Model free analysis of Small Angle Scattering data of mesoporous and microporous carbons

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Small Angle Scattering (SAS) with X-rays and neutrons is a powerful tool for structure analysis of meso- and microporous materials, i.e. carbons. Usually for analysis of SAS data, an assumption about the shape of the scatterer has to be made to fit the scattering curve. Structural investigations of microporous carbons are especially challenging as the shape of the pores inside the carbon matrix is still under debate.

We present a model free analysis approach of SAS data that allows a quantitative structural analysis of microporous materials in terms of a two-phase system. This allows the determination of the inner surface as well as the porosity with great precision in a range of pore sizes depending on the q-range. Special emphasis is put on the necessary data correction for carbonaceous materials.

Additionally, the pore scattering is analyzed by utilizing the chord length distribution (CLD). From the CLD a slit like pore shape with a considerable amount of sharp edges is concluded (see figure). Furthermore, mean pore sizes as well as pore wall sizes are extracted. The power of the CLD analysis is demonstrated on commercially available as well as synthesized carbon samples, i.e. carbon fiber cloth [1] and carbide derived carbons synthesized at different temperatures [2]. Furthermore, the effect on the structural parameters of the pores in the perspective of filling the micro pores with Sulphur via melt infusion [3] or electrode preparation by adding binder to carbon powder[4] will be presented and discussed.

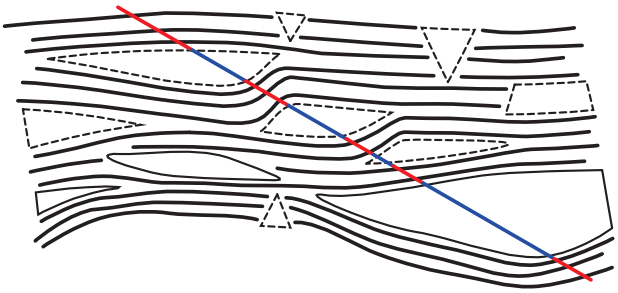

Figure 1. Pore structure (dashed areas) formed by distorted carbon layers (solid black lines). Selected chord going through pores (blue) and solid material (red).

References:
[1] Jafta, C. J.; Petzold, A. *et al.* (2017). *Carbon* **123**, 440-447.
[2] Härk, E.; Petzold, A. *et al.* (2019). *Carbon* **146**, 284-292.
[3] Petzold, A.; Juhl, A. *et al.* (2016). *Langmuir* **32** (11), 2780-2786.
[4] Härk, E.; Petzold, A. *et al.* (2019). *Microporous and Mesoporous Materials* **275**, 139-146.