The Pentasil Family

1. The Periodic Building Unit (PerBU) - 2. Type of Faulting - 3. The Layer Symmetry
4. Connectivity Pattern - 5. Ordered End-Members - 6. Disordered materials synthesized to date
7. Supplementary Information - 8. References

1. The Periodic Building Unit (PerBU) equals the \( bc \)-layer shown in Figure 1:

\[
\begin{array}{c}
\includegraphics[width=0.8\textwidth]{pentasil_layer.png}
\end{array}
\]

Figure 1: The Periodic Building Unit of the pentasil family of framework types

The PerBU in the pentasil family, the pentasil layer (Fig. 1(left)), is composed of T12-units (bold in Fig.1). T12-units, related by a rotation of 180° about \( c \) accompanied by a translation of \( \frac{1}{2}c \), form left- and right-handed chains along \( c \). The chains, related by a mirror plane \( m \) perpendicular to \( b \), are connected along \( b \) to give the characteristic \( bc \) pentasil layer. A parallel projection of the pentasil layer along \( b \) is shown at the right of Fig.1.

2. Type of faulting: 1-dimensional stacking disorder of the PerBU’s along \( a \).
3. The plane space group of the PerBU is P 1 m (1).

4. Connectivity pattern of the PerBU:

Neighbouring PerBU’s can be connected along a through O-bridges in two different ways:

(a): successive pentasil layers are connected after a rotation of 180° about a (or b) with respect to each other. The resulting connectivity exhibits inversion symmetry (i: o) between successive layers.

(b): successive pentasil layers are connected after a rotation of 180° about c. The connectivity now shows mirror symmetry (m: |) between successive layers.

Figure 2: Parallel projection along b of the connection modes (a) and (b) in the pentasil family of framework types

Once the distribution of the symmetry elements i and m between the layers stacked along [100] is known, the 3-dimensional structure is defined.

An example of an intermediate structure in the pentasil family of zeolites is shown in Figure 3:

Figure 3: Connectivity sequence of PerBU’s with m and i as symmetry elements
5. The simplest ordered end-members in the pentasil family are shown in Figure 4:

Pure MFI (1) and MEL (2) are obtained when neighbouring PerBU’s along $a$ are exclusively related by inversion and reflection, respectively.

6. Disordered materials synthesized and characterized to date:

Bor-D (3)
7. Supplementary material

Diffax-Simulation of X-ray powder pattern for the MFI-MEL intergrowth.

Figure 5: Intensity (I, a. u.) of simulated powder patterns versus diffraction angle ($2\theta$) of disordered materials in the MFI-MEL series in steps of 10% intergrowth. The 0% MFI pattern corresponds to the 100% MEL pattern.

8. References

