

Supporting Information

© Wiley-VCH 2005

69451 Weinheim, Germany

A New Minimal Surface and the Structure of Mesoporous Silicas

Michael W. Anderson, Chrystelle C. Egger, Gordon J.T. Tiddy, John L. Casci & Kenneth A. Brakke



Fig. 1 Penetration scans (brown images) of cetyltriethylammonium bromide with 5 wt% bromohexadecane in water showing presence of an isotropic mesophase below 32.8°C at concentrations between the hexagonal mesophase and isotropic solution. The top right figure shows a penetration scan of cetyltriethylammonium chloride in water showing the presence of three isotropic mesophases at concentrations between the hexagonal mesophase and isotropic solution. In all cases the concentration of surfactant decreases from right to left on the microscope slide.



Fig. 2 Two exponential functions added together according to equation 1 give two separate bodies when they are far enough apart but a single continuous wrapped surface as the bodies approach.



Fig. 3 Above typical synchrotron diffraction patterns for SBA-1 synthesised in 4M HCl for one week at 4°C followed by heating for one hour at 100°C; below after calcination at 550°C.

h	k	l	Table I
0	0	0	h, k, l coordinates
1	0	0	of 9 spheres
0	1	0	
0	0	1	
1	1	0	
1	0	1	
0	1	1	
1	1	1	
0.5	0.5	0.5	

h'	<i>k</i> '	l'	b_1	b_2	b_3
1	0.25	0.5	$1/f^{2}$	1	$1/f^{2}$
1	0.75	0.5	$1/f^{2}$	1	$1/f^{2}$
0	0.25	0.5	$1/f^{2}$	1	$1/f^{2}$
0	0.75	0.5	$1/f^2$	1	$1/f^{2}$
0.5	1	0.25	$1/f^{2}$	$1/f^{2}$	1
0.5	1	0.75	$1/f^{2}$	$1/f^{2}$	1
0.5	0	0.25	$1/f^{2}$	$1/f^{2}$	1
0.5	0	0.75	$1/f^{2}$	$1/f^{2}$	1
0.25	0.5	1	1	$1/f^{2}$	$1/f^{2}$
0.75	0.5	1	1	$1/f^2$	$1/f^{2}$
0.25	0.5	0	1	$1/f^{2}$	$1/f^{2}$
0.75	0.5	0	1	$1/f^{2}$	$1/f^{2}$

Table II: h', k', l' coordinates for 12 ellipsoids with the values of b_1 , b_2 and b_3 given in terms of f and the radii of the sphere and the short axis of the ellipsoid. 12 extra virtual ellipsoids were placed by changing coordinates 0.25 for -0.25 and 0.75 for 1.25. These are necessary to prevent adverse edge effects.

 $r_1 =$ radius of sphere

 r_2 = radius of short axis of ellipsoid

- $f = \frac{\text{radius long axis of ellipsoid}}{1}$
- $f = \frac{1}{radius of short axis of ellipsoid}$

 $C = e^{-r_1^2}$

 $a = r_2^2 + \ln(C)$



Fig. 4 Calculated x-ray diffraction patterns above of the atomistic structures below from analytical expression for the structure of SBA-1. The numbers to the left of the upper figure show the radii of the sphere, r_1 , and the short radius of the oblate ellipsoid, r_2 , as a fraction of the unit cell. In this case $r_1=r_2$ where the best fits were achieved. The oblateness as a factor inset for each of these calculations.