



Analysis of diffuse scattering from liquid and amorphous samples: protocols and software

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Fostered by third-generation synchrotron sources, experimental studies of physical and chemical properties of liquids at high pressure and temperatures are constantly pushed towards more and more extreme conditions, with applications ranging from Earth and planetary science, to material science, to fundamental physics.

In the last 20 years, many efforts have been dedicated to the development of a method to obtain structural information from the X-ray diffuse scattering signal of a liquid [1], allowing, for instance, to improve our understanding of the structure and evolution of deep planetary interiors. However, while data collection protocols are by now quite advanced and overall comparable across beamlines worldwide, data analysis largely differs depending on user and employed codes. To answer to the need of a unified data analysis tool for liquids and amorphous systems, we developed Amorpheus [2].

Amorpheus is an open-source, versatile, free and easy-to-use software for the analysis of X-ray diffuse scattering signal, allowing to perform a customizable analysis of a large amount of data and to invert for the density. Available on GitHub [3] it is fully accessible by the community. This software has been tested on data collected with DAC and with large volume presses and it is well adapted for the analysis of liquid metals and alloys, as well as of amorphous systems. Here we will present and discuss selected examples of data analysis performed by Amorpheus in order to determine local structure and density of liquid iron binary and ternary alloys at planetary core conditions.

[1] Eggert JH, Weck G, Loubeyre P, Mezouar M. Quantitative structure factor and density measurements of high-pressure fluids in diamond anvil cells by x-ray diffraction: Argon and water. *Phys Rev B*. 2002;65(17):174105. doi:10.1103/PhysRevB.65.174105

[2] Boccato S, Garino Y, Morard G, et al. Amorpheus: a Python-based software for the treatment of X-ray scattering data of amorphous and liquid systems. *High Press Res*. 2022;42(1):69-93. doi:10.1080/08957959.2022.2032032

[3] <https://github.com/CelluleProjet/Amorpheus>

