

### X-Ray diffraction study of stacking faults in silicoaluminophosphate SAPO-18/34

W. A. Sławiński<sup>1\*</sup>, D. S. Wragg<sup>1</sup>, D. Akporiaye<sup>2</sup> and H. Fjellvåg<sup>1</sup>

<sup>1</sup>Centre for Materials Science and Nanotechnology, Department of Chemistry, University of Oslo, PO Box 1126, 0315 Oslo, Norway

<sup>2</sup>SINTEF Materials and Chemistry, Forskningsvn 1, 0314 Oslo, Norway

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\*e-mail: w.a.slawinski@smn.uio.no

Silicoaluminophosphate framework structures have been widely studied because of their many technological applications. The most significant application of silicoaluminophosphate 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 (see Fig. 1). 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" AIPO-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.

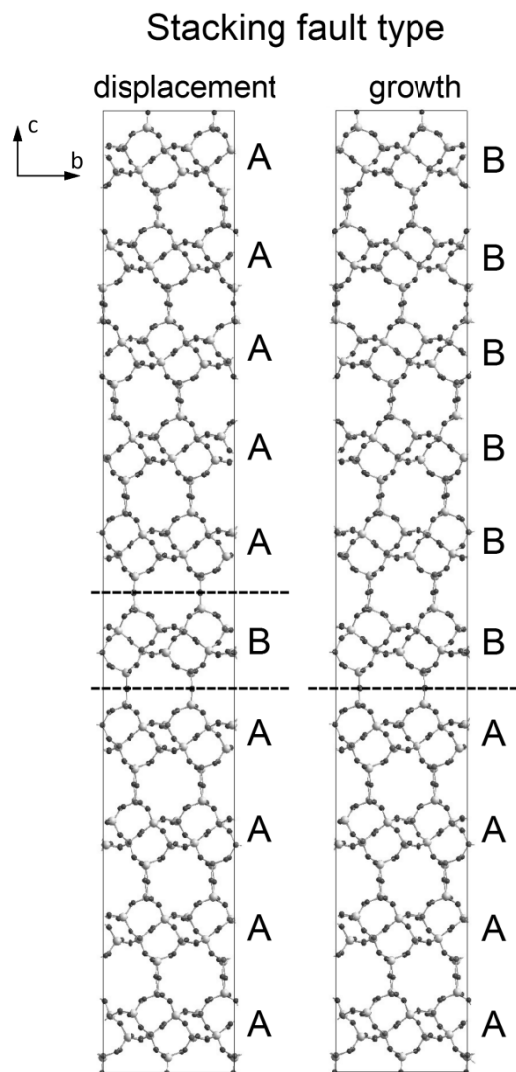


Figure 2. Displacement and Growth type of stacking faults in SAPO-18/34 structure

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