Pore Structure and Fluid Sorption in Ordered Mesoporous Silica. II. Modeling

Abstract

The nanostructure of SBA-15 ordered mesoporous silica is modeled by considering a full crystallite about 500 nm in size. The lattice sites of a 2D hexagonal lattice are occupied by circular mesopores that exhibit a size distribution and a rough pore wall. In addition, the walls of the ordered pores contain randomly distributed disordered pores. This model is introduced to quantitatively reproduce the experimental X-ray scattering profile from an evacuated SBA-15 sample considering both Bragg diffraction from the ordered pore lattice and the diffuse small-angle scattering from the disordered pores. In contrast to a previous form factor model which analyzed the Bragg diffraction peaks only, the present model reproduces correctly the total porosity of the material in good agreement with nitrogen sorption. The adsorption behavior of the model crystallite is studiedby introducing simple filling rules for the ordered and the disordered porosity. The filling of the disordered pores as well as film formation and capillary condensation in the ordered pores are reproduced by the model. Good agreement between the calculated and measured scattering profiles along the adsorption isotherm of a contrast-matching fluid is found. In particular, the change of the integral diffuse scattering intensity with increasing vapor pressure of the fluid is quantitatively reproduced by the model. The integrated intensities from the Bragg reflections show however some quantitative discrepancies. Comparing the density profiles derived from the present lattice model with the one obtained from direct form factor fitting of the experimental data, we conclude that the experimental system is also subjected to fluctuations of the fluid density on the pore walls.

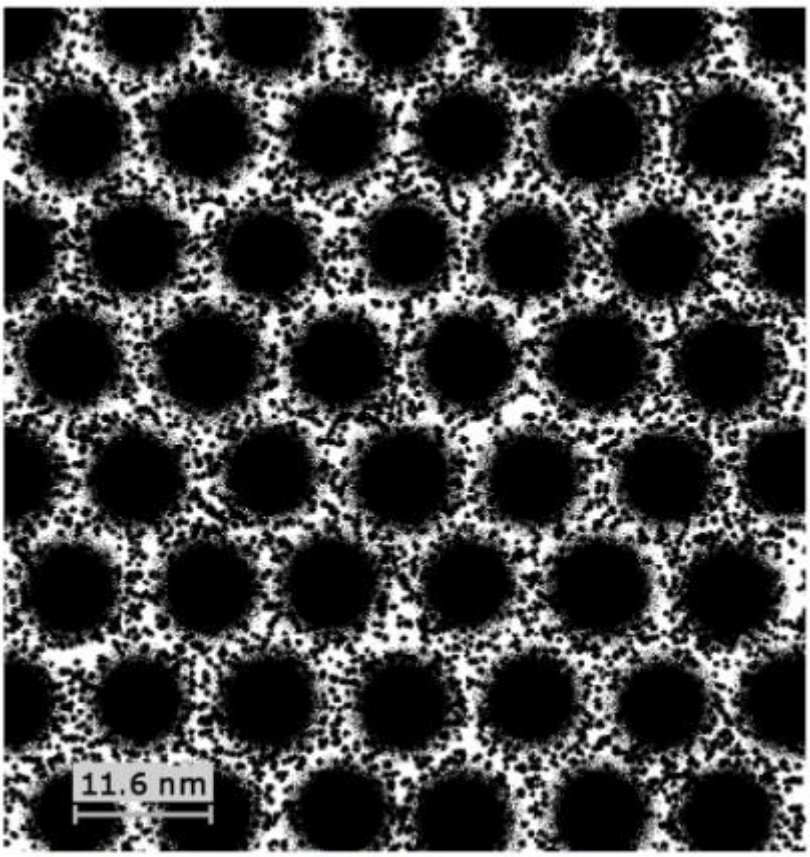

Figure 2. Cut-out of the SBA-15 model crystallite showing the 2D-hexagonal ordered pore lattice with additional random disordered pores.