An advanced evaluation method for the analysis of Wide-Angle X-ray Scattering (WAXS) data of non-graphitic carbons

Felix Badaczewski[1], Marc O. Loeh[1], Torben Pfaff[1], Bernd M. Smarsly[1]

[1](Institute of Physical Chemistry, Justus Liebig University,
Heinrich-Buff-Ring 17, 35392, Giessen, Germany)

Wide-angle X-ray scattering (WAXS) is next to Raman spectroscopy and transmission electron microscopy one of the few suitable techniques for the structural characterization of non-graphitic carbons. However, as non-graphitic carbons exhibit turbostratic disorder, WAXS patterns of these carbons usually contain only diffuse and overlapping reflections, which hinder the use of standard evaluation approaches like the Scherrer formula.

Therefore, we present an advanced evaluation technique for WAXS data of non-graphitic carbons in order to attain quantitative insights into the carbonaceous microstructure on the nanometer scale. The basic principle of this evaluation by Ruland and Smarsly is based on the fitting of the whole WAXS pattern by a theoretical function, providing a range of physically meaningful parameters describing the carbon microstructure, such as the average interlayer spacing, the average stack height, the lateral extent of the carbon layers.

The application of this model and the results of different studies are presented:

First, the temperature-induced evolution of the carbon microstructure of several coal tar pitches, which exhibit distinctly different elemental and molecular compositions, was systematically investigated. The results revealed an almost identical development of the carbon microstructure.

Second, the structural evolution of non-graphitizing carbons was investigated by a combined small- and wide-angle scattering analysis. The results yielded comprehensive insights into the relation between the graphene microstructure and the inaccessible porosity upon heat treatment of glassy carbons.

Third, the influence of spatial confinement on the microstructural development of carbon replicas experienced throughout a nanocasting process in monolithic SiO_2 is quantitatively examined.

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