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Measuring the structure factor of simple fluids under extreme conditions

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The structure and dynamics of fluids, although a long standing matter of investigations, is still far from being well established. In particular, with the existence of a first order liquid-liquid phase transition (LLT) discovered in liquid phosphorus at 0.9 GPa and 1300 K [1] it is now recognized that the fluid state could present complex structural changes. At present, very few examples of LLTs have been clearly evidenced, which may mean that a larger range of densities must be probed. First order transitions between a molecular and a polymeric liquid have been recently predicted by first principles calculations in liquid nitrogen at 88 GPa and 2000 K [2] and in liquid CO_2 at 45 GPa and 1850 K[3]. The only device capable of reaching these extreme conditions is the diamond anvil cell (DAC), in which, the sample is sandwiched between two diamond anvils of thickness 100 times larger. Consequently, the diffracted signal from the sample is very weak compared to the Compton signal of the anvils, and becomes hardly measurable for pressures above $\sim$20 GPa. A similar problem has been faced by the high pressure community using large volume press so as to drastically reduce the x-ray background from the sample environment. In the angle-dispersive diffraction configuration, it was proposed to use a multichannel collimator (MCC) [4]. This solution has been implemented to fit the constraints of the Paris-Edimburg (PE) large volume press and it is now routinely used on beamline ID27 of the European Synchrotron Radiation Facility [5,6]. In this contribution, we present our adaptation of the MCC device accessible at ID27 for the DAC experiment. Because of the small sample volume a careful alignment procedure between the MCC slits and the DAC had to be implemented. The data analysis procedure initially developed by Eggert et al. [7] has also been completed in order to take into account the complex contribution of the MCC slits. A large reduction of the Compton diffusion from the diamond anvils is obtained enabling quantitative structure factor measurement, even for the weakest x-ray scatterer liquid. Experimental results on fluid hydrogen will be presented to test the limits of this new setup. In collaboration with Gaston Garbarino, ESRF, France; Frederic Datchi, Sandra Ninet, Université Pierre et Marie Curie-Paris VI, France; Dylan Spaulding, Paul Loubeyre, CEA, DAM, DIF, France; and Mohamed Mezouar, ESRF, France.

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