

## High-pressure 3D C<sub>60</sub> fcc polymer

J. Laranjeira<sup>a</sup>, L. Marques<sup>a</sup>, M. Melle-Franco<sup>b</sup>, K. Strutyński<sup>b</sup>, M. Mezouar<sup>c</sup> and M. Barroso<sup>d</sup>,

<sup>a</sup> Departamento de Física and CICECO, Universidade de Aveiro, 3810 Aveiro, Portugal.

<sup>b</sup> Departamento de Química and CICECO, Universidade de Aveiro, 3810 Aveiro, Portugal.

<sup>c</sup> E.S.R.F., BP220 38043 Grenoble, France.

<sup>d</sup> Departamento de Física and I3N, Universidade de Aveiro, 3810 Aveiro, Portugal.

OA63

A new C<sub>60</sub> polymerized face-centered cubic (fcc) phase has been obtained at 9 GPa and 550°C. The high-pressure high-temperature polymerization process was followed *in situ* through synchrotron x-ray diffraction. The short lattice constant, 13.19Å, displayed by the recovered samples indicates that a three-dimensional polymer has been prepared, although the determination of its crystal structure was hampered by the low-resolution diffraction data. We have performed density functional theory (DFT) investigations of possible C<sub>60</sub> polymerized structures, with molecules adopting one of the two standard orientations, which are compatible with cubic crystal lattices. Ordered binary-alloy-type structures (AuCuI, Au<sub>3</sub>Cu, CuPt, “A<sub>2</sub>B<sub>2</sub>”) were used as prototypes in constructing these theoretical structures, with one standard orientation corresponding to the A atom and the other orientation to the B atom. The DFT calculations show that intermolecular bonds, 56/56 2+2 cycloaddition, are formed between molecules with different orientations but no bond is formed between molecules with the same orientation. Although the calculated distances between neighboring molecules, at room pressure and at 9.5 GPa, are close to the experimental value, these DFT structures display symmetries lower than cubic, suggesting that the experimental fcc structure is disordered/frustrated with the two standard molecular orientations, and thus the 56/56 2+2 cycloaddition bonds, occurring at random [1]. The electronic and elastic properties of such polymeric structures were also calculated, at room pressure and at 9.5 GPa. All these structures show metallic behavior [2] and their bulk moduli ranges between 88 and 132 GPa [3].

[1] J. Laranjeira, L. Marques, M. Mezouar, M. Melle-Franco, K. Strutyński, Phys. Stat. Sol. RRL 11 (2017) 1700343.

[2] J. Laranjeira, L. Marques, N. Fortunato, M. Melle-Franco, K. Strutyński, M. Barroso, Carbon 137, (2018) 511-518.

[3] J. Laranjeira, L. Marques, N. Fortunato, M. Melle-Franco, K. Strutyński (to be published).

Acknowledgement: part of this work was developed within the scope of the project POCI-01-0145-FEDER-031326 financed by FCT and co-financed by FEDER.

Presenting author: Jorge Laranjeira, CICECO, Complexo de Laboratórios Tecnológicos, Campus Universitário de Santiago 3810-193 Aveiro, Portugal. [jorgelaranjeira@ua.pt](mailto:jorgelaranjeira@ua.pt)  
00351914410266