

MODEL SHEET STRUCTURES FOR C-S-H

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Even though Portland cement has been in use for more than 100 years, the structure of the calcium silicate hydrates (C-S-H), its primary hydration product, is still a matter of debate. A common view is the description of C-S-H with a colloidal model, such by Jennings [1, 2]. These models can explain many measured properties of C-S-H but have difficulties explaining all aspects of C-S-H formation.

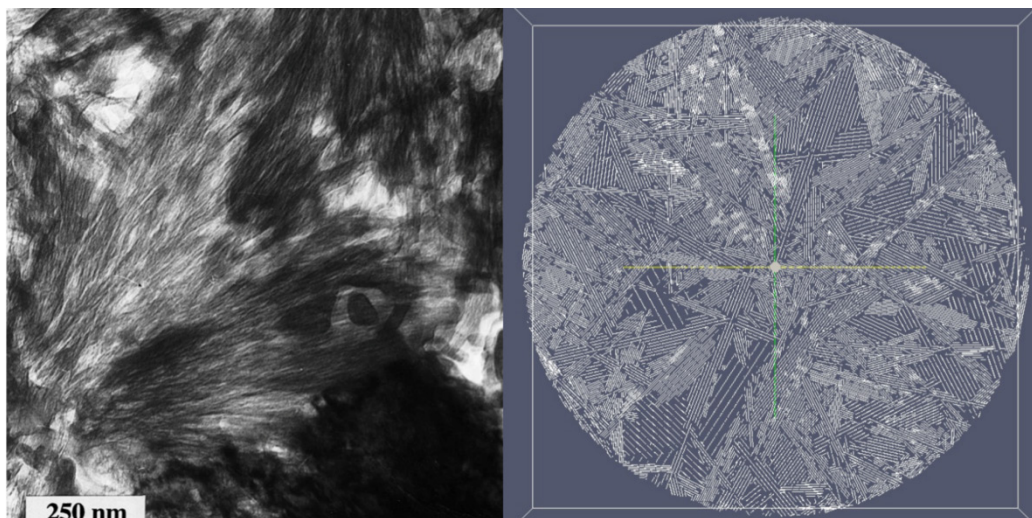
An alternative are sheet-models. Feldman and Sereda describe C-S-H as disordered sheets which fill the capillary pore space [3]. This agrees with micrographs, but it is unclear how such structures form and what general properties they have.

In this work, the interdependence between the formation and the properties of sheet-structures is studied. A computer model has been developed that can describe the growth of sheets within the confined space of a capillary pore. The four key ingredients of the model are:

1. Sheets start growing from initially placed nuclei, corresponding to the idea of a rapid nucleation period [4].
2. Sheets grow by adding material to their perimeter.
3. New sheets can start growing on existing sheets by placing new nuclei on top of existing sheets. This forms the interlayer space.
4. Sheets can neither grow in space outside the capillary pore nor in space already occupied by other sheets.

In this model, each sheet describes a single layer of calcium oxide covered with silica tetrahedra as suggested by Richardson and other authors [5].

In Figure 1 the cross section through an example structure is shown together with a micrograph of Portland cement.



*Figure 1: **Left:** micrograph for the outer product in PC, taken from Richardson [6]. **Right:** cross section through an example structure generated with the model presented in this work. The circular confinement has a diameter of 400 nm. Note the apparent similarity of both structures.*

It is found that the growth rate observed in these structures show qualitative similarity with the evolution of the heat flux or the chemical shrinkage rate in real cement systems; an example is shown in Figure 2 (left).

Additionally, it is shown that certain growth parameters lead to self-densifying structures as it has been suggested for cement systems [4].

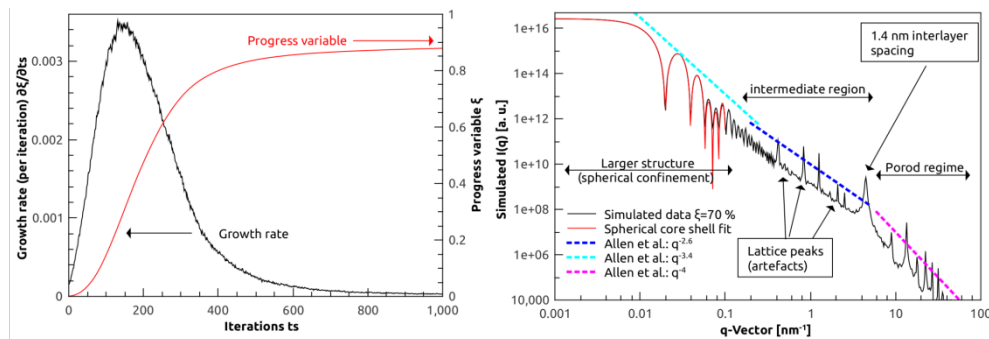


Figure 2: **Left:** example growth rate curve for a structure generated by the model presented. The progress variable ξ has a similar meaning in the model to the degree of hydration for a real cement system. The growth rate $\partial\xi/\partial t$ is analogue to the heat flux or the rate of chemical shrinkage. **Right:** example small angle scattering pattern simulated for a structure generated by the sheet growth algorithm. The power-laws use exponents given by Allen [7].

The model provides a 3D structural representation. This information can then be used to simulate experiments. The small scattering pattern (Figure 2 (right)) is computed and compared against literature data. For large q , a Porod regime is found. Intermediate q values yield power laws with exponents comparable to literature values reported for cement paste [7]. The far smoother appearance of the literature data can be understood by considering that the model represents only one pore size and shape, whilst the real system contains many pores of irregular shapes and sizes. Most of the peaks, as labelled in Figure 2, are artefacts corresponding to the underlying triangular lattice. An interlayer peak together with its higher order peaks is observed in the model.

These results show that the sheet structures proposed by the algorithm produce similar scattering pattern as observed for real cement structures. Sheet models, therefore, pose an alternative towards the well-known colloidal models.

Other properties, such as the implications of such structures on transport properties, can be evaluated using random media formalisms [8] or numerical tools such as lattice Boltzmann.

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