Structure of High-pressure Liquids: X-ray Diffraction and RMC Modelling

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With the arrival of the latest generation of synchrotron sources and the introduction of advanced insertion devices (wigglers and undulators), the high-energy (E > 30 keV) X-ray diffraction technique has become feasible, leading to new approaches in the quantitative study of the structure of simple liquids at high pressure.

We report reliable diffraction data of high-pressure liquids in a diamond anvil cell (DAC), measured at the SPring-8 high-energy X-ray diffraction beamline BL04B2 using 37.6 keV X-rays. Moreover, we performed reverse Monte Carlo modelling [1] to investigate structural modification of the liquids under high pressure. The resulting large structural models (sets of thousands of atomic coordinates) were subjects of geometrical analyses: distributions of the number of first neighbours, as well as local angular correlations have been calculated. In the cases of molecular liquids investigated (like the case of liquid O_2), correlations between orientations of neighbouring molecules have been characterized.

[1] McGreevy R.L., Pusztai L., *Mol. Simul.,* 1988, **1**, 359.

Keywords: high-pressure x-ray diffraction, diamond anvil cells, computer modelling liquids