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Size dependance of the photo-induced phase transition in Ti_3O_5 nanocrystals

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Recently, our group started exploring the possibility of using laser pulse induced long range lattice deformations for driving phase transitions [1]. We showed how strain waves drive a semiconductor (β-phase) to metal (λ-phase) phase transition in bistable trititanium pentoxide (Ti_3O_5) nanocrystals [2, 3] excited by an ultrashort laser pulse (~ 100 fs). Here, the electronic process occurs within 100 fs, whereas the phase transition propagated by the strain wave is completed within 20 ps. During this transition there is a significant change of volume and the two phases show distinct diffraction patterns, hence powder diffraction is suitable to follow structural changes. It is not trivial to determine which parameters affect this photo-induced phase transition, in order to control the light induced strain wave to a degree allowing high efficiency. We performed pump/probe x-ray powder diffraction at ESRF (ID09) on Ti_3O_5 nanocrystalline pellets to investigate the role of crystallite size and pump wavelength. We studied samples from 100 nm to 500 nm in size. The pellets were excited with a ps laser pump and probed with grazing x-rays at several delays ranging from 50 ps to 1 ms, thereby allowing to monitor the "elastic step" (~ 100 ps), the heat diffusion step (~10 ns depending on samples and fluence) and the complete relaxation (within 10 ms). Our results confirm that the strain waves provide an efficient pathway for insulator-to-metal transition, irrespective of crystallite size/morphology. The thermally induced transition between β and λ phases and the recovery of thermal equilibrium show significant dependence on the crystallite size, motivating further simulations to rationalize this result.

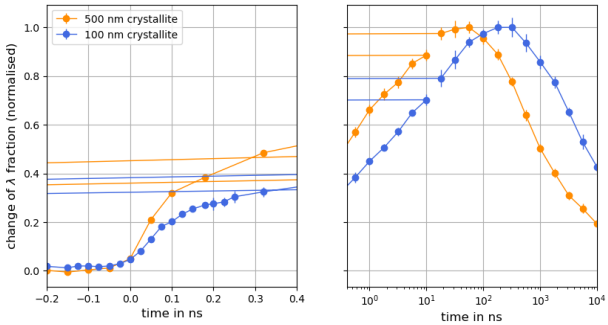

Figure: Change of the metallic (λ) fraction obtained from rietveld analysis of the time resolved powder pattern measured at ESRF, ID9 beamline for 100 nm [3] and 500 nm [5] samples.

[1] Bertoni, R. et al., *Nature Mater* 15,606–610 (2016).
[2] Mariette, C. et al., *Nat Commun* **12,** 1239 (2021).
[3] Ohkoshi, S. et al., *Nature Chem* 2, 539–545 (2010).
[4] Tokoro, H.et al., *Nat Commun* 6, 7037 (2015).
[5] Ohkoshi, Si. et al. *Sci Rep* 9, 13203 (2019).