Comparative microstructural analysis of non-graphitic carbons (NGCs) based on wide-angle X-ray (WAXS) / neutron (WANS) scattering as well as pair distribution function (PDF) analysis

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NGCs represent the most abundant class of sp^2-hybridized carbon materials and are made up of small graphene layer stacks possessing significant structural disorder both in the single graphene sheets and the stacking. Nevertheless, a quantitative description of this disordered sp^2 polyaromatic microstructure is desirable.

In 2002 Ruland and Smarsly introduced a novel NGC microstructural characterization approach based on WAXS data evaluation. The microstructure is described by several parameters describing physical dimensions (like the average graphene layer extent L_a) and disorder providing a meaningful structural characterization. However, WAXS suffers from experimental and physical limitations diminishing the general validity of the NGC analysis by WAXS. Therefore, using WANS instead provides fundamental advantages.

In this study first the aforementioned evaluation approach was adopted to WANS data and applied to several different NGC samples. The analysis yielded microstructural parameters which were compared with parameters obtained from WAXS data analysis. A good agreement within the error margin was found proving the model's validity for NGCs WANS data.

Second, we investigated how reliably the originary microstructure can be reconstructed from WAXS/WANS by fitting simulated WAXS/WANS curves being impaired both by different noise levels and 2θ-cut-offs. These analyses revealed that the quality of WAXS data acquired with a standard Cu-K_α laboratory diffractometer is sufficient for a reliable analysis of the NGC microstructure.

Third, the comparison of PDF and WAXS/WANS fitting analysis revealed the presence of small highly ordered oligoaromatic domains embedded in the larger graphene sheets of size L_a, contrasting the classical view on the NGC microstructure.