

MS44 O1

Tracking molecular motions in solution Marco Cammarata^a *European Synchrotron Radiation Facility (ESRF), Grenoble, France.*

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Keywords: molecular motion, time-resolved X-ray scattering

Thanks to unprecedented photon flux delivered by tailor made undulators and a fully synchronized laser system, ID09B has become a “molecular movie factory” where reactions in solution can be followed with 100ps time resolution.

The experimental challenges, the key elements of the beamline, and few examples of the research carried out at ID09B will be given. They include: a) the determination of the reaction kinetics and transient molecular structures of small molecules (where atomic resolution can be reached!) and b) the characterization of protein structural relaxations after photolysis.

These examples will show the richness of the reactions taking place in solution and how 3rd generation facilities can be used to answer fascinating scientific questions.

MS44 O2

Photoinduced transition of TTF-CA: Picosecond diffuse scattering investigations. Eric Collet^a, Marylise Buron^a, Laurent Guérin^b, Johan Hébert^a, Hervé Cailleau^a, Shin-ichi Adachi^b, Shin-ya Koshihara,^b *Institute of Physics, University of Rennes 1, France.* ^b *JST ERATO, Tsukuba, Japan.* ^c *KEK Tsukuba, Japan.* ^d *Tokyo Institute of Technology, Tokyo, Japan.* E-mail: eric.collet@univ-rennes1.fr

Keywords: photoinduced phase transition, time-resolved structural studies, solid-state phase-transition

Within the emerging field of ultra-fast x-ray science and the development of next generation sources, time-resolved diffuse scattering opens new opportunities to watch the generation, correlation and propagation of photoinduced excitations between the constituent molecules of solids. The investigation of such precursor phenomena is illustrated here by the detection, by 100 picosecond x-ray diffuse scattering, of cooperative charge-transfer charge-transfer exciton-strings of one-dimensional nature, in the first step of the photoinduced transition in the molecular crystal TTF-CA investigated by time-resolved diffraction [1,2].

The time-dependence of the intensity of Bragg reflections on the 100 fs, triggered by the generation of coherent atomic oscillations in a solid, was reported in different materials. X-ray diffuse scattering experiments on solids open the unique opportunity to get key information on local excitations and on the nature of the cooperative interactions between the constituent molecules of crystals. In that, they are very different from diffuse scattering from solution. We show here that such local photoinduced phenomena, which may be the precursor effects driving real photoinduced phase transitions, can be detected by this technique. Experiments were performed on the NW14 time-resolved beamline of synchrotron KEK-PFAR [3].

[1] Collet E. et al, *Science*, 2003, 300, 612.

[2] Guérin L. et al, *C. Chem. Phys.* 2004, 299.

[3] Nozawa S. et al, *J. Synch. Rad* in press.

MS44 O3

Antimony-containing anodes for Li-ion batteries – their reactivity and structure, Kristina Edström and Hanna Bryngelsson *Department of Materials Chemistry, Uppsala University Box 538, Uppsala, Sweden.*

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Keywords: In situ time-resolved powder diffraction, Lithium batteries, Intermetallics

To obtain a sufficiently large amount of energy storage based on battery technology the batteries need to be safer and cheaper than today's options. This problem is recognised as one of the key technology problems to solve. One of the main battery candidates is the Li-ion battery which has shown to be the rechargeable battery with highest energy density, higher than the NiMH and the lead-acid systems. Portable equipments such as laptops and mobile phones are mainly powered by this battery type and strong efforts are taken to find new cheap and environmentally materials that can allow a scale up of the battery to Hybrid Electrical Vehicle systems.

In this presentation the focus will be on antimony compounds as possible anode materials replacing the carbonaceous electrode used in today's commercial batteries. Antimony can alloy with three lithium-ions that give the material a theoretical capacity of 660 mAh/g compared to 372 mAh/g, which is that of graphite. The main reason why antimony has not yet been practically implemented in a better way stems from the fact that a large volume expansion of ~150 % will occur in the formation of the end product Li₃Sb. We will demonstrate several strategies to overcome this problem:

- Intermetallic systems can be used where the antimony atoms will be separated in a crystal structure with other metals that are either non-active to lithium alloying (Cu, Mn or Ni) or active to lithium alloying (Al, In or Sn).
- Nano-particles of antimony are used in a rubber-binder matrix that buffer for the volume changes.
- Thin film electrodes where the volume expansion can be handled.

For all these scenarios the use of *in situ* X-ray diffraction is vital for the understanding of the basic lithium-alloying processes. We use so-called “coffee bag” batteries consisting of polymer laminated aluminium pouches that can be easily sealed to prevent the battery from exposure to air and moisture and that are only 0.2 mm thick. This means that the structural response to charge and discharge can be monitored in transmission mode. We use both in house and synchrotron radiation for our studies.

We will discuss whether the lithium insertion reactions occur by a topotactic reaction or by a restructuring at the atomic level. As examples we will show how lithium is inserted into Cu₂Sb, MnSb and Mn₂Sb and discuss the common features as well as the difference in mechanisms.

We will also comment the influence of microstructure of the electrode composite on the insertion mechanism as well as the importance of different volume buffering media for nano-particle and thin film electrodes based on the results of synchrotron based *in situ* X-ray diffraction measurements.