Carbon clathrates from fullerite under high pressure

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C60 fullerite displays a very rich phase diagram with a plethora of interesting new phases with new structural architectures. At pressures below 8 GPa different C60 polymers, based on 2+2 cycloaddition polymeric bond, have been found: a 1D polymeric phase and two 2D polymeric phases, involving square or triangular polymerized planes [1]. It must be noted that these high-pressure polymeric phases can be quenched to room conditions. Also in this pressure range but for temperatures above 850ºC, C60 cages collapse irreversibly transforming into an amorphous sp2-carbon phase. Despite its graphitic nature this amorphous phase displays remarkable super-hard properties [2]. At pressures above 8GPa, and in contrast to low-pressure range, the phase diagram of C60 fullerite is not elucidated. We have used the Paris-Edinburgh large-volume press, employing sintered diamond anvils, to extend the analysis of the fullerite phase diagram to higher pressures [2]. The synchrotron diffraction patterns displayed by C60 samples compressed above 10GPa are complex indicating heterogeneous samples composed of several different phases and/or partial transformed grains. Despite this complexity the x-ray diffraction analysis clearly shows that C60 fullerite forms 3D polymers. The molecular near-neighbor (NN) distances in these 3D polymers are much smaller than the one corresponding to the 2+2 cycloaddition bond characteristic of the low-pressure polymers. This indicates that new intermolecular bonding schemes come into play at these pressures. Unfortunately the poor-crystallized samples, in addition to its heterogeneity, did not permit to obtain the detailed atomic structure of these new 3D polymeric phases, preventing the elucidation of the intermolecular bonding active at these pressures. It must be noted, and in contrast to low-pressure polymers, that the transformations above 10GPa are not reversible and thus these 3D polymers can be better viewed as carbon clathrates.

References

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