STRUCTURAL STUDIES OF DISORDERED CARBONS - COMPARISON OF SIMULATIONS AND HIGH-ENERGY X-RAY DIFFRACTION DATA

L. Hawelek [1*], A. Brodka [1], J.C. Dore [2], V. Honkimaki [3], and A. Burian [1]

[1] *A. Chelkowski Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland*

[2] *School of Physical Sciences, University of Kent, Canterbury, CT2 7NR, UK*

[3] *European Synchrotron Radiation Facility, BP 220, 38043 Grenoble, France*

Keywords: X-ray diffraction, activated carbons, structure, molecular dynamic, density functional theory

**) e-mail: hawelek@us.edu.pl*

The X-ray diffraction measurement was carried out for sample of disordered, commercially produced carbon CXV on the ID15B beam-line at the European Synchrotron Radiation Facility (ESRF), Grenoble, France (Fig. 1).

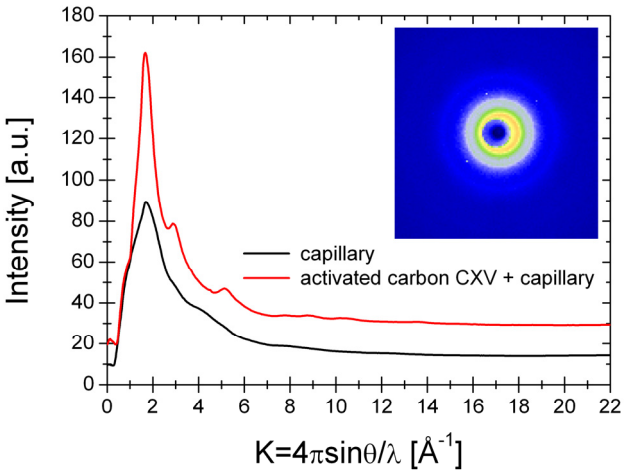

Figure 1. Comparison of the experimental intensities for the activated carbon CXV with capillary and the empty capillary. The 2D diffraction intensity for the CXV sample presented in the inset.

The obtained results show that the structure of the studied sample consists of two graphite like layers, stacked without spatial correlations. The size of the ordered region was described by the model of 4.5 Å in radius. The disordered structure was simulated by introducing the Stone-Wales defects (pair of two pentagons and two heptagons), randomly distributed in the network. The optimisation of those disordered carbon structure was performed by combining the classical molecular dynamic simulation using the REBO2 (the reactive bond order) potential [1] with the density functional theory using B3LYP functional method [2,3]. In Fig. 2 the relaxed atomic arrangement using the REBO2 potential is displayed. The Grimme's empirical Van der Waals correction was used [4]. Finally, the HOMO-LUMO molecular orbitals calculated using the 6-31g* basis set for such carbon were compared.

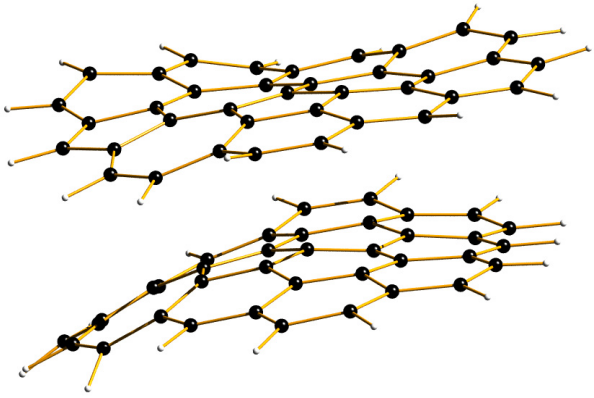

Figure 2. Arrangement of carbon (black) and hydrogen (grey) atoms for the model of the CXV after geometry optimisation using molecular dynamics simulation with REBO2 potential.

References

[1] D.W. Brenner, O.A. Shenderova, J.A. Harrison, S.J. Stuart, N. Boris, S.B. Sinnott, "A second-generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons", *J. Phys.: Condens. Matter* **14** (2002) 783–802.

[2] A.D. Becke, "Density-functional thermochemistry. III. The role of exact exchange", *J. Chem. Phys.* **98** (1993) 5648–5652.

[3] C. Lee, W. Yang, R.G. Parr, "Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density", *Phys. Rev. B* **37** (1988) 785–789.

[4] S. Grimme, "Semiempirical GGA-type density functional constructed with a long-range dispersion correction", *J. Comput. Chem.* **27** (2006) 1787–1799.