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Multscale real-time XRD probing of the semiconductor to metal ultrafast phase transition in Ti_3O_5 nanocrystals

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Last decades have seen tremendous technical progress in the development of pulsed Xray sources. Synchrotron sources can now produce 100ps duration pulses with enough photons to allow quantitative analysis. The emergence of free electron laser brought the pulse duration a step shorter, typically 10fs, and even more bright. This leads to the ability to probe electrons and atoms on the time scale of their respective motions, opening a completely new field of investigation to physicians and material scientists: the science of out-of-equilibrium processes.

Since the 2000s and the pioneering time resolved XRD experiments, we can now "see" atomic motions in real time on fs time scales. Today's challenge is not only to see but also to be able to "act" on matter in an ultra-fast and controlled manner. This means inducing an ultrafast permanent change, ultimately reversible, in a material. This requires a deep understanding of the ultrafast structural dynamics but also the propagation process of the induced deformation on longer time and space scales. It was recently demonstrated experimentally and theoretically a self-amplified responsiveness in a spin-crossover material [1] during its delayed volume expansion.

Time-resolved XRD is a direct probe of volume changes and structural rearrangement in materials.

Such experiments are still highly challenging. However we will show how that the implementation of quantitative structural analysis (rietvelt refinement) can be extended to these out-of-equilibrium studies. Our talk will focus on Titanium Pentaoxide (Ti3O5), a protype of multistability which undergoes phase transitions between different forms (so called α, β, λ), that can be monitored by temperature, pressure, electric field and laser pulses. The stability of the phases is strongly related to the size of the crystallites. In particular λ phase is more stable in nanocrystals thus making the system bi-stable at ambient temperature with obvious interest for pure as well as applied science[2] (fig. 1). We will present the study of this ultrafast phase transition in Ti3o5 nanocrystals, for which we performed three major experiments:

- Time resolved powder XRD on ps time-scale (Swissfel, Bernina)[3]
- Multiscale (from 100ps to millisecond) time resolved XRD (beamline ID9, ESRF).
- Multiscale optical spectroscopy pump/probe measurements (IPR , rennes).

We will show how this combined approach gives us new insight into this reversible semi-conductor to metal ultrafast phase transition

References:

[1] R. Bertoni et al., Elastically driven cooperative response of a molecular material impacted by a laser pulse, Nat. Mat. 15, 606–610 (2016)
[2] S. Ohkoshi et al., Synthesis of a metal oxide with a room-temperature photoreversible phase transition. Nat. Chem 2, 539-545 (2010)
[3] https://www.psi.ch/swissfel/first-pilot-experiment (2017)

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