484
doi:10.1017/S1431927610056527
Microsc. Microanal. 16 (Suppl 2), 2010

"Making the Molecular Movie": Quest for the Structure-Function Correlation in Biology

R. J. Dwayne Miller

Departments of Chemistry and Physics and Institute for Optical Sciences, University of Toronto, 80 St. George St., Toronto ON, M5S 3H6, Canada.

Femtosecond Electron Diffraction (FED) harbours great potential for providing atomic resolution to structural changes as they occur, essentially watching atoms move in real time --- directly observe transition states. This experiment has been referred to as "making the molecular movie" and has been previously discussed in the context of a gedanken experiment. With the recent development of femtosecond electron pulses with sufficient number density to execute nearly single shot structure determinations, this experiment has been finally realized [1]. A new concept in electron pulse generation was developed based on a solution to the N-body electron propagation problem involving up to 10,000 interacting electrons that has led to a new generation of extremely compact and bright electron pulsed sources that minimizes space charge broadening effects [2]. Figure 1 shows table-top FED setups based on a compact electron guns, 3rd and 4th generations. Previously thought intractable problems of determining t=0 and fully characterizing electron pulses on the femtosecond time scale have now been solved through the use of the laser ponderomotive potential to provide a time dependent scattering source [3, 4]. Synchronization of electron probe and laser excitation pulses is now possible with an accuracy of 10 femtoseconds to follow even the fastest nuclear motions. The camera for the "molecular movie" is now in hand. Through the Debye-Waller factors, it is now possible to directly observe lattice heating and discern thermal from electronic effects on lattice potentials [5]. It has been possible to study rarified states of matter up to conditions corresponding to warm dense matter [6] as well as optical manipulation of electron distribution and associated bonding on ultrafast timescales [7].

Unprecedented results on cooperative effects in strongly correlated electron-lattice systems involving superlattices as a consequence of charge density waves (CDW) in TaS_2 [9], a 2-dimensional system, will be shown (see figure 2 (a)). In addition, some preliminary results obtained for a molecular crystal [10] (see figure 2 (b) and (c)) will be discussed in the context of developing the necessary technology to directly observe the structure-function correlation in biomolecules – the fundamental molecular basis of biological systems [8].

References

[1] B.J. Siwick, *et al.* Science 302 (2003) 1382.
[2] B.J. Siwick *et al. J. Appl. Phys.* 92 (2002) 1643.
[3] C.T. Hebeisen *et al. Opt. Lett.* 31 (2006) 3517.
[4] C.T. Hebeisen *et al. Opt. Express* 16 (2008) 3334.
[5] M. Harb *et al. Phys. Rev. Lett.* 100 (2008) 155504.
[6] R. Ernstorfer *et al. Science* 323 (2009) 1033.
[7] G. Sciaini *et al. Nature* 458 (2009) 56.
[8] R.J.D. Miller *et al. Acta Cryst. Acta A* (2010) in press.
[9] M. Eichberger, H. Schäfer, J. Demsar, H. Berger, G. Moriena, G. Sciaini, and R.J.D.Miller. (to be submitted).

[10] H. Jean-Ruel *et al.* (to be submitted).

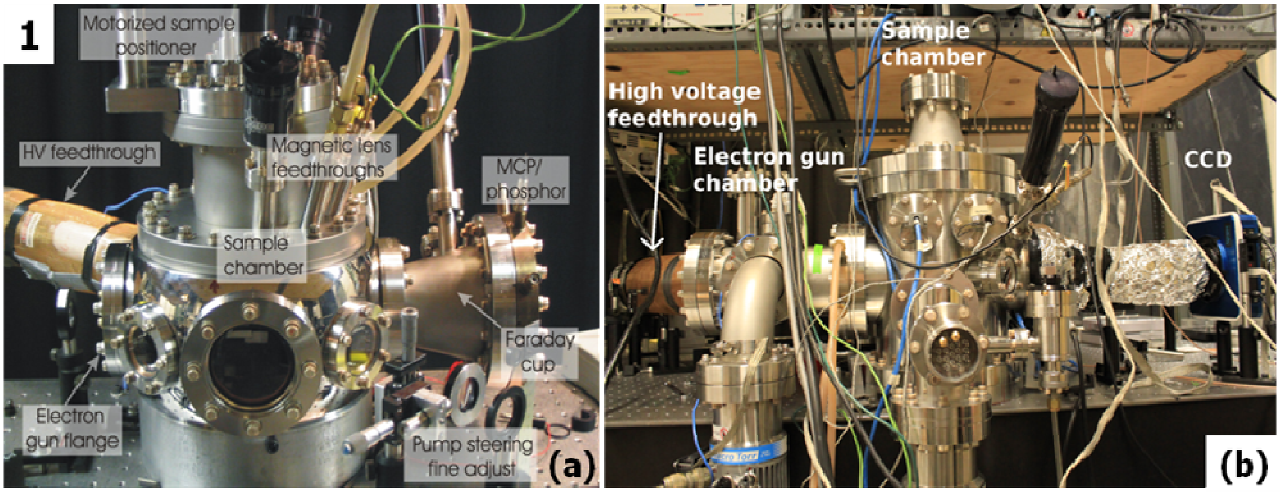

FIG. 1. Photos of the FED setups used at University of Toronto. (a) 3rd generation 30 keV FED setup and (b) 4th generation FED upgraded to 60 keV. The setups compromise a compact high voltage DC electron gun, a sample chamber and a detection system based on a micro-channel plate/phosphor screen and a charge coupled device camera.

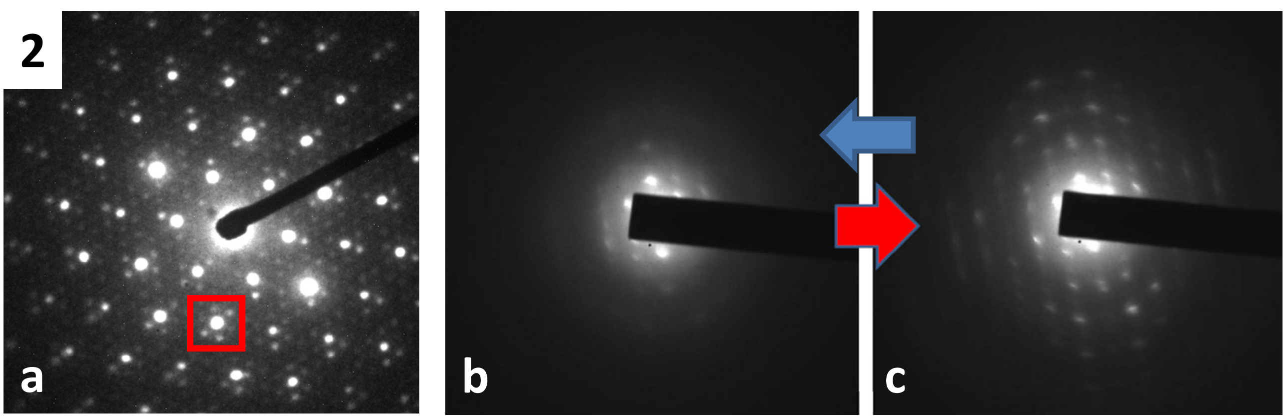

FIG. 2. Panel (a) Diffraction pattern of TaS_2. The modulation of the CDW can be noted around each Bragg spot. In the red square the 6-fold symmetry of the CDW can be observed [from ref. 9]. Panels (b) and (c) show the diffraction patterns of an organic molecular crystal [from ref. 10]. (b) After UV irradiation (266 nm). (c) After He-Ne irradiation (633 nm). A photoinduced crystalline phase transition takes place due to an opening-close ring isomerization reaction in the molecular basis. The sample supports about 10^4 cycles.

https://doi.org/10.1017/S1431927610056527 Published online by Cambridge University Press