The Decasil Family

1. The Periodic Building Unit (PBU) equals the chain shown in Fig. (a) :

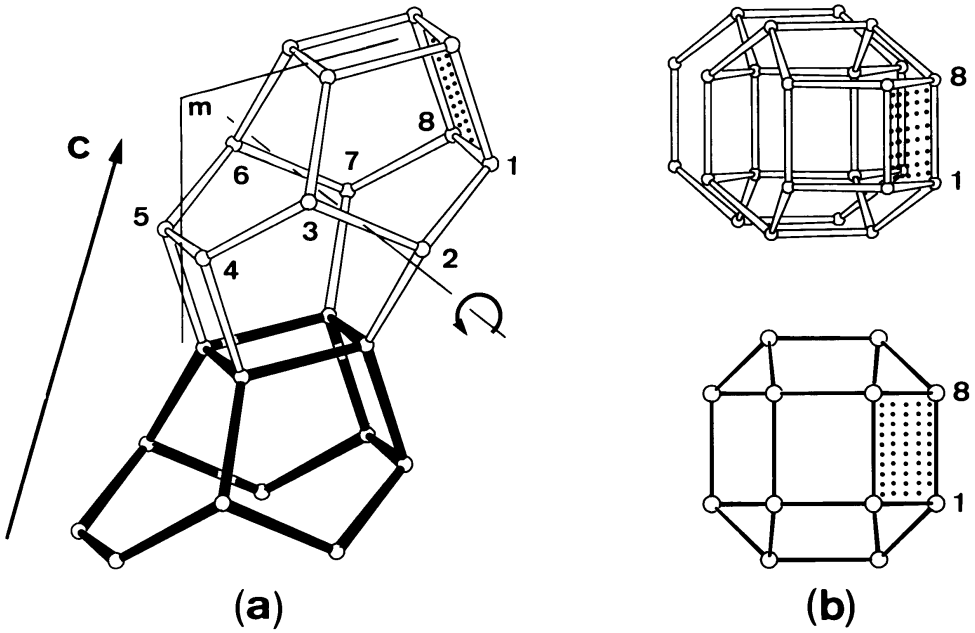

Figure 1: The Periodic Building unit of the decasil family of structures.

The PBU of the decasil family of structures, is formed by connecting T12-Units (in bold) related by pure translations along **c**. As orientation sensitive indicator one of the T4-rings is shaded. The numbered T atoms are used in describing the connection modes. A perspective and parallel view down the chain axis is shown in (b).

2. Type of faulting: 2-dimensional stacking disorder of the PBUs along [100] and [010].

3. The rod symmetry (2/m) is indicated in the Figure.

4. Connectivity pattern of the PBU.

Neighbouring PBUs can be connected via O-bridges in several ways:
The connection modes 2 and 3, 5 and 7 , and 6 and 8 are pairwise identical. The modes in each pair are related by a 180^0 rotation about an axis parallel to the connecting TOT bridges.

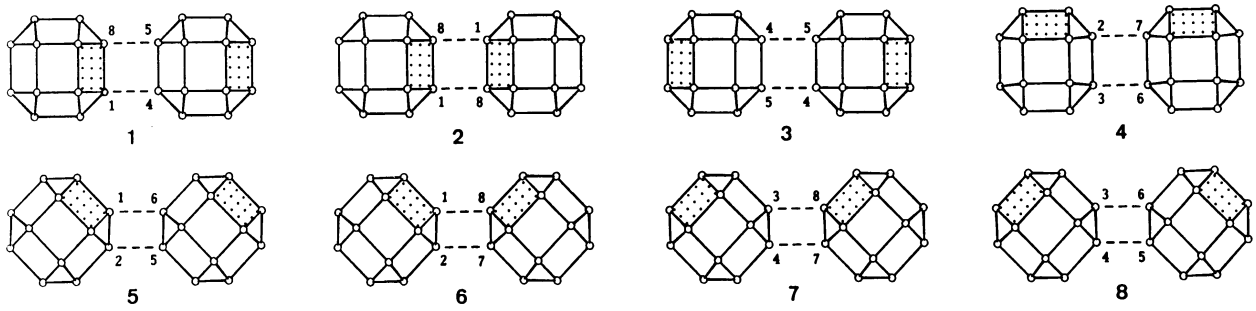

Figure 2: Connectivity od neighbouring PBU's.

Once the distribution of the connection modes in two dimensions is known, the 3-dimensional framework is defined.

5. The simplest ordered end-members in the decasil family are given below. Only end-member 1 has been observed as single crystal material and represents the structure type with code RTE (1).

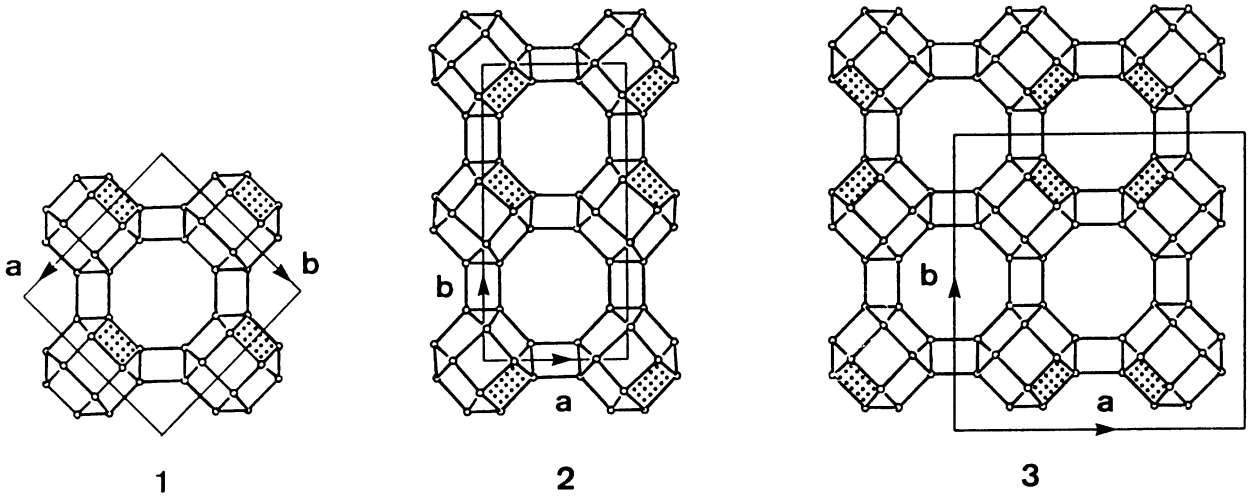

Figure 3: The three simplest periodic end-member structures of the decasil family

End-Member	*Sequence of the Connection Modes along **a** and **b**: (along **a**, ...; **b**, ...)*	*Space Group Symmetry*
1	(5,5,....;7,7,.....)	C2/m *
2	(7,7....;8,6,8,...)	P2/m
3	(8,6,8,...;8,6,8,...)	P4/m mm

* This is the end-member with structure type code RTE (1); the sequence of the connection modes is along (**-a** + **b**) and (**a** + **b),** respectively.

6. Faulted structures synthesized so far:

RUB-4 (1,2)

7. Supplementary Material

7.1 Simulated diffraction pattern of decasils

A theoretical analysis of the diffractiong properties of the 2-dimensionally disordered material RUB-4 has been reported by Daniels (3). Since the diffuse intensities in the diffraction experiments are brought about by the disorder of the one dimensional PBU, two dimensional diffuse scattering is observed. Therefore, single crystal photographs have been simulated. The examples in Figure 4 show that 0-layer experiments always give sharp reflections. Higher layer photographs with the normal running parallel to the PBU, however, show diffuse intensities extending in two dimensions.

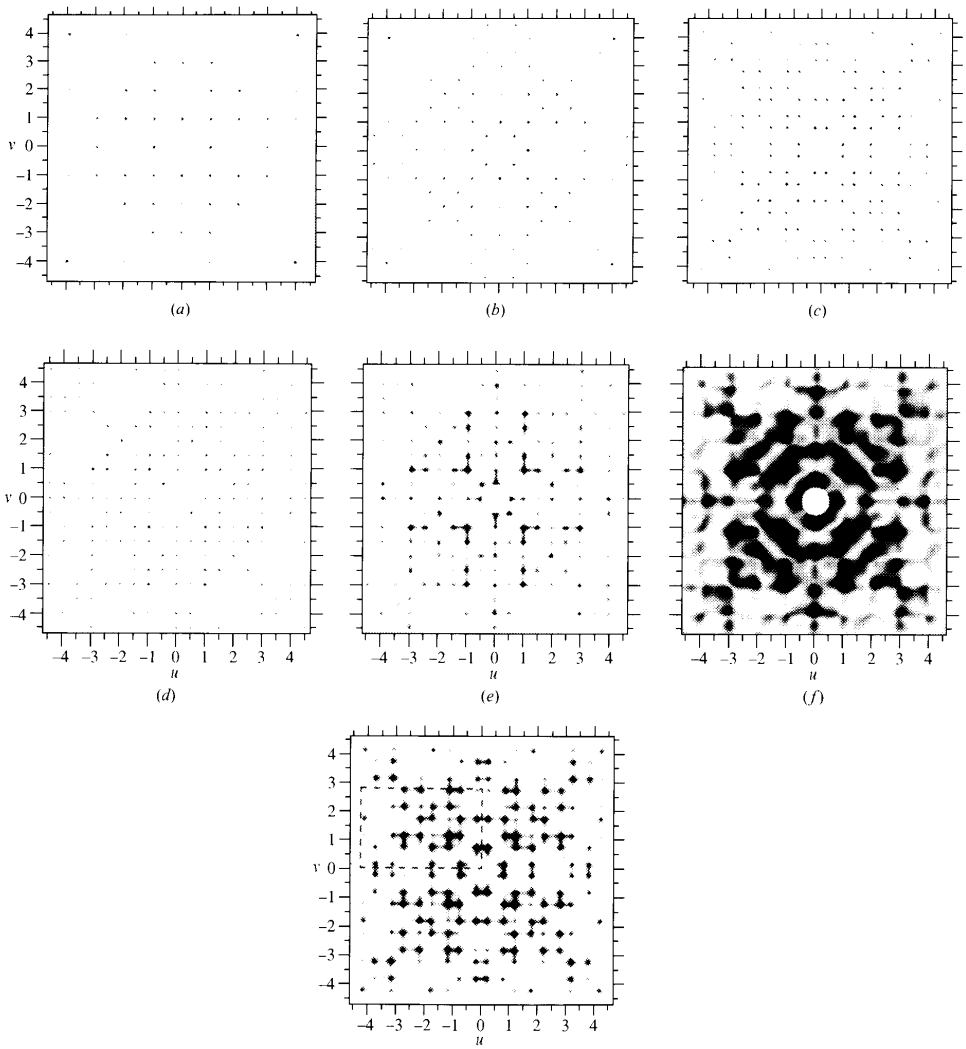

Figure 4: Sequence of simulated diffraction pattern in plane *a*, *b* perpendicular to *c* with various indices *l* and different stacking seqeunces α_{11} demonstrating the influence of the degree of disorder on the distribution of diffracted intensities in the X-ray diagram: a) $l = 0$ with $\alpha_{11} \neq 0$, b) $l = 0$ with $\alpha_{11} = 0$, c) to g) $l = 1$ and $\alpha_{11} = 1.0$, 0.0, 0.25, 0.50, and 0.75 respectively (after Daniels (3)).

The comparison between the experimental precession photograph and the results of the simulation is shown in Figure 5. Visual inspection suggests that the degree of disorder is close to $\alpha_{11} = 0.75$ which is an intergrowth of type 1 and 3.

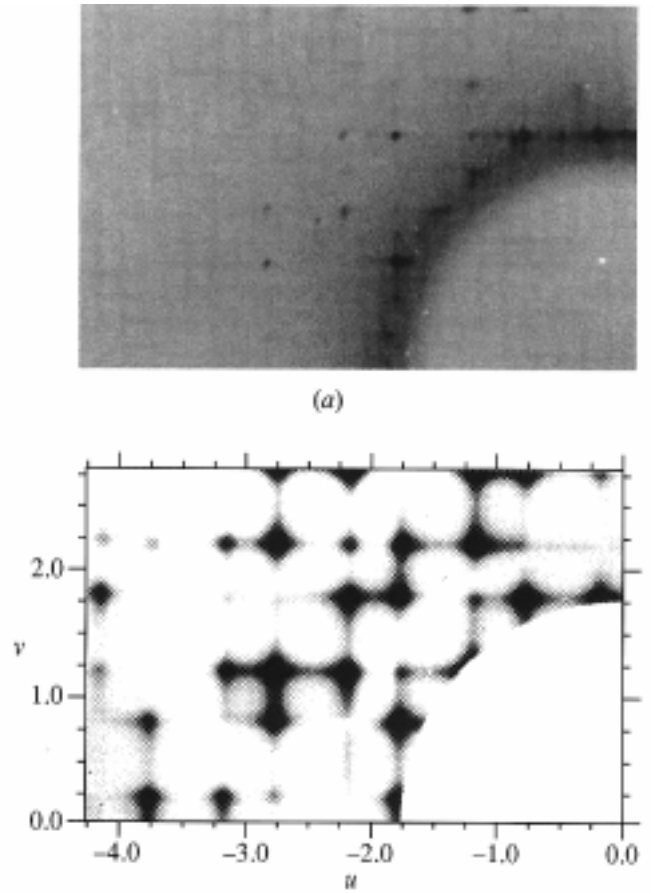

Figure 4: (a) Experimental and (b) simulated diffraction diagram of RUB-4

7.2 Experimental powder diffraction diagrams of the materials RUB-3 and RUB-4

In the following Figures 5 and 6 the experimental diffraction diagram of RUB-3 and RUB-4 are shown in comparison.

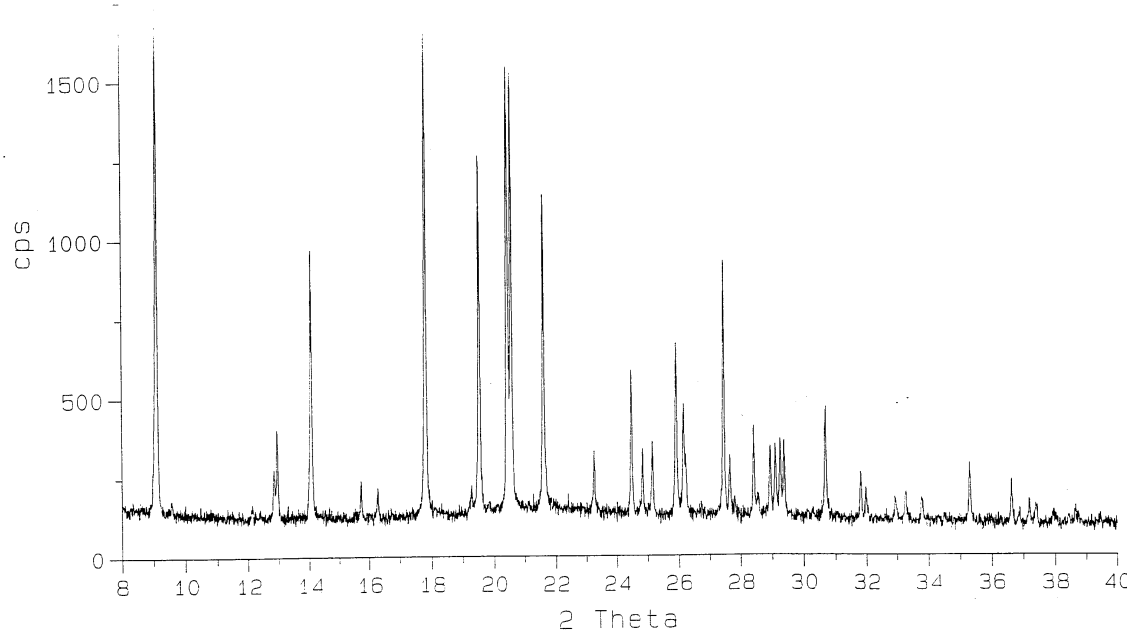

Figure 3: Powder X-ray diffraction diagram (wavelength CuKα_1) of the ordered material RUB-3. For a detailed reference see the Atlas of Zeolite Structure types and the Collection of simulated Powder Pattern.

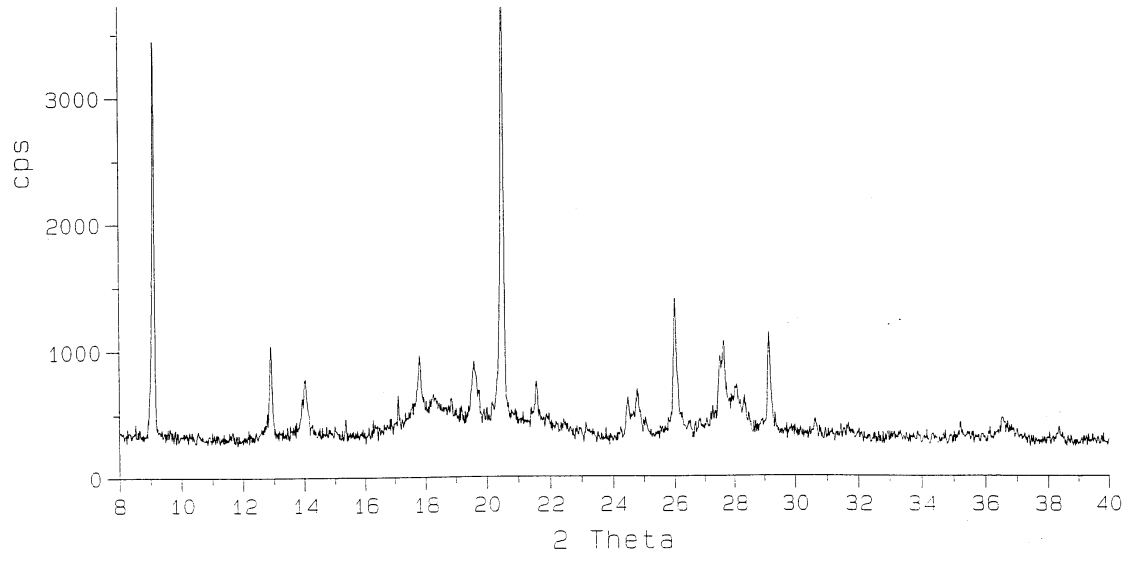

Figure 4: Powder X-ray diffraction diagram (wavelength CuKα_1) of the disordered material RUB-4 (2). Peak broadening and the increased backgrounf in the 2θ-range between 12 and 30° is clearly seen. The peak maxima affected by the disorder don't coincide with the Bragg peaks of the ordered material and, therefore, indexing of the pattern is obsolete.

8. References

(1) B. Marler, A. Grünewald-Lüke, H. Gies, Zeolites **15,** 388 (1995).

(2) A. Grünewald-Lüke and H. Gies, Microporous Mater. **3**, 159 (1994).

(3) P. Daniels: *Appl. Cryst.* ***31***, 559 (1998).