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High pressure pair distribution function study of amorphous silica in helium

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We characterized a-SiO_2 in helium by the high pressure PDF measurements of. High-pressure high-quality data were obtained using 61 Kev photons up to 22 $Å^{-1}$, Figure 1.

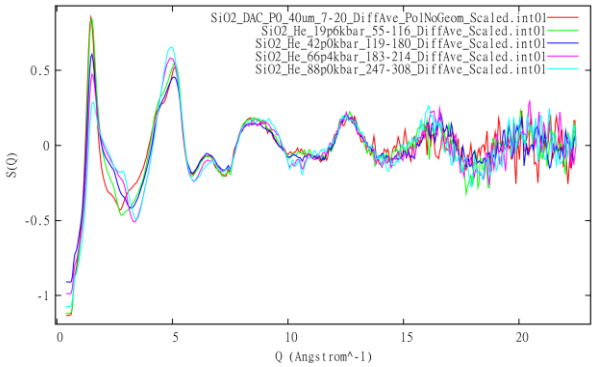

Figure 1 : High pressure PDF measurements of a-SiO_2 in helium up to 8.8 GPa.

The total scattering data was refined by the reverse Monte Carlo (RMC) method[1] in order to obtain changes to bond-angle distributions and network topology of a-SiO_2 in helium as a function of pressure. Figure 2 shows helium adsorbed on silica as a function of pressure which are in perfect agreement with theoretical predictions[2].

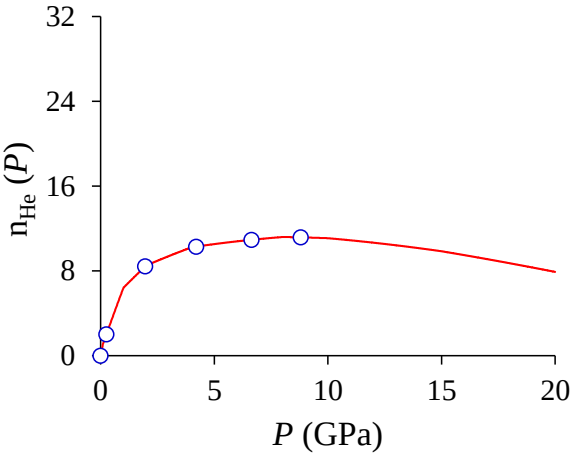

Figure 2 : Pressure dependence of the amount of He atoms adsorbed by SiO_2 silica based on PDF data (open blue dot) and predicted by the poroelastic model in unjacketed conditions[2] (red line).

Partial PDFs were obtained, Figure 3, and permitted to understand the structural modifications induced by the helium adsorption at high pressure which consist in: i) a broadening of the Si-Si bond distribution(inter-tetrahedra distances) in the first and second coordination shells; as a consequence appearance of a new

contribution is also observed above 3 Å for the Si-O PDF, ii) a decrease in the O-He distance distribution with increasing pressure which becomes more ordered as a result of helium confinement.

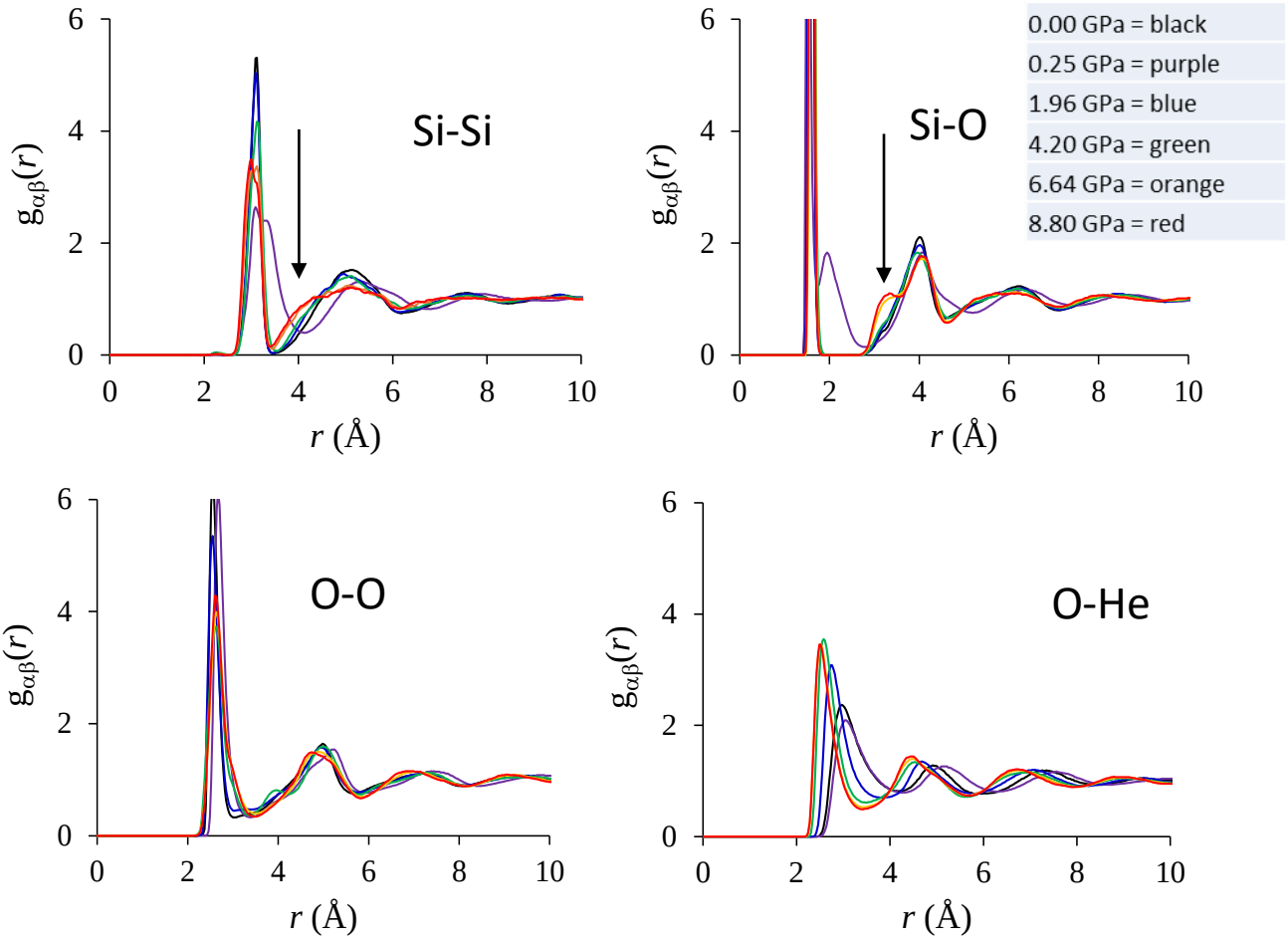

Figure 3 : Partial PDFs obtained based on RMC method. Note that data obtained at 0.25 GPa has to be ignored as data subtraction from the empty DAC (without helium) did not remove entirely the Bragg contribution from the diamond.

References

[1] M. G. Tucker, D. A. Keen, M. T. Dove, and K. Trachenko, Journal of Physics-Condensed Matter **17**, S67 (2005).

[2] B. Coasne, C. Weigel, A. Polian, M. Kint, J. Rouquette, J. Haines, M. Foret, R. Vacher, and B. Ruffle, J Phys Chem B **118**, 14519 (2014).