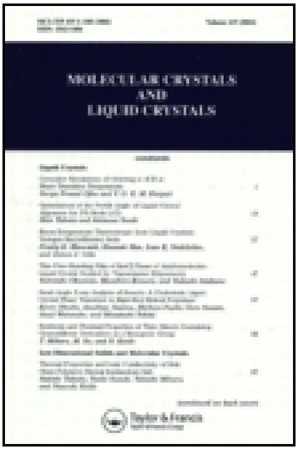

Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

Evaluation of Interparticle Pore Network of Porous Carbon Material Using Macro Crystal Model

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Version of record first published: 18 Oct 2010

To cite this article: Takaomi Suzuki, Hideaki Ito & Shuji Oishi (2002): Evaluation of Interparticle Pore Network of Porous Carbon Material Using Macro Crystal Model, Molecular Crystals and Liquid Crystals, 388:1, 63-66

To link to this article: http://dx.doi.org/10.1080/713738881

Mol. Cryst. Liq. Cryst., Vol. 388, pp. [477]/63–[480]/66
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1058-725X/02 $12.00 + .00
DOI: 10.1080/10587250290113871

EVALUATION OF INTERPARTICLE PORE NETWORK OF POROUS CARBON MATERIAL USING MACRO CRYSTAL MODEL

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Capillary rise of cyclohexane and water on graphite powder was measured in order to evaluate the interparticle pore network. The reduced diameter (d) of the pore network was determined from the sorbed height of cyclohexane using Young-Laplace equation. The effectiveness of the d* value was examined by calculation of the contact angle of water on graphite powder surface from the sorbed height of water. It was clear that d* has serious relationship with the average pore width of this macro crystal model. Though we have a possibility to adopt the idea of d* on micropore system, the real meaning of d* is still not clear.*

Keywords: porous carbon; capillary rise; pore network

INTRODUCTION

The micropore of activated carbon fiber (ACF) is often approximated as slit-shaped pore, and there are several established methods of analysis of nitrogen adsorption isotherms [1,2]. We tried to reproduce nitrogen adsorption isotherms using grand canonical Monte Carlo (GCMC) simulation with slit-shaped micropore model, but simulated isotherms were not close to experimental nitrogen adsorption isotherms [3]. Microporous carbons, such as activated carbons, are composed of micro graphitic crystallites, and the interstice of the graphitic crystallites composes complicated network of micropore. Ideal slit-shaped part of micropore in the real ACF system is rare. Therefore, a simple slit-shaped model is too crude for approximation of micropore system in porous carbon such as ACF. We also have observed dynamic structural change of graphitic crystallites of ACF during molecular adsorption using in situ X-ray diffraction [4]. For example, d_{002} of cellulose base ACF decreases from 0.43 nm to 0.34 nm by saturated water adsorption. The structural change of pore wall should accompany the structural change of micropores. The above-mentioned phenomena indicate that the idea of "pore size" for porous carbon is very ambiguous. Here we introduce a macro crystal model in order to study the quantitative treatment of the complicated pore network of porous carbon.

EXPERIMENTAL

SP1 graphite (Union Carbide) was used as power-like sample, and cyclohexane (Wako 98%) and distilled water were used as liquid samples. The crystal size of SP1 graphite was 20–150 μm. The SP1 graphite crystals were divided into different crystal size groups through stainless steel mesh sieve and were filled in glass tubes with inside diameter of 8 mm. The glass tubes filled with SP1 graphite crystals were supported vertically, and the bottoms of the glass tubes were immersed into flask containing the liquid sample. The systems were kept at 303 K. The capillary rise of cyclohexane or water to the samples filled in the glass tube was observed as the height of the sorbed liquid surface.

RESULTS AND DISCUSSION

The heights of sorbed cyclohexane and water by capillary rise as functions of average particle size, $\bar{x}$, of SP1 are shown in Figure 1. Though there are some exceptions, the smaller crystal size was, the larger amount of sorption was observed. In order to indicate the size of interstice, we determined the reduced diameter, d^*, as following Young-Laplace equation:

$$d^* = \frac{4\gamma \cos\theta}{h\rho g} \tag{1}$$

where γ, θ, h, ρ, and g, are surface tension, contact angle, sorbed height, density of the liquid, and gravity constant, respectively. This reduced pore diameter is considered to depend on the average diameter of interstice network between the crystals. Cyclohexane droplet well wetted the graphite surface, and the contact angle was approximated as zero. The relationship between d^* determined by cyclohexane sorption and $\bar{x}$ is shown in Figure 2.

The sorbed height of water by capillary rise was less than half of that of cyclohexane as shown in Figure 1. Because the contact angle of water on graphite surface was difficult to determine, d^* was not determined from the sorbed height of water. Therefore, we calculated the contact angle of water from d^* determined by cyclohexane sorption and the sorbed height of water using Eq. (1), and it was 87 ± 2 degree. The regularity of the

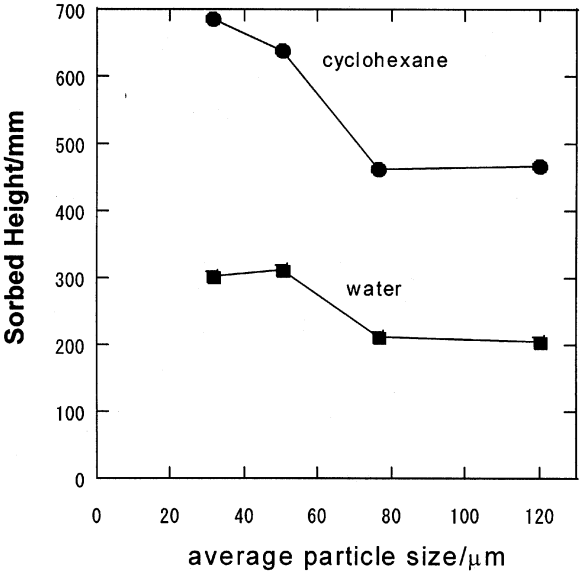

FIGURE 1 Sorbed height of cyclohexane and water on SP1 graphite crystals as functions of average particle diameter of the crystals.

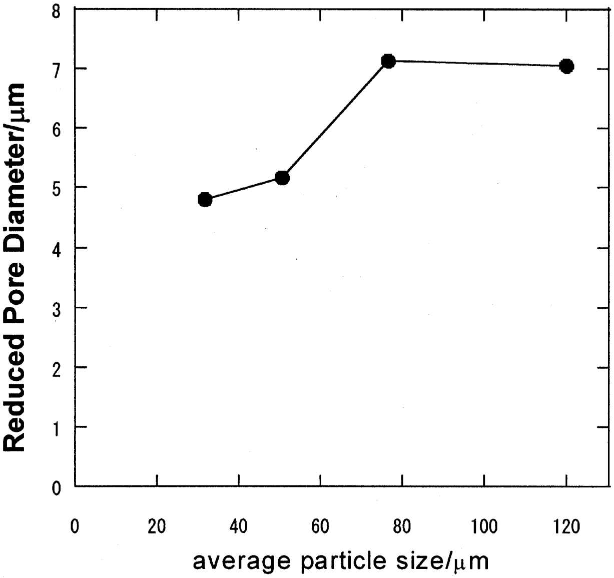

FIGURE 2 Reduced pore diameters of interparticle pore network of SP1 crystals as functions of average particle diameter calculated by capillary rise result of cyclohexane.

contact angle of water for different $\bar{x}$ system indicates the effectiveness of the value of d^*.

The geometrical meaning of d^* should be made clear in order to adopt d^* in micropore system. So far we have no evidence that reduced diameter, d^*, is regarded as so-called average pore diameter. First of all, what is the meaning of average pore size? The ratio $d^*/\bar{x}$ calculated from the values in Figure 2 is 0.06–0.15, indicated that the "size" of pore is 0.06–0.15 times of that of particle. On the other hand, the void ratio of the system, calculated from the bulk density of the SP1 powder and solid density of graphite crystal was approximately 80%. This large void ratio looks difficult to consistent with the small ratio of $d^*/\bar{x}$. Though d^* closely related with average pore width of the complicated interparticle pore network, d^* is not simply equal to the average pore width. In order to make this point clear, we are now constructing more preferable model to explain the meaning of d^*.

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