The atomic structure of glassy carbon foams

Karolina Jurkiewicz*†[1,2], Cyril Schmidt[3], Barbara Liszka[4], Stanisław Duber[4], and Andrzej Burian[1,2]

[1]Institute of Physics, University of Silesia in Katowice (POLAND) – Poland
[2]Silesian Centre for Education and Interdisciplinary Research (POLAND) – Poland
[3]Ecole d'Ingénieur CESI (FRANCE) – Ecole d'Ingénieur CESI (FRANCE) – France
[4]Faculty of Earth Sciences, University of Silesia in Katowice (POLAND) – Poland

Abstract

Recently, there has been an intense interest in carbon foams for a variety of engineering applications due to their superior mechanical, electrical and thermal properties. Glassy carbon foams are produced by the pyrolysis process using organic resins as the precursors. By controlling the synthesis conditions it is possible to adjust the porous structure of the foams in terms of bulk density, cell size and connectivity, but also the atomic structure which directly affects their final properties. Glassy carbon foams have disordered structure that is intermediate between crystalline graphite and amorphous carbon. Since the atomic arrangement is complex allowing coexistence of different bonds between carbon atoms, and very sensitive to the synthesis temperature, there is a need to use advanced tools for their characterization. Here, we use methodology based on the molecular dynamics simulations and their experimental verification by the wide-angle X-ray scattering to describe the atomic structure of glassy carbon foams pyrolyzed at different temperatures. The obtained diffraction data are converted to a real space representation in the form of the atomic pair distribution function. The applied pair distribution function analysis shows that the glassy carbon foams have a local order extending on the length scale of nanometers, in which carbon atoms are arranged in fullerene-related, curved units. The results of the computer simulations suggest that the curvature can arise from the presence of topological defects in the form of nonhexagonal carbon rings.

Keywords: glassy carbon foams, atomic structure, pair distribution function

*Speaker
†Corresponding author: karolina.jurkiewicz@us.edu.pl