamber, shown in Fig. 2, is constrained to be 8.5 m from the gun.

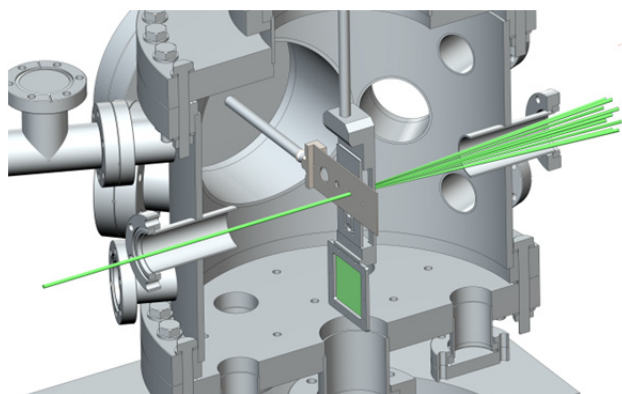


Figure 2: Interchangeable sample holders, each supporting a number of samples and a YAG screen are mounted on a motorised VG Omniax manipulator. An aperture (0.5 – 2 mm diameter) can be positioned directly in front of the sample to shape the electron beam.

The diffraction pattern is captured on a fluorescent Fine Lanex Screen (Kodak Carestream, supplied without backing by Hospital Engineering, Manchester M41 7HS) which is photographed with single-photon sensitivity with an ANDOR iXon3 camera. Table 2 lists the d-spacing of the low index planes of aluminium and gives the 2θ diffraction angle from Bragg's Law for 4 MeV electrons of wavelength = 2.5×10^{-3} Å. By locating the screen at 3.4 m from the sample and arranging 1:1 magnification onto the camera detector we make optimum use of the detector area, as detailed in Fig.3.

Table 2: Diffraction from aluminium. X is the displacement of the diffracted beam relative to the undiffracted beam on the screen 3.4 m from the sample. For polycrystalline Al (random orientation of crystal planes) these diffracted beams give rings around the central spot.

Crystallographic planes	d spacing (Å)	2θ (mrad)	X (mm)
111	2.338	1.070	3.6
200	2.024	1.235	4.2
220	1.431	1.747	5.9
311	1.221	2.048	6.9

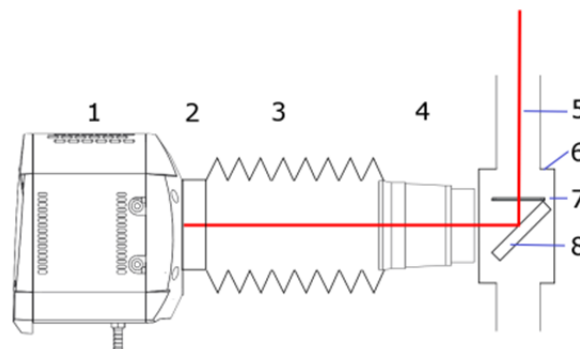


Figure 3: An Andor iXon3 image intensifying camera (1) with shutter (2) equipped with a Samyang 85mm f/1.4 lens (4) on a Nikon bellows (3) allows up to 1:1 imaging of the Lanex screen (7) onto the 13x13 mm sensor of the camera via the 45 degree mirror (8) with on-axis hole to transmit the undiffracted electron beam. At 1:1 magnification the front element of the lens is 125 mm from the screen. The shortest available distance is 87 mm.

The extremely short depth of field when working at maximum aperture requires that the Lanex screen and mirror assembly moves on rails for reproducible positioning.

A Faraday cup can be inserted into the beam immediately upstream of the screen.

ELECTRON BEAM MODELING

In this short paper we present only data on the electron bunch length.

The shortest bunch that can be delivered from the VELA photoinjector is determined by (1) the laser pulse length (2) the cathode response time and (3) the space charge. The minimum laser pulse is 76 fs rms (Gaussian temporal profile). The copper photocathode response is <10 fs and is neglected in these simulations. Space charge effects can be reduced by operating at low bunch charge and by proper choice of laser spot size on the photocathode for each specific bunch charge.

The bunch expands due to both space charge and also any time-energy chirp from the gun. The phase of the RF gun can be used to control the time-energy correlation of the beam emerging from the gun, but the space charge expansion still occurs. This effect is stronger for a shorter beam as can be seen in Fig. 4.

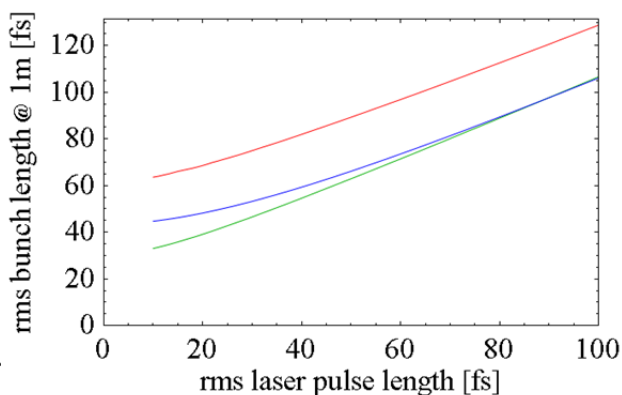


Figure 4: Electron bunch length as a function of laser pulse length for a 1 pC bunch with laser spot diameters of 0.5 mm (red), 1 mm (green), and 2 mm (blue).

In the current layout of VELA the large distance between the gun and the sample means that even at 1 pC bunch charge, space-charge dominates and causes the bunch to lengthen. In addition, transverse focussing causes the bunch to lengthen further. Fig. 5 shows both these cases. Therefore in the phase 1 experiments the bunch length will be ~150 fs at the sample point.

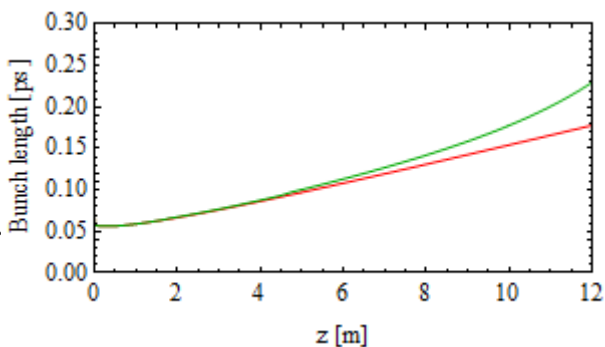


Figure 5: Bunch length along the beam line with (green) and without (red) transverse focussing.

FUTURE DEVELOPMENTS

A number of options are available for future time-resolved electron diffraction experiments on VELA.

Following our initial experiments the opportunity will arise to reconfigure VELA and move the diffraction chamber directly after the gun, allowing the bunch lengths as shown in Fig. 4 to be achieved. This would essentially be a standalone electron diffraction station and give ideal beam properties.

Another benefit of moving the sample chamber to a location close to the gun, is the ability to use a “streaking” scheme, as described in [7], and shown schematically in Fig. 6. In this screen a long electron pulse is diffracted from the sample and a slit is used to pick out a horizontal slice of the diffraction pattern. A transverse deflecting cavity (TDC) then streaks these beams vertically, allowing the time dependant structural changes to be followed. Such a TDC will be tested later this year on VELA.



Figure 6: Layout of a “streaking” scheme for diffraction.

Other options include using the CLARA Front-End due to be installed in 2015[8]. This gun is followed by a 2 m long S-band RF linac that is normally used to accelerate the beam, but can also be used in “velocity bunching” mode to compress the beam longitudinally. A dogleg will then transport the beam to the diffraction chamber. Further details and simulations of this velocity bunching scheme are required.

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