MS42.O05

Modeling of SAPO-18/34 intergrowth crystal structure

W. Slawinski[1], D. Wragg[1], D. Akporiaye[2], H. Fjellvag[1]

[1]*University of Oslo, Centre for Materials Science and Nanotechnology, Department of Chemistry, Oslo, Norway,* [2]*SINTEF Materials and Chemistry, Oslo, Norway*

Aluminophosphate framework structures have been widely studied because of their many technological applications. The most significant application of aluminophosphate type framework catalysts is in the methanol-to-olefin (MTO) conversion process [1], catalysed by SAPO-34 (the silicoaluminophosphate form of the chabazite (CHA) zeolite framework with silicon substituted into its structure). The effectiveness of SAPO-34 in the MTO process is due to both the shape selective properties of the framework and the concentration and strengths of the acid sites created by silicon substitution [2]. Another aluminophosphate framework MTO catalyst is SAPO-18 (zeolite framework type (AEI)), which has a very closely related structure to SAPO-34 and can form intergrowths with it. It has been suggested that the level of intergrowth can affect the efficiency of the MTO process [3], however, assessment of the level of intergrowth has remained difficult. We present a consistent model of the crystal structure of SAPO-18/34 family members which can accurately determine the level of intergrowth. The model utilises two types of stacking fault: Displacement and Growth which have significantly different effects on the diffraction pattern. A series of powder diffraction patterns is calculated using the Discus software package. Changes in the level of intergrowth and stacking fault type strongly affect the calculated pattern. A series of patterns has been calculated to illustrate this. The structure of an intergrown SAPO-34 sample with 4.8% Si content is modelled and refined using Displacement stacking faults. An example of "defect-free" AlPO-18 (0% Si content) is then presented. Refinement of the model shows that even this contains a small amount of stacking faults. Finally, a simple method for defect level estimation is proposed based on FWHM (Full Width at Half Maximum) ratios for selected Bragg reflections.

[1] D. Chen, K. Moljord, T. Fuglerud, et al. Microporous and Mesoporous Materials 1999, 29, 191-203, [2] F. Bleken, M. Bjrgen, L. Palumbo, et al., Topics in Catalysis, 2009, 52, 218-228, [3] M. Janssen, A. Verberckmoes, M. Mertens,et al., Exxon-Mobile Chemical Europe Inc., 2007, patent no. EP 1 365 992 B1

Keywords: stacking faults, intergrowth, SAPO