MICROSCOPIC INVESTIGATION OF LASER SHOCKED GLASSY GEO$_2$

Emanuele Colonna (ESRF, FR),
Raffaella Torchio (ESRF, FR),
Carlo Meneghini (Roma Tre, IT),
J.A. Hernandez Colonna (ESRF, FR),
N. Sevelin-Radiguet Colonna (ESRF, FR),
T. Vinci (Ecole Polytechnique, FR),
M. Bethkenhagen (Ecole Polytechnique, FR),
A. Benuzzi (Ecole Polytechnique, FR),
F. Dorchies (CEA, FR),
V. Recoules (CEA-DIF, FR)

Abstract
Germanium dioxide (GeO_2) is an important structural and chemical analogue of SiO_2. Investigating GeO_2 can be advantageous thanks to its simple phase diagram under moderate (<100 GPa) static P, T conditions[1] and being more accessible to hard X-rays synchrotron techniques.
However, the analogy between GeO_2 and SiO_2 is still not fully established at more extreme and dynamic conditions. In particular, none of the GeO2 polymorphs – quartz, rutile and glass – has been investigated under dynamic P, T conditions using X-rays microprobes.
In this study, we have explored the structural and electronic evolution of glassy GeO_2 under laser-driven shock compression at High Power Laser Facility (HPLF) of the ESRF[2], up to 200GPa and 15000K, by ultrafast (100 ps) X-ray Absorption (XAS) measurements.
Online VISAR diagnostics and hydrodynamic simulations using the MULTI code, provide the pressure–temperature conditions reached along the Hugoniot and along release states. The XAS spectra reveal clear modifications of the local atomic structure, consistent with an increase in Ge coordination under compression. In parallel, we observe marked changes in the electronic structure and optical properties, indicating a progressive closure of the band gap.
These observations are supported by Principal Component Analysis (PCA), used to identify distinct structural regimes along the compression path, Fig. 1, and DFT-MD simulations, which reproduce the evolution of the electronic density of states and provide insight into the microscopic mechanisms driving the gap closure.
Our results provide the first direct microstructural constraints on glassy GeO_2 under dynamic compression up to 200GPa and establish ultrafast XAS as a powerful tool to probe structural and electronic evolution under extreme conditions.

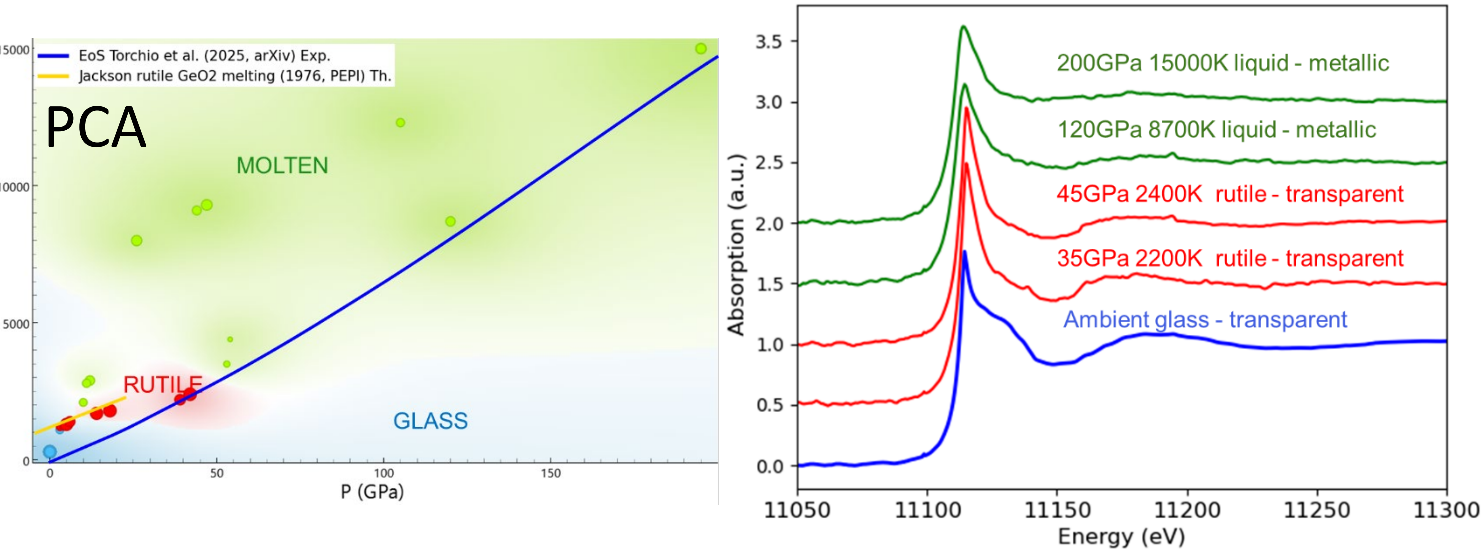

Fig. 1

[1]Prakapenka, Journal of Physics and Chemistry of Solids Volume 65, Issues 8–9, 2004, Pages 1537-1545
[2]Hernandez, The high power laser facility at beamline ID24-ED at the ESRF, High Pressure Research, 2024