

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:

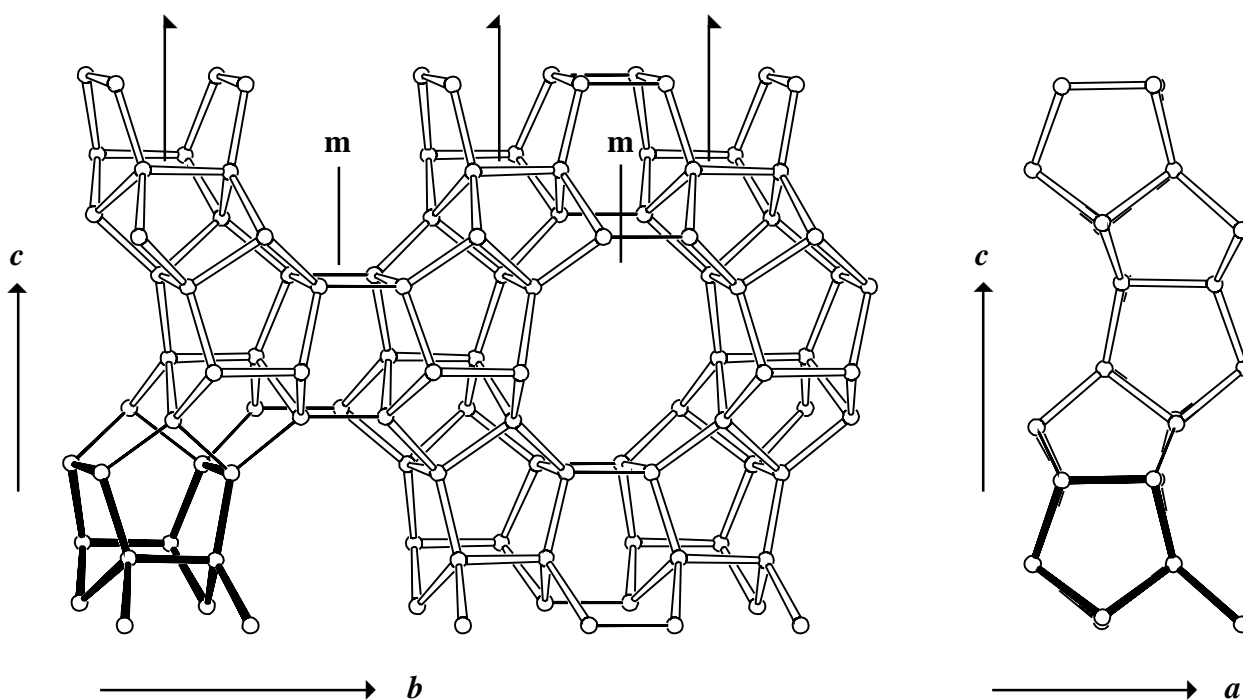


Figure 1: The Periodic Building Unit of the pentasil family of framework types

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**: \circ) 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.

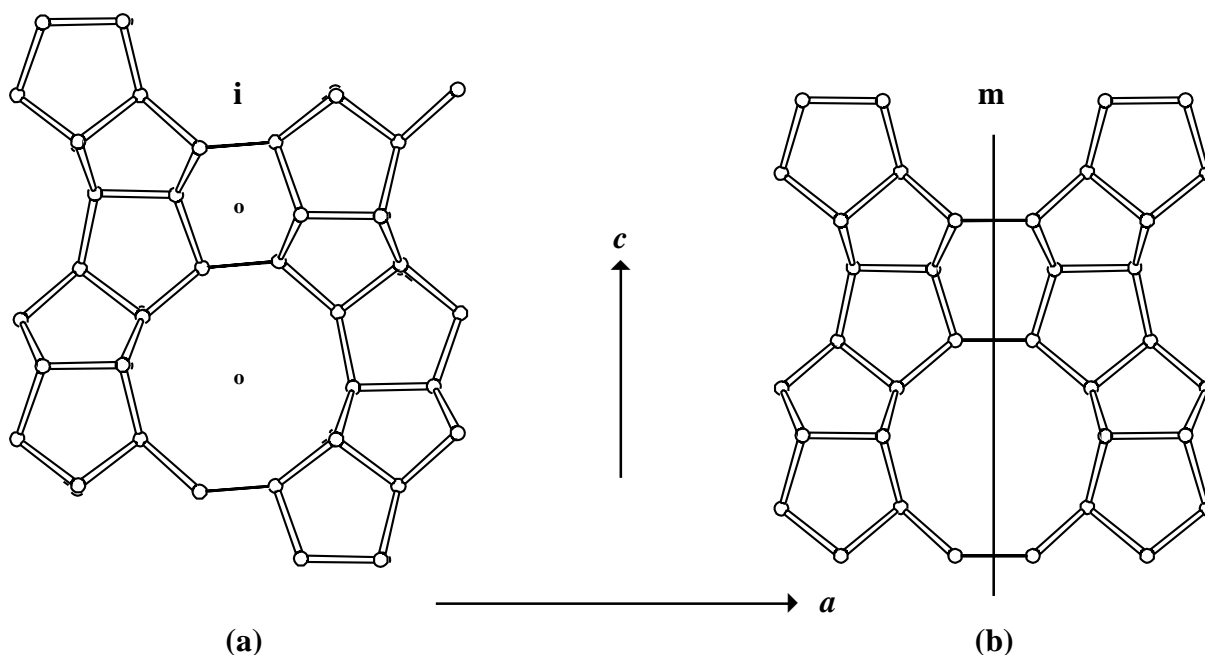


Figure 2: Parallel projection along b of the connection modes (a) and (b) in the pentasil family of framework types

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:

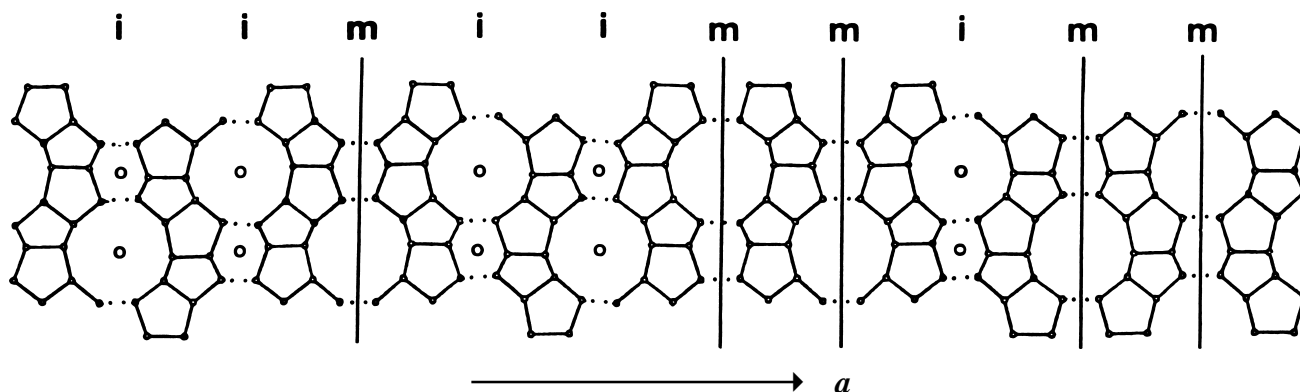


Figure 3: Connectivity sequence of PerBU's with **m** and **i** as symmetry elements ▲

5. The simplest ordered end-members in the pentasil family are shown in Figure 4:

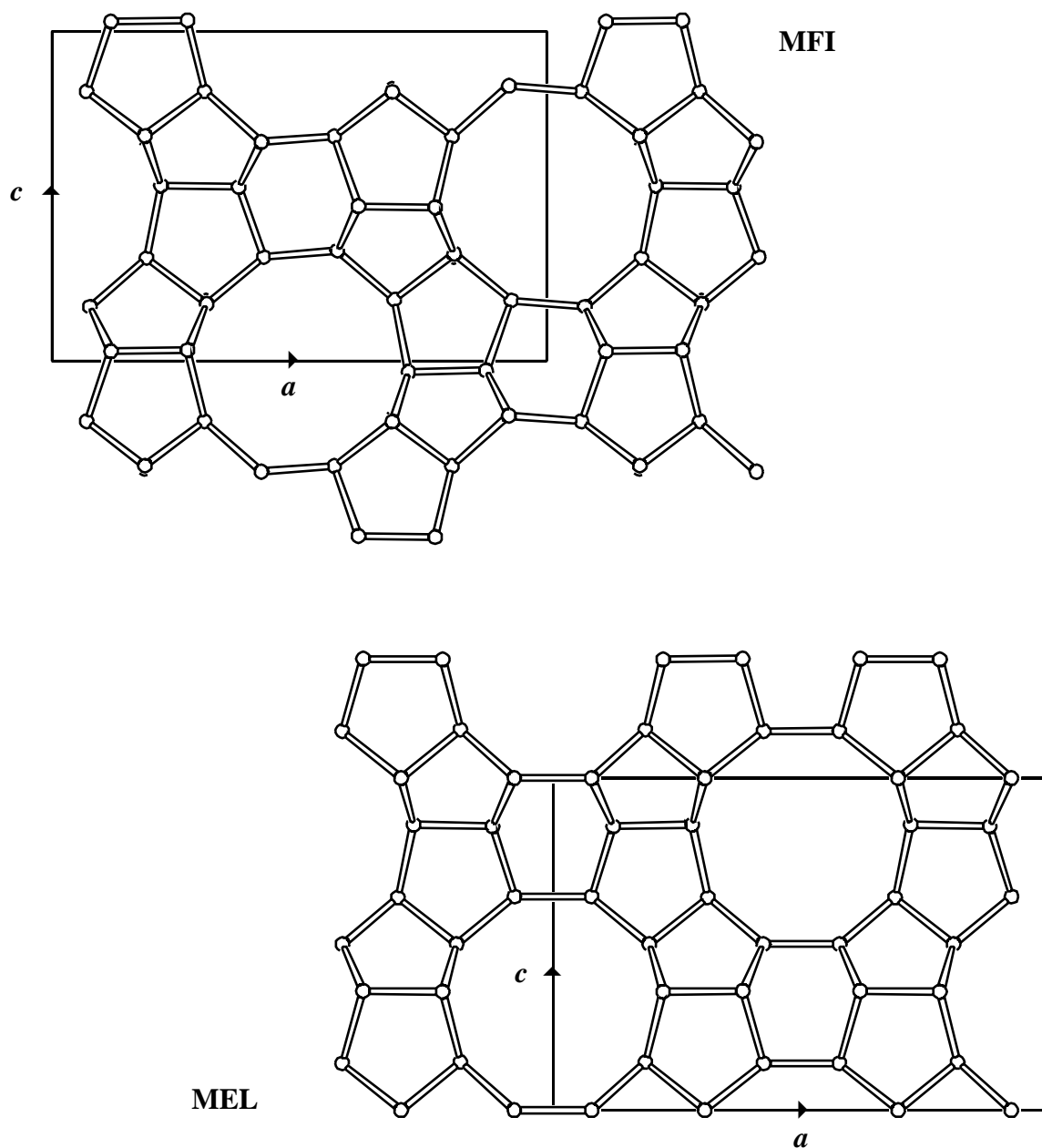


Figure 4: Parallel projection of the unit cell content along b of the two simplest ordered end-members of the Pentasil family: MFI (top) and MEL (bottom)

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 powdrex pattern for the MFI-MEL intergrowth.

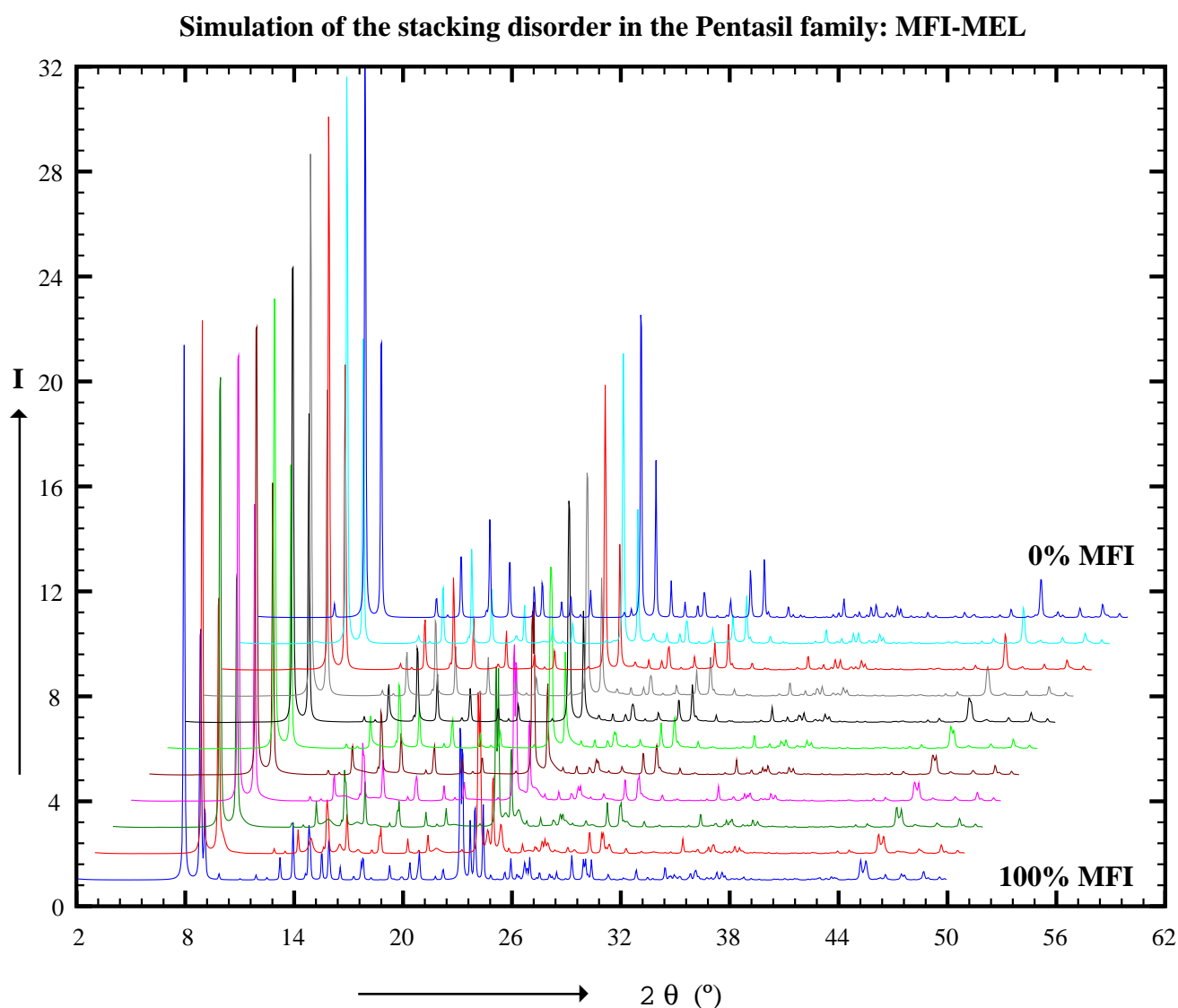


Figure 5: Intensity (I , a.u.) of simulated powder patterns versus diffraction angle (2θ) of disordered materials in the MFI-MEL series in steps of 10% intergrowth. The 0% MFI pattern corresponds to the 100% MEL pattern

8. References

- (1) G.T. Kokotailo, S.L. Lawton, D.H. Olson and W.M. Meier, *Nature* **272**, 437 (1978).
- (2) G.T. Kokotailo, P. Chu, S.L. Lawton and W.M. Meier, *Nature* **275**, 119 (1978).
- (3) G. Perego, M. Cesari, *J. Appl. Cryst.* **17**, 403 (1984). ▲