

3D-Printed Devices for *In Situ* X-ray Pair Distribution Function Experiments

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Total x-ray scattering for pair distribution function (PDF) analysis is a powerful and versatile tool for probing nanoparticle structures that are crystalline, partly disordered, or amorphous. Samples can be analyzed in a variety of different states *e.g.*, dry powders and liquid suspensions. Synchrotron PDF measurements can enable *in situ* investigations of dynamic processes such as nanoparticle crystallization, surface reactions (*e.g.*, adsorption), and phase transformations. However, real-time experiments need custom reactors that are both compatible with total x-ray scattering instruments and can achieve the desired fluid mixing and flow characteristics of a particular system. The most effective reactor designs are simple, yet adaptable for a wide variety of research objectives while being fabricated quickly and at low cost. Meeting these requirements will advance the development of structure-property-reactivity relationships for important types of natural and synthetic nanoparticles.

Desktop stereolithography (SLA) 3D printing can be used to fabricate custom experimental devices rapidly and at significantly lower cost than traditional manufacturing approaches (Michel *et al.*, 2018, *Appl Geochem* 89, 86-91). The 3D printed polymer used for fabrication is stable at a wide range of pH conditions and therefore highly suitable for aqueous (geo)chemical studies (Kletetschka *et al.*, 2018, *Appl Geochem* 98, 121-126). Digital input files for the reactors can be easily adapted and shared among research groups. We have begun using relatively large-volume (5-25 mL) 3D-printed mixed flow reactors for experimental PDF studies aimed at understanding calcium phosphate and ferric hydroxylsulfate mineral nucleation and growth.

We have also been developing novel 3D-printed microfluidics reactors for *in situ* PDF experiments. Microfluidics use small sample volumes and can operate at extremely short (<1 sec) to intermediate (10's of min) timescales. They can also be designed to achieve unique laminar fluid flow patterns with diffusive mixing conditions. Important reactions are known to occur at these conditions in geological environments (*e.g.*, soil pores, rock fractures), biological systems (microbial biofilms), and technological applications (porous filter media), but are challenging to study in the lab because laminar flow can be difficult to produce and control. This talk will provide an overview of SLA 3D printing, describe several reactor designs, and give examples of PDF structural data collected *in situ* from nanoparticle crystallization experiments.