NANO-SILICA UNDER EXTREME CONDITIONS : FROM NANO-POWDER TO GLASS TRANSITION

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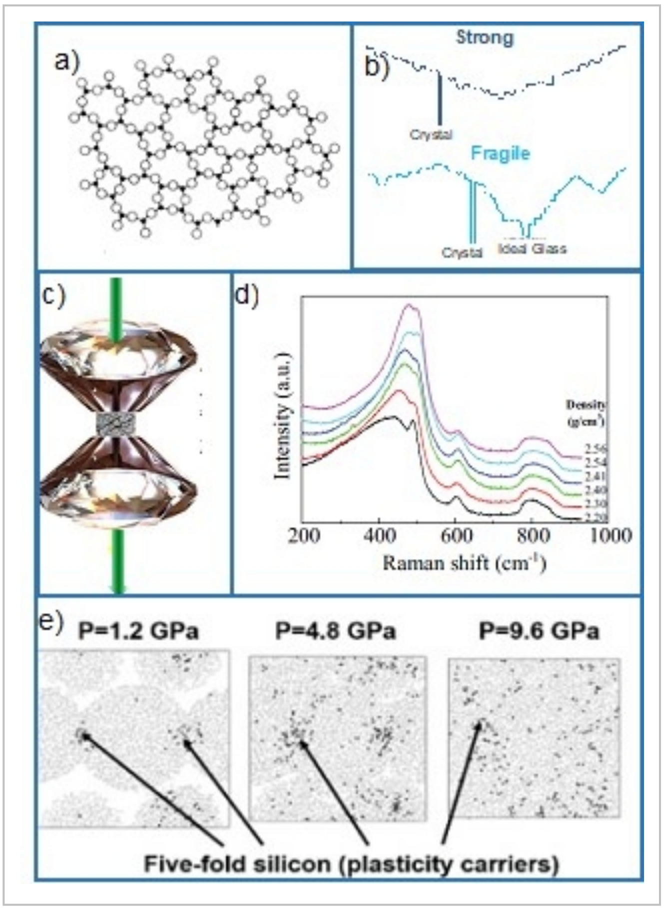
SCIENTIFIC CONTEXT :



Silicate glasses are ubiquitous in a many of applications, but their main drawback remains their fragility. Recent theoretical and experimental advances suggest that glass resulting from the compaction of nanoparticles could be the key to reducing this limitation. By adjusting factors such as the size of the nanoparticles or the consolidation pressure, it is possible to observe transition from the brittle phase to the ductile phase. The fundamental objective of this PhD proposal is to study and understand the mechanisms of the nano-meso transition of this amorphous phase when a pressure is applied. The aim of this study is to highlight a new amorphous silica phase, nano-compacted, with increased toughness compared with conventional SiO_2 glass resulting from the quenching of the supercooled liquid. Theoretical studies resulting from numerical simulations of molecular dynamics have confirmed the ductile behaviour of densified amorphous nanoparticles as the size of the silica nanoparticles decreases (fig.e)[1,2].

In this research, we aim to study the potential of these nanocompacted silicas to: (i) improve the ductility of amorphous silica (ii) explore the effect of nanometric size in the P-T phase diagram, possibly leading to new glassy states, and (iii) further our understanding of the elasto-plastic properties of free and compacted silica nanoparticles.

MISSIONS :

The PhD student will carry out in-situ and ex-situ vibrational spectroscopic studies of nano-silica under pressure (fig.c and fig.d). To do this, they will have to carry out these experiments under diamond anvil or belt press cells (pressure of up to 20 GPa) and at various temperatures (from room temperature to 1000°C). The spectroscopic monitoring carried out during and after the thermodynamic transformation will provide access to the structural deformations (size of the SiO_4 rings shown in Fig. a, for example) and to the changes in elastic and plastic properties undergone by the glass nanoparticles during compaction [3]. In subsequent studies, once the glass has been synthesised, it will be possible to access the elastic constants of the new glass (modulus of elasticity, Poisson's ratio, etc.) thus formed.

OUTLOOKS :

A more ductile glass

New glassy states

A better understanding of the physics of glass

BIBLIOGRAPHY :

[1] Brittle to ductile transition during compression of glassy nanoparticles studied in molecular dynamics simulations, M. Akl et al, J. Appl. Phys. 134, 035104 (2023)

[2] Silica Glass Toughened by Consolidation of Glassy Nanoparticles,Y. Zhang et al, Nano Lett. ,19, 8, 5222–5228(2019)

[3] Memory effect in the plasticity of a silicate glass densified at room temperature, T. Deschamps, C. Martinet et al., PR, 105 (22), 224206 (2022)