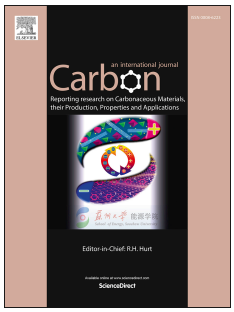
Accepted Manuscript



The suitability of infinite slit-shaped pore model to describe the pores in highly porous carbon materials

H. Kurig, M. Russina, I. Tallo, M. Siebenbürger, T. Romann, E. Lust

PII: S0008-6223(16)30049-5

DOI: 10.1016/j.carbon.2016.01.061

Reference: CARBON 10681

To appear in: *Carbon*

Received Date: 14 October 2015

Revised Date: 12 January 2016

Accepted Date: 15 January 2016

Please cite this article as: H. Kurig, M. Russina, I. Tallo, M. Siebenbürger, T. Romann, E. Lust, The suitability of infinite slit-shaped pore model to describe the pores in highly porous carbon materials, *Carbon* (2016), doi: 10.1016/j.carbon.2016.01.061.

The suitability of infinite slit-shaped pore model to describe the pores in highly porous carbon materials

H. Kurig,[1] M. Russina,[2] I. Tallo,[1] M. Siebenbürger,[2] T. Romann,[1] E. Lust[1]*

[1] *Institute of Chemistry, University of Tartu, Ravila 14a, 50411 Tartu, Estonia*

[2] *Helmholtz Zentrum Berlin, 14109 Berlin, Germany*

Abstract

The slit-shaped pore model is often assumed to be the most suitable to describe the pores in micro-/mesoporous carbon materials. This article analyses the suitability of this assumption when pore size distribution of carbon materials is calculated applying non-local density functional theory (NLDFT) to nitrogen adsorption isotherms. For further insight, three micro-/mesoporous carbide derived carbons (CDC-s) synthesised from SiC, TiC and Mo_2C, respectively, and denoted as SiC-CDC, TiC-CDC and Mo_2C-CDC, were characterized with nitrogen sorption, small angle neutron scattering (SANS) and Raman spectroscopy methods. Although the SANS and NLDFT with slit-shaped pore model produced coinciding results for pore widths, it was found that the pores in all three carbon materials have different shapes and width-to-length ratios. Pores in SiC-CDC can be approximated to sphere-like, in TiC-CDC to cylinder-like and in Mo_2C-CDC to slit-like shape. It was also suggested that the pore length may contribute significantly to the pore size distribution calculated using NLDFT model. Thus, the shape of pores in the carbon material investigated should be verified before the performance of carbon materials is explained in detail by the size and porous structure of micro-/mesoporous carbon materials.

* Corresponding Author: e-mail: enn.lust@ut.ee