

# Literature Review

Joshua Torrance

May 8, 2012

# 1 Introduction

The University of Melbourne’s cold-atom electron source aims to be able to create high-brightness, high-coherence electron bunches for use in coherent electron diffractive imaging. Imaging of nanoscale objects such as biological molecules [1, 2] and defects in solid-state devices [3] by ultrafast, single-shot electron diffractive imaging would provide important information about structure and dynamic processes of nanoscale objects.

Membrane proteins, for example, are very important for some reason (*ASK VIVIEN get some references*). Determining the structure of these molecules is a key step in understanding their chemical and biological function. The importance of knowing the atomic structure of biomolecules is exemplified by the enormous progress made in various fields of biology once the double-helical structure of DNA was determined from x-ray images in 1953 [4]. Once a protein’s structure and function are known then it becomes possible to design drugs [5] where needed and to more fully understand how the protein behaves in its biological system.

In order to determine the structure of these biological molecules atomic, sub-nanometre imaging resolution is required. A number of techniques are available for determining these structures [6–8] however the most successful to date has been x-ray crystallography [9, 10]. Unfortunately the process of crystallising these membrane proteins is difficult and to date relatively few have been crystallised [11].

New imaging techniques and light sources such as x-ray free electron lasers and ultrafast single-shot diffraction have been driven by the goal of overcoming the limitations of x-ray crystallography. Ultrafast single-shot diffraction imaging also has the potential to determine dynamic structure of biological molecules. The Melbourne cold-atom electron source is aims to produce bright, coherent bunches of electrons for use in diffractive imaging.

## 1.1 Ultrafast, single-shot, coherent diffractive imaging with electrons

X-ray diffraction from crystals was first observed a century ago [12] and resulted in a Nobel prize being awarded to William Bragg and his son. Since then coherent diffractive imaging (CDI) has been performed on a myriad of different samples with coherent beams of x-rays and electrons.

Electrons have a shorter wavelength than x-rays thus allowing a higher limit on the attainable resolution for CDI. [REFERENCE would be nice]

### 1.1.1 Single-shot diffractive imaging

Single-shot diffractive imaging with an x-ray source of sufficient brightness should be able to produce a diffraction pattern from scattered x-rays from a single molecule before the molecule is destroyed by the Coulomb explosion which follows photoionisation within the molecule [13,14]. Single-shot imaging aims to avoid the need for crystallisation with x-ray imaging since with a sufficiently bright source should allow imaging of any molecule.

With femtosecond timescale single-shot imaging it becomes possible to observe such things as molecular vibration and dynamic chemical processes [15] with the sophisticated imaging techniques currently in development it will become possible to create “molecular movies” [1] of these processes.

## 1.2 Melbourne cold-atom electron source

The University of Melbourne’s cold-atom electron source project aims to produce an electron source for coherent diffractive imaging. If bright, coherent, femtosecond long bunches of electrons can be produced then CDI can be performed on a range of structures.

The cold-atom electron source operates by first illuminating laser-cooled rubidium atoms with a resonant 780 nm excitation laser followed by a 5 ns 480 nm ionisation laser pulse. The electrons are then accelerated in a uniform electric field and guided and focused onto the target.

[CHANGE THE FIGURE SO IT DOESN’T HAVE THE DIPOLE TRAP]

When extracting the ionised electrons from the atom cloud it is necessary to turn off the magnetic trapping fields [AND THE ZEEMAN SLOWER?] in order to prevent magnetic distortions of the electron bunches’ paths. This means that just before electron extraction the cloud is no longer trapped and is beginning to expand. The use of trapping mechanisms that do not interfere with the electron bunches, such as an ODT, will help prevent this expansion and thus stabilise the initial position of the electron bunches which tend to drift at present due to dispersal of current, and hence magnetic field, in the magnetic coils and their power supplies.

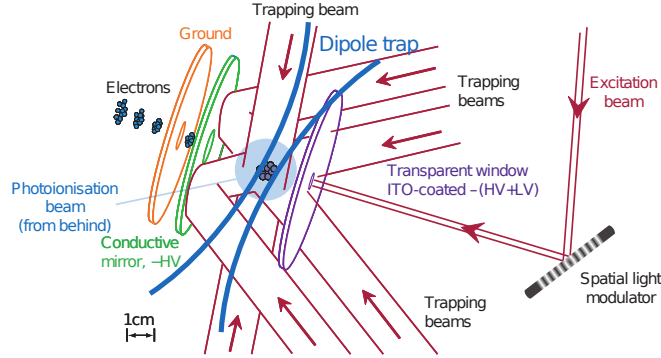


Figure 1: Quasi mirror MOT with optical dipole trap (ODT)

Using an ODT in this system will also allow an increase in the brightness and coherence of the source due to higher atom cloud densities during the ionisation process.

### 1.2.1 Brightness

Brightness is important in single-shot CDI due to the need to maximise the scattered signal and thus ensure sufficient sampling of the specimen within the exposure time.

For the cold-atom source the transverse brightness at the source is given by [16]

$$B_{\perp} = \frac{I_p m_e c^2}{4\pi^2 \sigma_x \sigma_y k_B T}, \quad (1)$$

where  $\sigma$  is the root mean squared source size and  $I_p$  is the peak electron current.

A pulse of electron's brightness can be increased by a reduction in the length of the bunches, by increasing the density of the bunches or by increasing the number of electrons in the bunch. A short bunch is necessary for ultrafast electron diffraction.

The use of an ODT will allow an increase of the atom-cloud density which will in turn result in an increase of the electron bunch density.

### 1.2.2 Coherence

Unsurprisingly coherence is an important factor in CDI since this technique relies on the interference of the diffracted waves. The transverse coherence

length of a imaging beam must be approximately twice the width of the object being imaged [17].

For a quasi-homogeneous source [18], the transverse coherence length  $L_c$  can be related to the transverse momentum spread, and hence the temperature, through [19]

$$L_c = \hbar / \sqrt{m_e k_B T}. \quad (2)$$

The transverse coherence is determined solely from the temperature of the electrons which is proportional to the temperature of the electron source and the ionisation energy.

The coherence of our electron bunches will be increase with the correct use of an ODT since the trap will serve to reduce the temperature of the atom cloud, and hence the electron bunches.

## 2 Optical Dipole Trapping

The use of ODTs in the cold-atom electron source will allow greater stability of the atom cloud during ionisation and extraction as well as increasing the density of the atom cloud during these phases with corresponding increases in density.

### 2.1 History of optical dipole trapping

The use of the optical dipole force as a confining mechanism was first proposed by Askar'yan in 1962 [20] for plasmas and neutral atoms. Ashkin successfully demonstrated the trapping of micron-size latex spheres suspended in water using a focused Gaussian lasers in 1970 [21]. The first optical trapping of atoms was demonstrated by Chu et. al. in 1986 [22] where a ODT was used to trap sodium atoms.

### 2.2 Theory of Dipole Trapping

ODTs are sometimes considered to be the simplest form of atom trap since then consist solely of a focused, Gaussian laser beam detuned from the atomic resonances.

#### 2.2.1 Trapping potential

The intensity of a Gaussian laser beam at the beam waist varies with  $r$  as

$$I(r) = I_0 e^{-r^2/w_0^2}, \quad (3)$$

where  $I_0$  is the intensity at the centre of the beam at the waist,  $r$  is the radial distance from the centre of beam and  $w_0$  is the beam radius at the focus.

The ground state light shift is given by [23]

$$\Delta E_g = \frac{\hbar \Omega^2}{4\delta}, \quad (4)$$

where the Rabi frequency  $\Omega^2 = \gamma^2 I / 2I_s$  and  $\gamma$  is the linewidth,  $I$  is the light intensity and  $I_s$  is the saturation intensity. Thus the light shift is larger at points of high intensity such as the centre of the beam and the beam focus.

In order to trap the laser is detuned below the resonances such that  $\delta = \omega_l - \omega_a < 0$  where  $\omega_l$  is the laser frequency and  $\omega_a$  is the atomic resonance frequency. With negative detuning the ground-state light shift is negative everywhere and thus atoms feel a force towards the centre given by the gradient of the light shift, and for  $\delta \gg \Omega$  and  $\delta \gg \gamma$  the force is given by

$$F \simeq -\frac{\hbar}{4\delta} \nabla(\Omega(r)^2) = -\frac{\hbar\gamma^2}{8\delta I_s} \nabla I(r). \quad (5)$$

At the focus of a Gaussian beam this force is

$$F \simeq \frac{\hbar\gamma^2}{4\delta} \frac{I_0}{I_s} \frac{r}{w_0^2} e^{-r^2/w_0^2}, \quad (6)$$

and thus the transverse trapping potential is given by

$$U = -\int dr F \simeq \frac{\hbar\gamma^2}{8\delta} \frac{I_0}{I_s} e^{-r^2/w_0^2}. \quad (7)$$

It is easy to see with this equation how a negative (red) detuning will result in an inwards, trapping force and a positive (blue) detuning will result in a outwards, repulsive force. Blue detuned lasers can be used for trapping if the beam has a low intensity centre however [24–27].

### 2.2.2 Scattering rates

More general expressions for the trapping potential can be used to compare the potential to the scattering rate due to photon absorption [28]

$$U_{dip}(\vec{r}) = \frac{3\pi c^2}{2\omega_0^3} \frac{\gamma}{\delta} I(\vec{r}) \quad (8)$$

$$\Gamma_{sc}(\vec{r}) = \frac{3\pi c^2}{2\hbar\omega_0^3} \left(\frac{\gamma}{\delta}\right)^2 I(\vec{r}) \quad (9)$$

The scattering rate should be kept to a minimum in order to prevent the heating atoms in the trap. Fortunately the relationships are such that for large detunings  $U_{dip} \gg \Gamma_{sc}$ . Such far detuned lasers however do create shallower traps and thus require more powerful lasers to create similar trap depths.

## 2.3 Using an optical dipole trap in a cold-atom electron source

An ODT can serve several purposes in the cold-atom electron source including increasing the brightness and coherence of the electron bunches as described earlier.

A number of design choices in the development of this dipole trap are under consideration such as the wavelength of the trap, the configuration of the trapping beam/s and the size of the beam waist.

### 2.3.1 Available equipment

Two main options are available as far as light sources for the trap,

- a 20mW, 780nm diode laser amplified by a tapered amplifier to 1.8W,
- a 20W, 1064nm fibre laser.

The 780nm diode laser that seeds the tapered amplifier can be tuned away from the 780nm resonance [HOW FAR EXACTLY? what does this do to the TA?] up to [SOME NUMBER] nm. The 1064nm laser is extremely far away from the resonances which will result in reduced scattering rates however lasers with power as high as 20W require more caution in there use as well as suitable high-power optics.

### 2.3.2 1064nm optical dipole traps

ODTs with a wavelength near 1064nm are frequently used when rubidium Bose-Einstein condensates (BECs) are being formed [29–34]. These BECs are used for many different applications including the creation of atom-lasers [29–31], atomic clocks [35] and obviously further studies into BECs themselves and related trapping mechanisms [32–34].

ODTs with wavelengths at 1064nm are not only used in rubidium BECs. They have to used to form BECs of caesium [36], chromium [37], double-species BECs [38], and even molecular BECs [39].

### 2.3.3 “Near” 780nm optical dipole traps

Traps made from lasers “near” 780nm are more often used when studying and developing trapping methods [possibly due to reduced costs?]. Such



traps have detunings that vary from 0.5nm [42] to over 60nm [40,41] and are usually referred to as far-off-resonance traps (FORTs). Some of the things that these laser have been used to study are dipole trap loading [43], trapping single atoms [41] and the combination of an ODT with Sisyphus cooling [42].

#### 2.3.4 Configurations

The simplest ODT consists simply of a focussed Gaussian beam [22] and many of the references use this simple configuration.

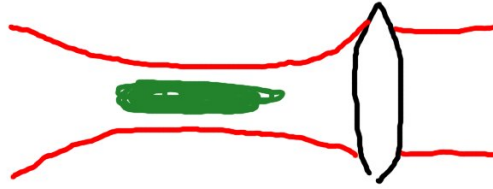


Figure 2: A simple ODT configuration

Crossed dipole trap [cite a selection of references] are a more complicated configuration that can provide a stronger trap as well as control over the shape of the trap and the trapping potentials in various directions. [Examples] Unlike simple dipole traps which create long cigar-shaped traps crossed dipole traps can create spherical traps.

Something about the angles involved. [refind the reference]

Not trapping at the focus. [refind the reference]

#### 2.3.5 Waist size

Not really to do with the literature.

Fix last lens, vary collimated beam size incident on the final lens using a beam expander.

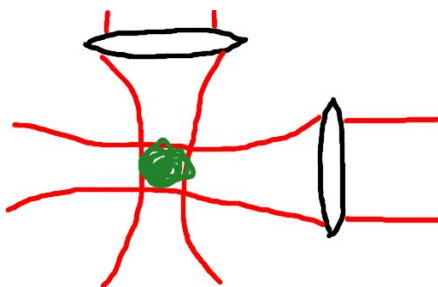


Figure 3: A crossed ODT configuration

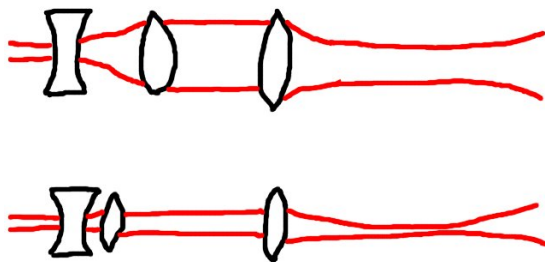


Figure 4: An example setup for controlling the beam waist

# Glossary

**BEC** Bose-Einstein condensate.

**CDI** coherent diffractive imaging.

**ODT** optical dipole trap.

# References

- [1] J. R. Dwyer, C. T. Hebeisen, R. Ernstorfer, M. Harb, V. B. Deyirmenjian, R. E. Jordan, and R. J. Dwayne Miller. Femtosecond electron diffraction: ‘making the molecular movie’. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 364(1840):741–778, March 2006.
- [2] J. C. Williamson, J. Cao, H. Ihee, H. Frey, and A. H. Zewail. Clocking transient chemical changes by ultrafast electron diffraction. , *Published online: 13 March 1997*; | *doi:10.1038/386159a0*, 386(6621):159–162, March 1997.
- [3] B. J. Siwick, J. R. Dwyer, R. E. Jordan, and R. J. Dwayne Miller. An Atomic-Level view of melting using femtosecond electron diffraction. *Science*, 302(5649):1382–1385, November 2003.
- [4] J. D. Watson and F. H. C. Crick. Molecular structure of nucleic acids: A structure for deoxyribose nucleic acid. , *Published online: 25 April 1953*; | *doi:10.1038/1711737a0*, 171(4356):737–738, April 1953.
- [5] L. H. Pinto, L. J. Holsinger, and R. A. Lamb. Influenza virus m2 protein has ion channel activity. *Cell*, 69(3):517–528, May 1992.
- [6] J. E Nettleship, J. Brown, M. R. Groves, and A. Geerlof. Methods for protein characterization by mass spectrometry, thermal shift (ThermoFluor) assay, and multiangle or static light scattering. *Methods in Molecular Biology (Clifton, N.J.)*, 426:299–318, 2008. PMID: 18542872.
- [7] D. I. Svergun and M. H. J. Koch. Small-angle scattering studies of biological macromolecules in solution. *Reports on Progress in Physics*, 66(10):1735–1782, October 2003.

- [8] S. J. Opella and F. M. Marassi. Structure determination of membrane proteins by NMR spectroscopy. *Chemical Reviews*, 104(8):3587–3606, August 2004. PMID: 15303829.
- [9] J. C. Kendrew, G. Bodo, H. M. Dintzis, R. G. Parrish, H. Wyckoff, and D. C. Phillips. A Three-Dimensional model of the myoglobin molecule obtained by X-Ray analysis. , *Published online: 08 March 1958*; | *doi:10.1038/181662a0*, 181(4610):662–666, March 1958.
- [10] I. Usón and G. M. Sheldrick. Advances in direct methods for protein crystallography. *Current Opinion in Structural Biology*, 9(5):643–648, October 1999. PMID: 10508770.
- [11] A. Geerlof, J. Brown, B. Coutard, M. P. Egloff, F. J. Enguita, M. J. Fogg, R. J. C. Gilbert, M. R. Groves, A. Haouz, J. E. Nettleship, P. Nordlund, R. J. Owens, M. Ruff, S. Sainsbury, D. I. Svergun, and M. Wilmanns. The impact of protein characterization in structural proteomics. *Acta Crystallographica. Section D, Biological Crystallography*, 62(Pt 10):1125–1136, October 2006. PMID: 17001090.
- [12] W. H. Bragg. X-rays and crystals. *Nature*, 90:219, October 1912.
- [13] R. Henderson. The potential and limitations of neutrons, electrons and x-rays for atomic resolution microscopy of unstained biological molecules. *Quarterly Reviews of Biophysics*, 28(2):171–193, May 1995. PMID: 7568675.
- [14] R. Neutze, R. Wouts, D. van der Spoel, E. Weckert, and J. Hajdu. Potential for biomolecular imaging with femtosecond x-ray pulses. *Nature*, 406(6797):752–757, August 2000.
- [15] A. H. Zewail. 4d ultrafast electron diffraction, crystallography, and microscopy. *Annual Review of Physical Chemistry*, 57(1):65–103, 2006.
- [16] M. Reiser. *Theory and Design of Charged Particle Beams*. John Wiley & Sons, August 2008.
- [17] J. C. H. Spence, U. Weierstall, and M. Howells. Coherence and sampling requirements for diffractive imaging. *Ultramicroscopy*, 101(2-4):149–152, November 2004. PMID: 15450660.

- [18] K. A. Nugent. Coherent methods in the x-ray sciences. *Advances in Physics*, 59(1):1–99, 2009.
- [19] T. van Oudheusden, E. F. de Jong, S. B. van der Geer, W. P. E. M. op’t Root, O. J. Luiten, and B. J. Siwick. Electron source concept for single-shot sub-100 fs electron diffraction in the 100 keV range. *Journal of Applied Physics*, 102(9):093501–093501–8, November 2007.
- [20] G. Askar’yan. Effects of the gradient of a strong electromagnetic beam on electrons and atoms. *Soviet Physics - Journal of Experimental and Theoretical Physics*, 15(1088), 1962. INSPEC:10786990.
- [21] A. Ashkin. Acceleration and trapping of particles by radiation pressure. *Physical Review Letters*, 24(4):156–159, January 1970.
- [22] S. Chu, J. E. Bjorkholm, A. Ashkin, and A. Cable. Experimental observation of optically trapped atoms. *Physical Review Letters*, 57(3):314–317, July 1986.
- [23] H. J. Metcalf and P. van der Straten. *Laser Cooling and Trapping*. Springer, 1999.
- [24] N. Davidson, H. Jin Lee, C. S. Adams, M. Kasevich, and S. Chu. Long atomic coherence times in an optical dipole trap. *Physical Review Letters*, 74(8):1311–1314, February 1995. PMID: 10058988.
- [25] H. J. Lee, C. S. Adams, M. Kasevich, and S. Chu. Raman cooling of atoms in an optical dipole trap. *Physical Review Letters*, 76(15):2658–2661, April 1996.
- [26] R. Ozeri, L. Khaykovich, and N. Davidson. Long spin relaxation times in a single-beam blue-detuned optical trap. *Physical Review A*, 59(3):R1750–R1753, March 1999.
- [27] N. Friedman, L. Khaykovich, R. Ozeri, and N. Davidson. Compression of cold atoms to very high densities in a rotating-beam blue-detuned optical trap. *Physical Review A*, 61(3):031403, February 2000.
- [28] R. Grimm, M. Weidemüller, Y. B. Ovchinnikov, Benjamin Bederson, and Herbert Walther. Optical dipole traps for neutral atoms. In *Advances In Atomic, Molecular, and Optical Physics*, volume Volume 42, pages 95–170. Academic Press, 2000.

- [29] A. P. Chikkatur, Y. Shin, A. E. Leanhardt, D. Kielpinski, E. Tsikata, T. L. Gustavson, D. E. Pritchard, and W. Ketterle. A continuous source of Bose-Einstein condensed atoms. *Science*, 296(5576):2193–2195, June 2002.
- [30] A. Couvert, M. Jeppesen, T. Kawalec, G. Reinaudi, R. Mathevet, and D. Guéry-Odelin. A quasi-monomode guided atom laser from an all-optical Bose-Einstein condensate. *EPL (Europhysics Letters)*, 83(5):50001, September 2008.
- [31] G. Kleine Büning, J. Will, W. Ertmer, C. Klempt, and J. Arlt. A slow gravity compensated atom laser. *Applied Physics B: Lasers and Optics*, 100(1):117–123, 2010.
- [32] Y.-J. Lin, A. R. Perry, R. L. Compton, I. B. Spielman, and J. V. Porto. Rapid production of  $^{87}\text{Rb}$  Bose-Einstein condensates in a combined magnetic and optical potential. *Physical Review A*, 79(6):063631, June 2009.
- [33] K. J. Arnold and M. D. Barrett. All-optical Bose-Einstein condensation in a  $1.06\ \mu\text{m}$  dipole trap. *Optics Communications*, 284(13):3288–3291, June 2011.
- [34] Zhengkun Fu, Pengjun Wang, Shijie Chai, Lianghai Huang, and Jing Zhang. Bose-Einstein condensate in a light-induced vector gauge potential using 1064-nm optical-dipole-trap lasers. *Physical Review A*, 84(4):043609, October 2011.
- [35] G. Kleine Büning, J. Will, W. Ertmer, E. Rasel, J. Arlt, C. Klempt, F. Ramirez-Martinez, F. Piéchon, and P. Rosenbusch. Extended coherence time on the clock transition of optically trapped rubidium. *Physical Review Letters*, 106(24):240801, June 2011.
- [36] C.-L. Hung, X. Zhang, N. Gemelke, and C. Chin. Accelerating evaporative cooling of atoms into Bose-Einstein condensation in optical traps. *Physical Review A*, 78(1):011604, July 2008.
- [37] Q. Beaufiles, R. Chicireanu, T. Zanon, B. Laburthe-Tolra, E. Maréchal, L. Vernac, J.-C. Keller, and O. Gorceix. All-optical production of chromium Bose-Einstein condensates. *Phys. Rev. A*, 77(6):061601, June 2008.

- [38] G. Thalhammer, G. Barontini, L. De Sarlo, J. Catani, F. Minardi, and M. Inguscio. Double species Bose-Einstein condensate with tunable interspecies interactions. *Physical Review Letters*, 100(21):210402, May 2008.
- [39] M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, S. Gupta, Z. Hadzibabic, and W. Ketterle. Observation of Bose-Einstein condensation of molecules. *Physical Review Letters*, 91(25):250401, December 2003.
- [40] J. D. Miller, R. A. Cline, and D. J. Heinzen. Far-off-resonance optical trapping of atoms. *Physical Review A*, 47(6):R4567–R4570, June 1993.
- [41] M. Weber, J. Volz, K. Saucke, C. Kurtsiefer, and H. Weinfurter. Analysis of a single-atom dipole trap. *Physical Review A*, 73(4):043406, April 2006.
- [42] Kurt W. Miller, Stephan Dürr, and Carl E. Wieman. rf-induced sisyphus cooling in an optical dipole trap. *Physical Review A*, 66(2):023406, 2002.
- [43] S. J. M. Kuppens, K. L. Corwin, K. W. Miller, T. E. Chupp, and C. E. Wieman. Loading an optical dipole trap. *Physical Review A*, 62(1):013406, June 2000.