Containerless PDF of Low-Density Materials Enabled by Acoustic Levitation

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Characterising short-range order in low-density or weakly scattering materials can be challenging when using X-ray total scattering experiments, which rely on high-Q data for real-space resolution. The form factors are Q-dependent, damping the signal at higher Q. During the data processing, corrections applied amplify the noise faster than the coherent signal and it can potentially lead to a misinterpretation of the structural information.

One of the corrections applied to the data is background subtraction, which includes contributions from the sample container (typically made of borosilicate glass or quartz). These materials alone can present higher scattering power than organic or low-density samples. As a result, small inaccuracies in background subtraction can be amplified by subsequent high-Q corrections, leading to spurious features in the generated PDF.

This study presents a containerless approach to total scattering data collection using acoustic levitation with the *SuperLev*. The SuperLev is a compact levitator with strong acoustic traps, developed by Bordes et al. [1] and further advanced by Docker et al. [2]. This method eliminates container scattering entirely and enables stable, controllable sample positioning during data collection.

The results obtained so far demonstrate that acoustic levitation provides a practical platform for containerless measurements, particularly in systems where weak scattering impedes accurate short-range structural analysis. The potential application of the SuperLev extends beyond PDF experiments, facilitating in-situ studies such as real-time crystallisation, minimising preferred orientation effects in powder diffraction, monitoring chemical reactions and investigate surface tension effects across a range of scattering techniques. Development and testing are underway at multiple beamlines at Diamond Light Source and in lab-based instruments to evaluate the extent of the applicability of SuperLev and to identify limitations associated with processing data from levitated samples.



Figure 1. *A droplet of liquid stabilised in the trap of the SuperLev.*

[1] Argyri et al., Journal of Colloid and Interface Science 640 (2023)
[2] Morris et al., Scientific Reports 9 12431 (2019)

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