Porosity and local structure studies of carbon materials using synchrotron radiation

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The synthesis of disordered carbons with a precisely controlled porosity and degree of graphitic order is desirable for a wide range of applications, e.g., for electrode materials. Considerable research efforts have been directed towards the creation of micro- and nanostructured electrode designs with complex systems of pores reaching sizes from the nano-dimensions up to the macro-scale [1]. The materials contain both open and closed pores, which are unattainable by standard gas sorption methods. Moreover, the atomic-scale structure of a wide range of porous carbons is not crystalline and its thorough characterization requires the use of advanced analysis of the diffraction data going beyond the crystallography. The situation is even more complicated when the carbon structure is linked in a composite system with another material.

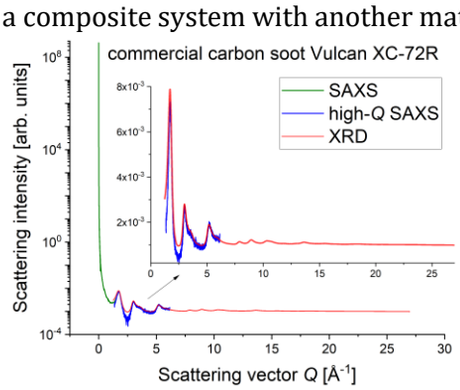

Figure 1. Combination of synchrotron SAXS and XRD data for carbon soot.

Here, we used the high-energy X-ray scattering (diffraction) combined with the pair distribution function (PDF) and small-angle X-ray scattering (SAXS) to derive a description of the arrangement of atoms within carbon individual layers, inter-layer correlations and the porous structure over wide range of length scales for a series of disordered carbons. The use of the connected SAXS and X-ray diffraction data offers an opportunity of their joint Fourier transform providing total information about the porous structure as well as the atomic structure [3]. This will allow for construction of realistic structural models of carbon materials and is critical for predicting their properties and design of their applications.

We present preliminary results from the measurements collected at the 9-ID-B,C (SAXS) and 11-ID-B (PDF) beamlines at the Advanced Photon Source and the methods of their analysis. As an example, Figure 1 shows the combination of the collected X-ray scattering data from the two beamlines, at the SAXS and PDF-dedicated diffraction instruments. Whereas the oscillating component of the PDF gives information about the interatomic distances within the material [3], the PDF baseline is related to particle shape which has its origin in the SAXS, but is usually disregarded in standard diffraction experiments. Given the relationship between the PDF and SAXS data, there is potential benefit in simultaneous analysis of both function for refinement of structural models of materials.

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