



	Experiment title: Equation of state of superhard 3D C60 polymers	Experiment number: HS1209
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Report:

C60 molecules polymerise under high-pressure high-temperature (HP-HT) forming, according to Pressure-Temperature conditions, 1D, 2D and 3D crystalline polymers. 3D polymers form a three-dimensional network of covalent bonds between cages (zeolite-network type) and are expected to exhibit high hardness [1]. Indeed, theoretical calculations predict for this material bulk modulus as high as 300-400 Gpa (just below the diamond value) [2]. It can thus be considered a low-density super-hard material.

The compressive properties of the 3D polymers have been studied at room temperature using diamond anvil techniques. A methanol-ethanol mixture and argon have been used as pressure transmitting medium ensuring hydrostatic conditions. Up to the maximum pressure reached, 35Gpa, the 3D polymers are stable [3]. Therefore, they have larger pressure-domain stability than the C60 monomer that collapse into sp³ carbon at 20Gpa.

Preliminary data analysis shows that the Debye–Sherrer ellipses displayed by the 3D C60 polymers are conserved up to the maximum pressure indicating that both kinds of bonds resist equally to the applied pressure. From lattice parameters dependence on pressure, the equation of state has been derived and the bulk modulus obtained. The large bulk modulus observed, around 300 Gpa [3], indicate that 3D polymers are low compressible materials although more compressible than diamond., in contrast to what has been stated by Serebryanaya and co-workers [4]. This systems with a density of 2.64g/cm³ can be classified as a low-density low-compressibility material.

The ellipsoidal nature of the Debye-Sherrer patterns was an additional problem in modelling the pressure dependence of peak positions and then in determining the equation of state. The determination of pressure stability of these systems is intended to be pursued by demanding extra beam time allocation at the ESRF.

[1] L.Marques et al. *Science*, 283, 1720 (1999); M.Mezouar et al. *ESRF Newsletter* n°33, 7 (1999).

[2] E. Burgos et al. *Phys. Rev. Lett.* 85, 2328 (2000); S.Okada et al. *Phys. Rev. Lett.* 83, 1986 (1999); A. San Miguel et al. 83, 5290 (1999).

[3] M. Mezouar, L.Marques, J-L. Hodeau, V. Piscedda M. Núñez-Regueiro (submitted to *Phys. Rev. Lett.*)

[4] N. Serebryanaya et al. *Sol. State Comm.* 118, 183 (2001)