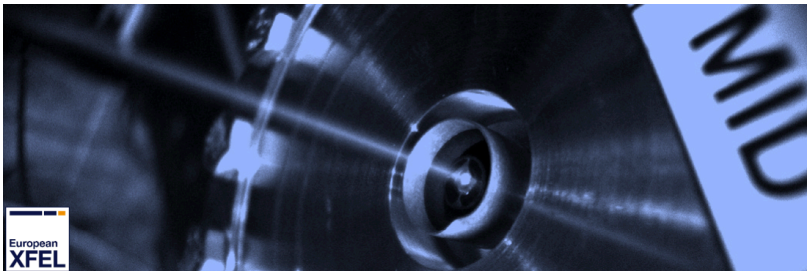

Contribution ID: **10** Type: **Poster**

Towards Femtosecond Structural Dynamics of Small Unit Cell Systems and Non-Crystalline Materials

Thursday 19 January 2023 19:23 (7 minutes)

In recent years, molecular dynamics of macromolecules has benefitted immensely from the femtosecond timescales of X-ray Free Electron Lasers (XFELs)[1]. However, the progress for small unit cell systems has been slow. Thus, Dr. L. Krause and B. Svane have developed a data reduction pipeline for small unit cell systems, including peak hunting, indexing, integration, and post-refinement[2]. Using the pipeline, data measured on single crystals of a I4/m polymorph of $K_4[Pt_2(P_2O_5H_2)_4]\ 2H_2O$ (PtPOP) at the SPring-8 Compact Free-Electron Laser (SACLA) have been reduced to structure factors that allow direct methods to solve the structure (R1 ~ 9.3%)[3]. Hopefully, the pipeline will allow for ultrafast structural dynamics, tracking for example the changes taking place upon photoexcitation of PtPOP.
Other structural dynamics studies that could benefit from femtosecond time resolution are the tracking of nanoparticle nucleation and growth (N&G). Pair Distribution Function (PDF) analysis is often the method of choice for following the N&G from precursor solutions[4]. Currently, the time resolution of in situ PDF studies performed at synchrotrons is on the order of ms, but many interesting processes occur on shorter timescales. Therefore, data measured at SACLA on HfO_2 nanoparticles in a liquid jet have been used to obtain a femtosecond PDF. This PDF has been compared to in situ PDF data measured on a capillary containing a suspension of HfO_2 nanoparticles at PETRA III, Deutsches Elektronen-Synchrotron (DESY)[5]. The SACLA PDF reproduce many of the features observed in the PETRA PDF with the same Q_{max}-value, but a higher Q_{max} is required to obtain better PDFs.

References

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Session Classification: Poster Session

Track Classification: Dynamics of functional materials