First observation of the FCC to Rhombohedral transition of dimerized C_{60} under high-pressure

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Subjecting the monomeric FCC phase of C_{60} to high-pressure leads to the progressive disordering and hardening of this material whilst preserving its symmetry. By contrast, the application of high-pressure to a preformed polymeric phase such as 1D-Immm [1] or 2D-Immm [2] yields new polymerized phases with 3D ordering.

The present work focuses on the influence of high-pressure on the crystal structure of a pure dimeric phase of C_{60} by making use of in-situ high-pressure laboratory X-ray powder diffraction in a diamond anvil cell.

The starting FCC dimeric C_{60} material was carefully characterized using synchrotron X-ray powder diffraction at the ESRF/SNBL BM01A beamline operated with a wavelength of 0.4989 Å. The cubic symmetry was confirmed, with a lattice parameter a = 14.0 Å.

The in-situ high-pressure experiment was carried out using Mo Kα laboratory X-rays. The cubic to rhombohedral transition was observed in the 1.2 to 8 GPa pressure range. The volume per C_{60} unit was deduced from Le Bail fits to X-ray powder diffractograms and estimated to decrease from 689 $Å^3$ (at ambient pressure) to 560 $Å^3$ (at 8 GPa).

Whereas the transformation within this pressure range was found to be reversible, a further increase of pressure leads to the irreversible formation of a disordered phase. A possible mechanism which may account for the observed cubic to rhombohedral transition will be presented.

[1] R. Le Parc, C. Levelut, J. Haines, V.A. Davydov, A.V. Rakhmanina, R.J. Papoular, E.E. Belova, L.A. Chernozatonskii, H. Allouchi and V. Agafonov, *Chem. Phys. Lett.* **438**, 63 (2007).

[2] D.H. Chi, Y. Iwasa, T. Takano, T. Watanuki, Y. Ohishi, S. Yamanaka, *Phys. Rev. Phys. B.* **68**, 153402 (2003).