Overcoming Challenges in High-Pressure Total Scattering: Radial Diffraction with Low-Z Metallic Glass Gaskets

A. Herlihy[1], S. Boccato[2], P. Botella[3], P. Chater[1], K. Georgarakis[4], J. L. Rodrigo-Ramon[3], S. Anzellini[3]

1 Diamond Light Source Ltd., Harwell Science & Innovation Campus, Diamond House, Didcot, OX11 0DE, UK, 2 Sorbonne Université, Muséum National d'Histoire Naturelle, UMR CNRS 7590, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, IMPMC 75005 Paris, France, 3 Departamento de Física Aplicada - Instituto de Ciencia de Materiales, Matter at High Pressure (MALTA) Consolider Team, Universidad de Valencia, Edificio de Investigación, C/Dr. Moliner 50, Burjassot, Valencia, 46100, Spain, 4 School of Aerospace, Transport and Manufacturing, Cranfield University, Cranfield, UK

anna.herlihy@diamond.ac.uk

Total scattering provides a powerful tool for resolving the local and long-range structural evolution of materials under extreme conditions. However, performing these measurements in diamond anvil cells (DACs) is technically demanding due to the intense parasitic scattering from the diamond anvils, which can obscure the sample signal in standard axial geometries.

While radial diffraction [1] through weakly scattering gaskets significantly mitigates this "contaminant" scattering, traditional gasket materials (e.g., Be, Boron-epoxy) often lack the mechanical or chemical compatibility required for many pressure-transmitting media.

In this work, we present a novel experimental approach developed at Diamond Light Source, utilizing low-Z metallic glass gaskets [2] to perform high-pressure total scattering. This setup allows for the recovery of high-quality local structure information from both amorphous and crystalline systems up to pressures of ~15 GPa. We discuss the optimization of radial scattering approaches and the data processing workflows necessary to extract reliable pair distribution functions (PDFs). Our results demonstrate that these metallic glass gaskets offer a robust alternative for high-pressure research, enabling new insights into several research areas including geophysics and the design of functional materials by providing a clearer window into local structural changes under pressure.

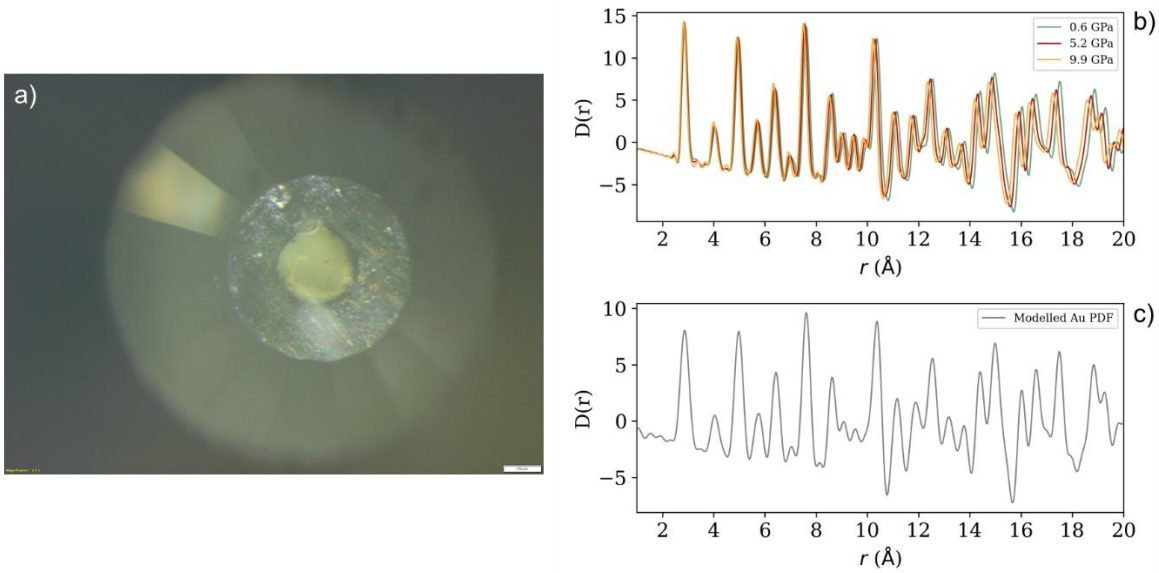


Figure 1. *a) Au loaded in a metallic glass gasket. b) PDFs generated from measurements of Au in a radial DAC equipped with a metallic glass gasket. c) A model Au PDF to show the excellent comparability between measured and modelled data.*

[1] S. Merkel & T. Yagi, Rev. Sci. Instrum. (2005) 76, 046109.

[2] W. Dong, K. Glazyrin, S. Khandarkhaeva, T. Fedotenko, J. Bednarčík, E. Greenberg, L. Dubrovinsky, N. Dubrovinskaiac & H.-P. Liermann, J. Synchrotron Rad. (2022). 29, 1167–1179.