Alkali-Silica Reaction

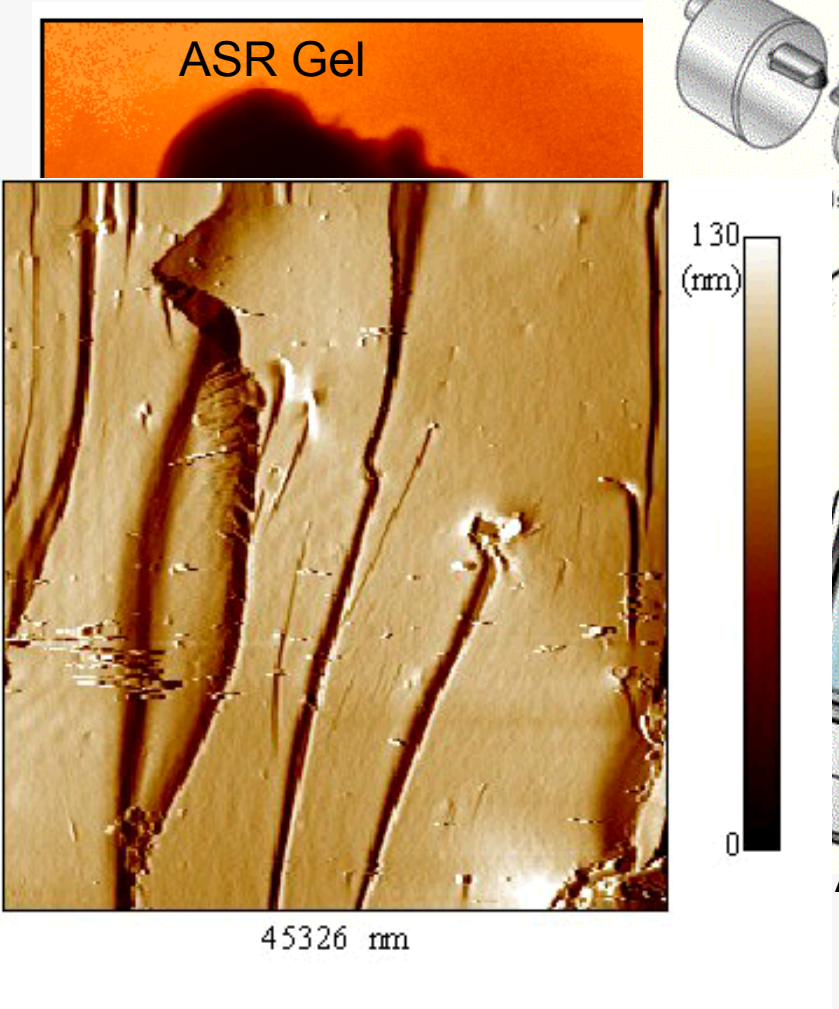
Research done at Berkeley

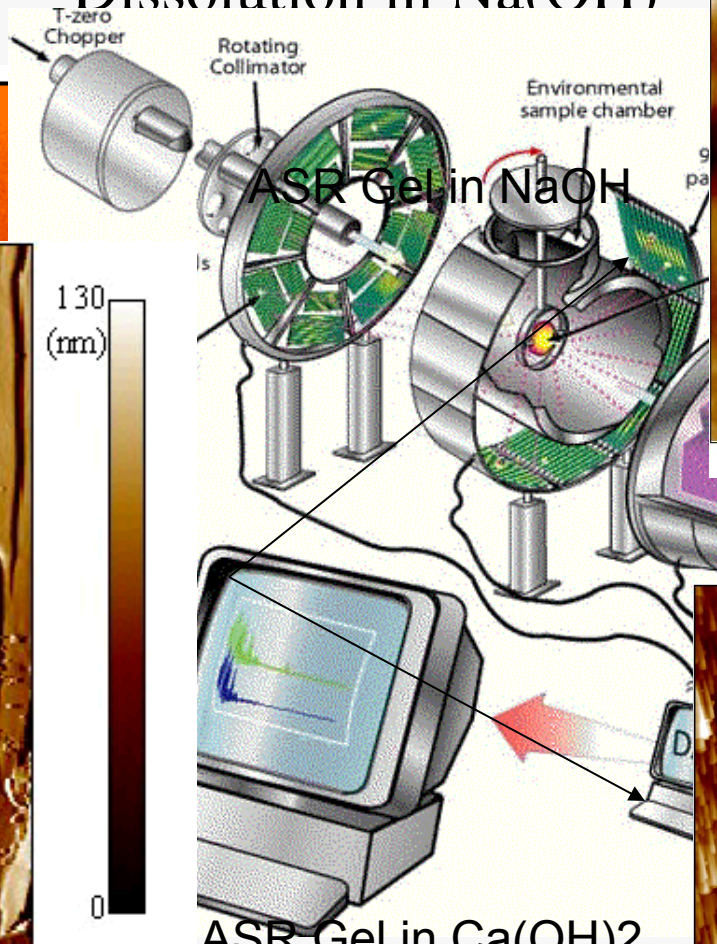
- Mathematical model using double layer theory
- Neutron diffraction of reactive aggregates
- Soft X-ray microscopy of the expansive gels
- Characterization of the ASR gel
- Repair strategies

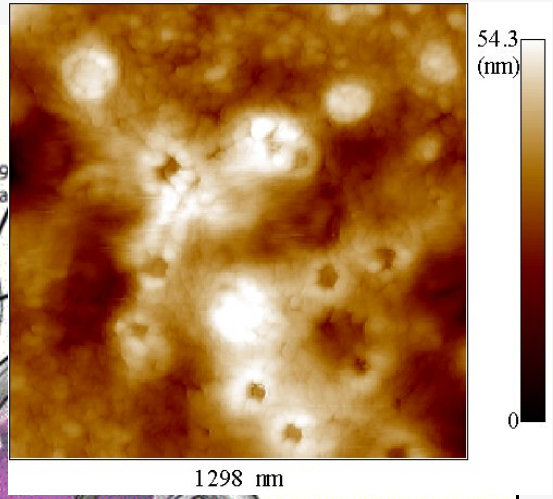
Integration with various methods

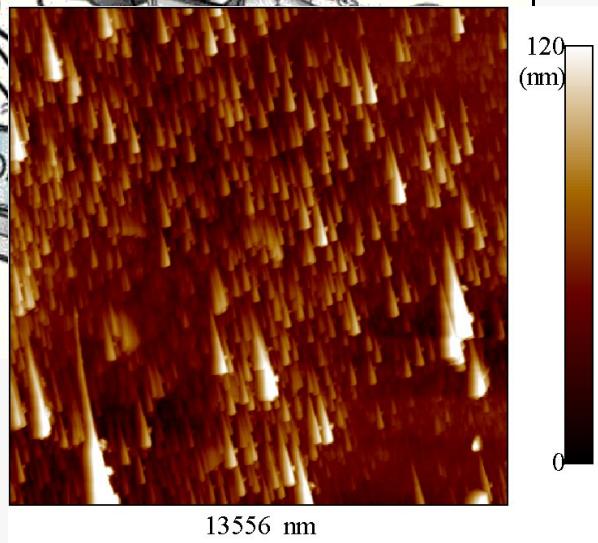
AFM
X-ray microscopy
Neutron Diffraction

Dissolution in Na(OH)



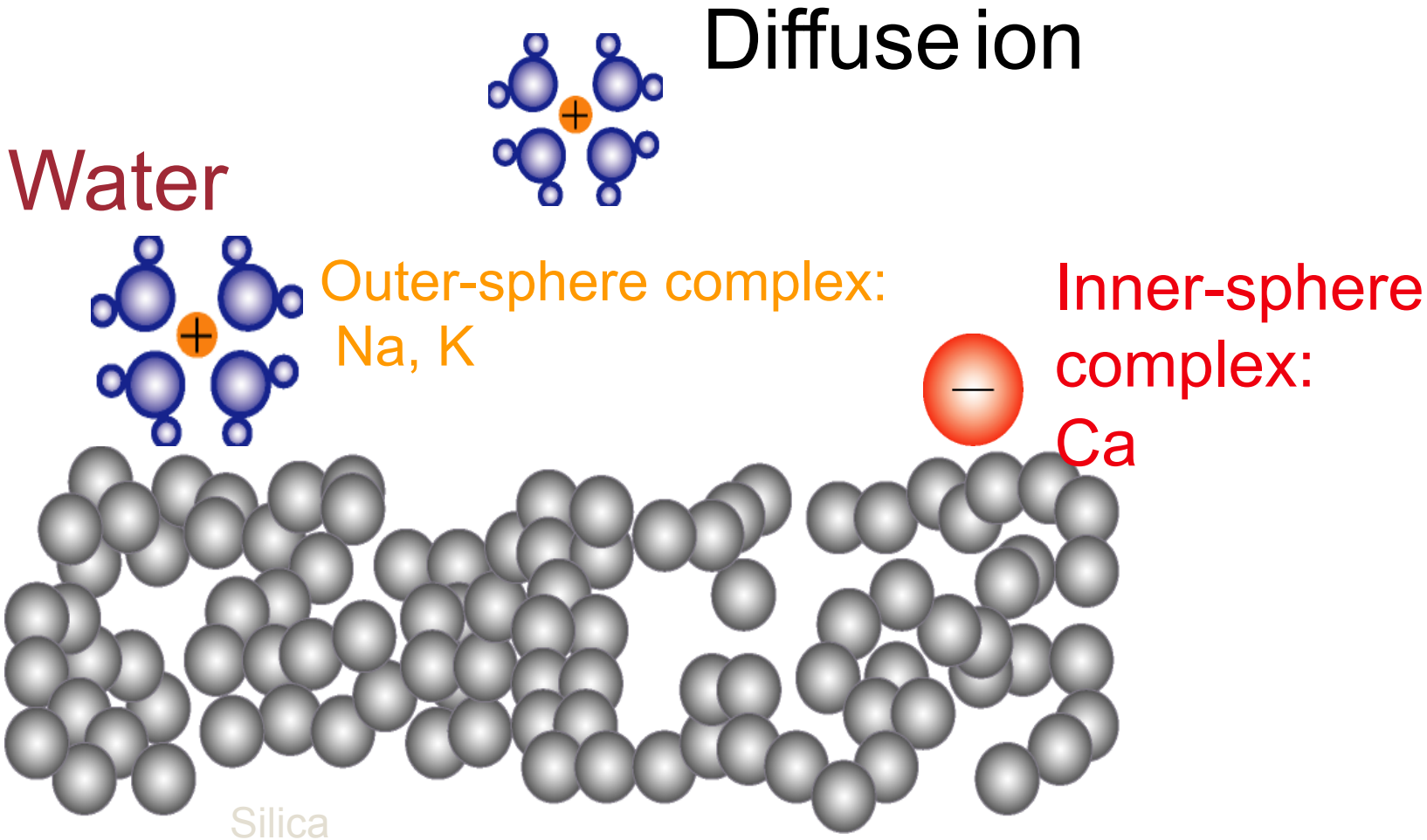




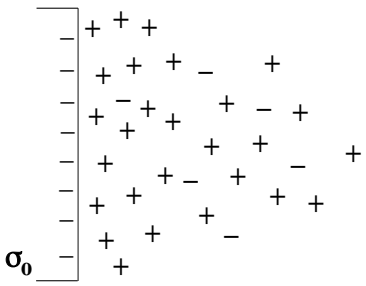


Use of double layer models to predict the stresses and damaged caused by the ASR gel

Double Layer Model



Fundamental Equations



$\sigma_d = \Sigma(\sigma_{d+} + \sigma_{d-})$

$\sigma_o + \sigma_d = 0$

σ_o = Surface charge

σ_d = Diffuse layer charge

Local pressure gradient the two particles and the electrolyte solution,

$$\nabla P + \rho \nabla \Psi = 0$$

where P is pressure, ρ is the net ion charge density, and ψ is the electric potential

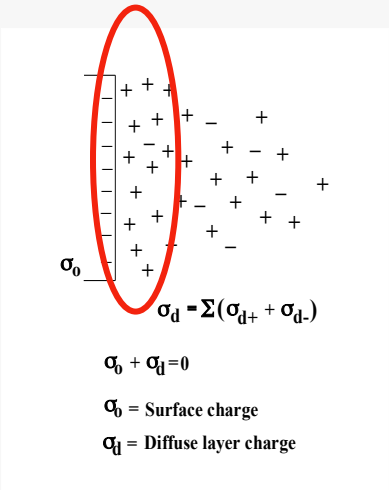
Integrating the net ion charge density:

$$\rho(\Psi) = C_o F \exp(- F \Psi / RT) - C_o F \exp(F \Psi / RT)$$

Computation of the stress

$$\Delta P = C_o R T [\exp(-\Psi_o / \Psi_D) + \exp(\Psi_o / \Psi_D) - 2]$$

where ΔP is the difference in pressure corresponding to an electric potential Ψo (relative to the bulk electrolyte solution as datum. The potential scaling factor Ψ_D = R T / F = 25.69 mV at 25 oC.

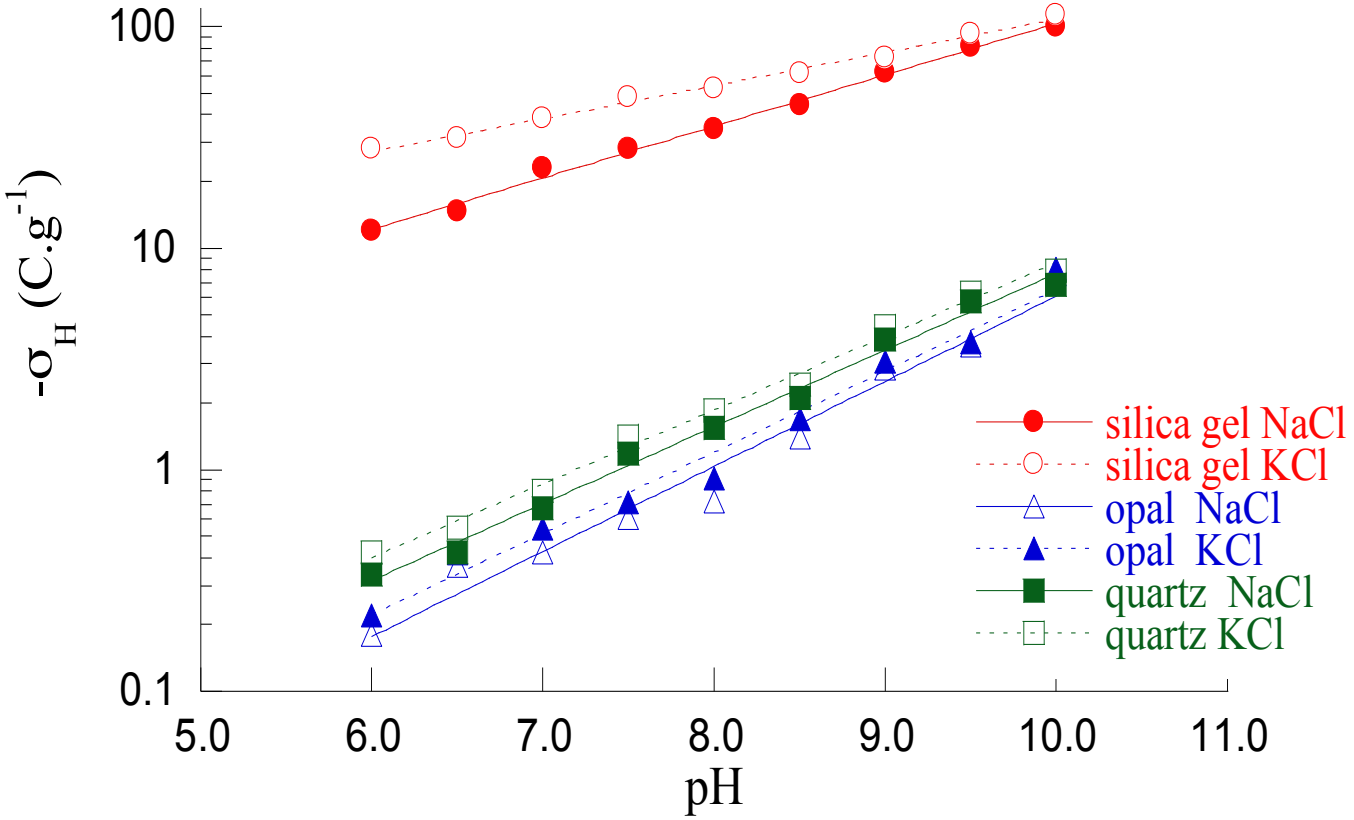


Need information of surface charge density of silica and silicates at high pH

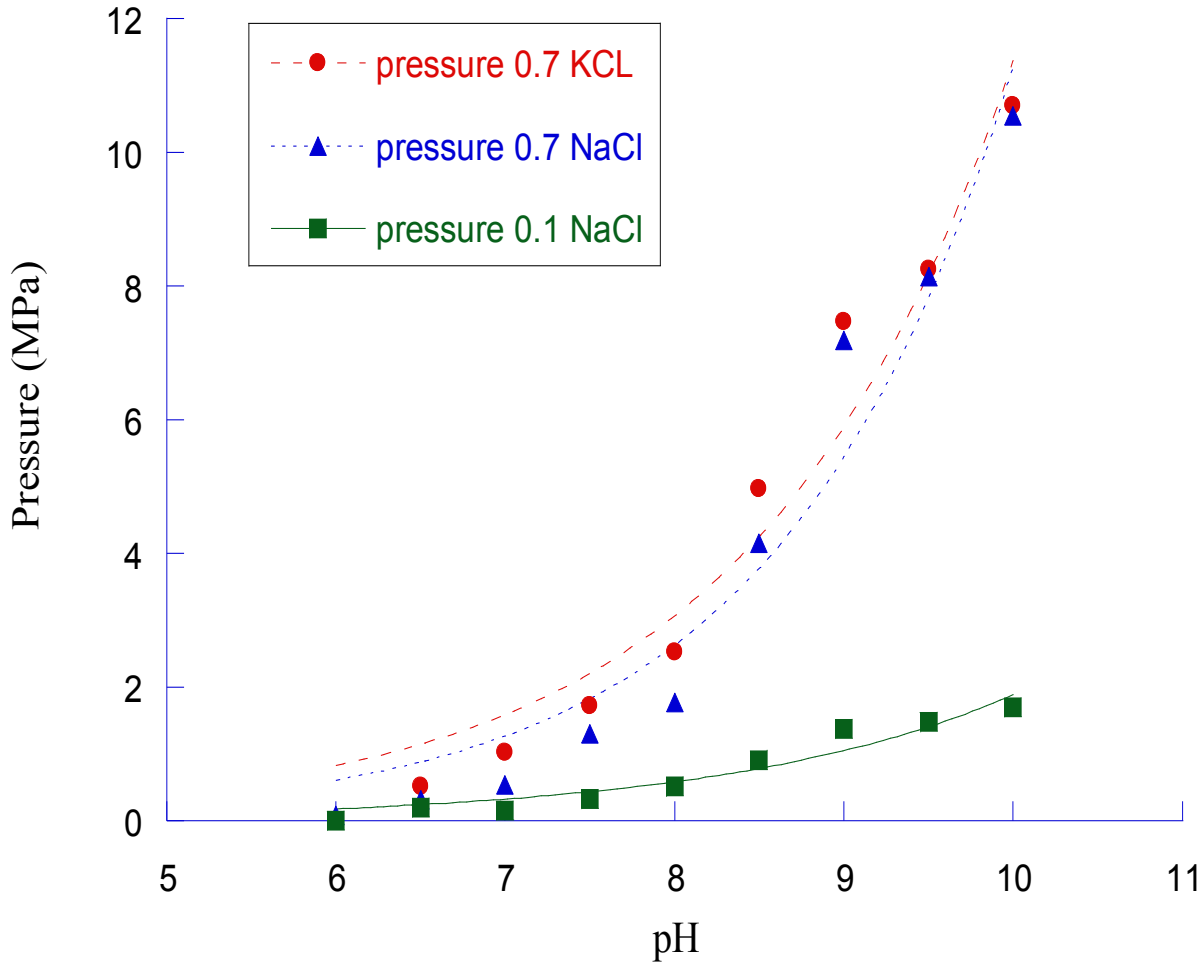
Experimental Research

- Surface charge density of silica at high values of pH and ionic strength
- Surface charge density of ASR gel at high values of pH and ionic strength

Phase I: Silica

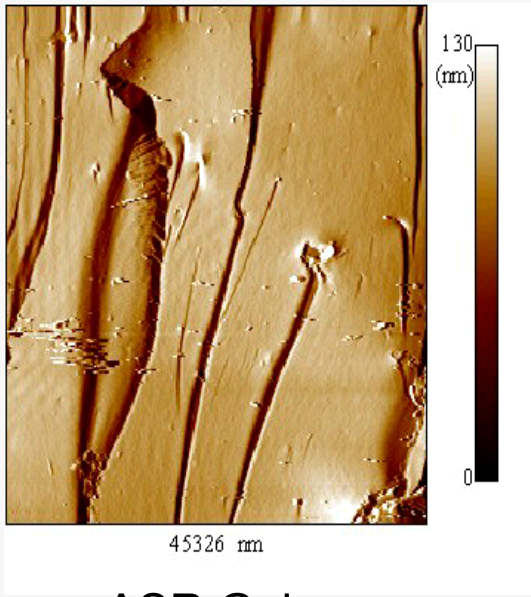


Pressure: opal



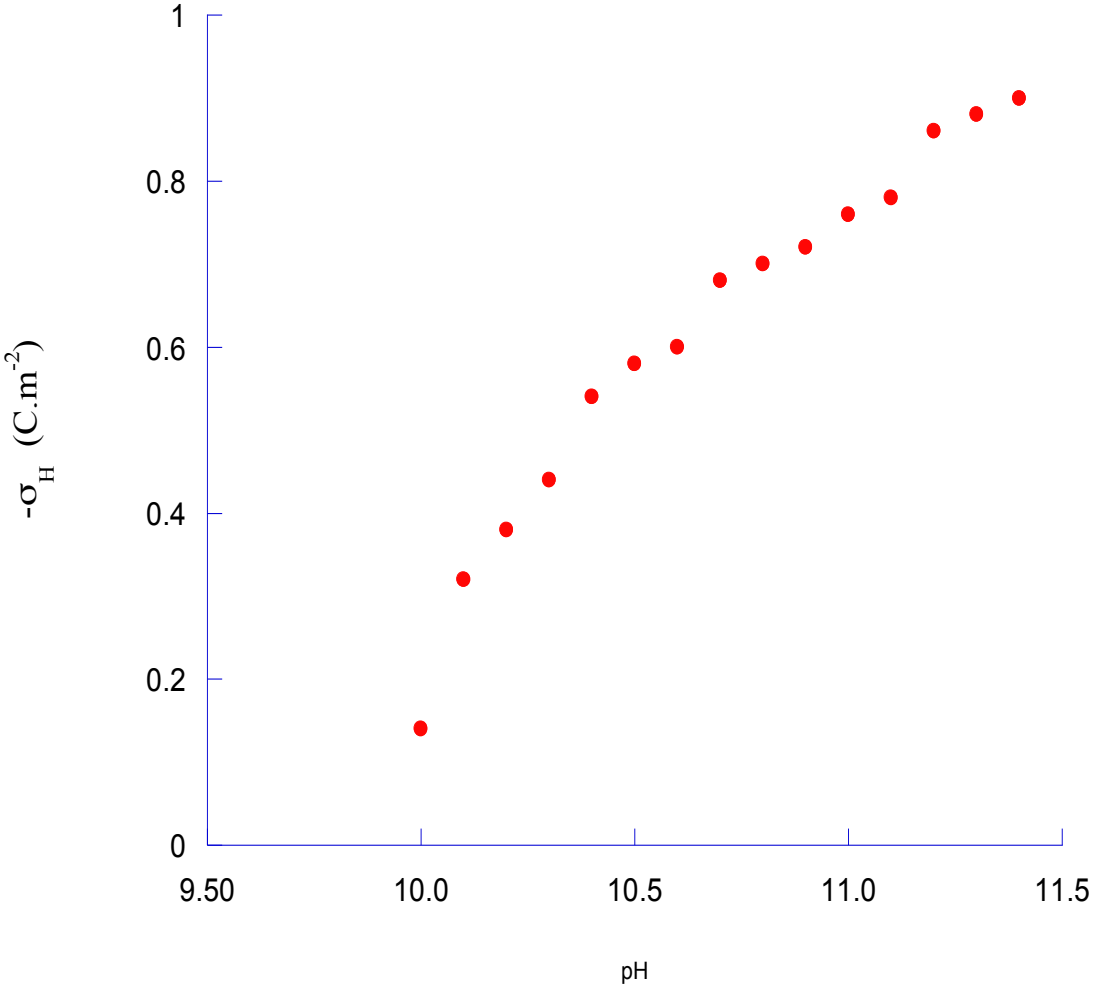
Phase II: ASR Gel

From the galleries

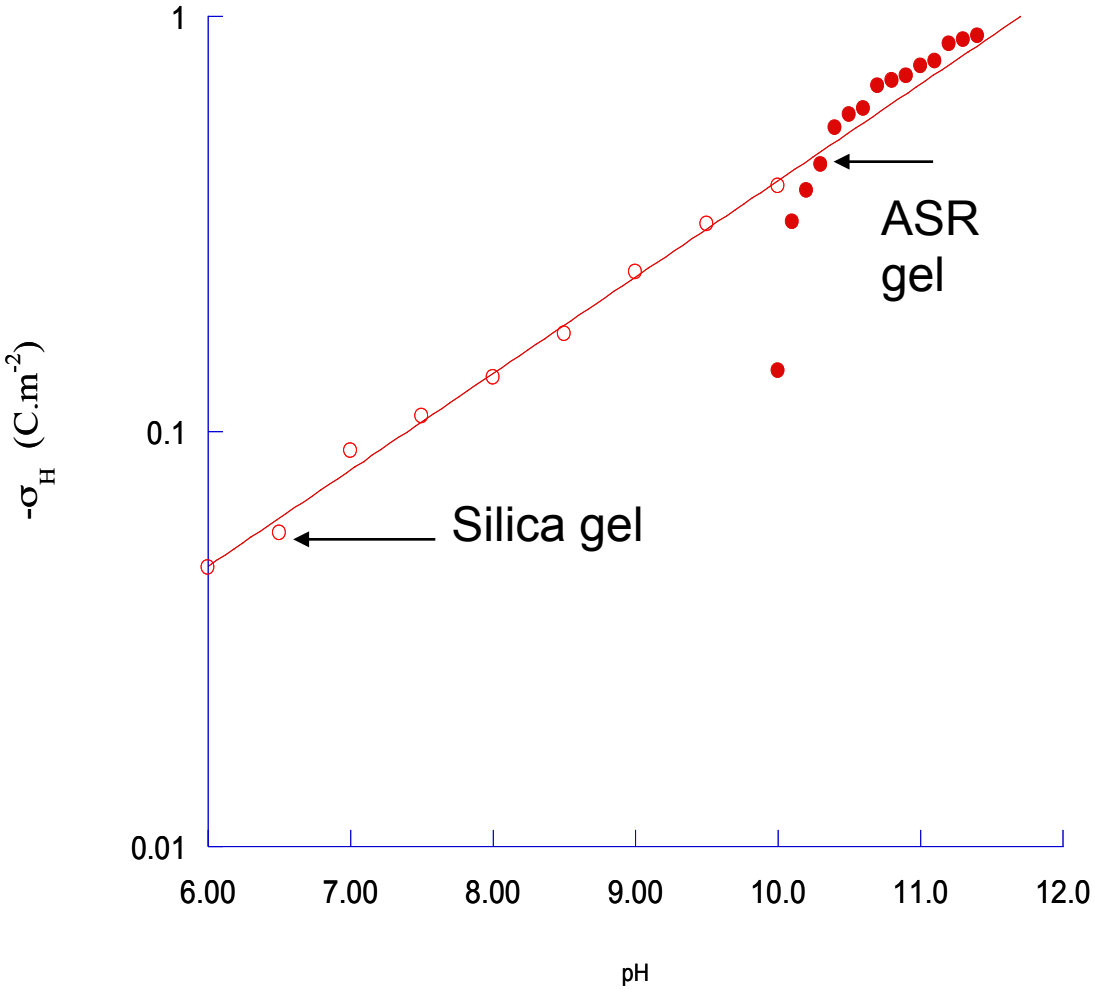


ASR Gel

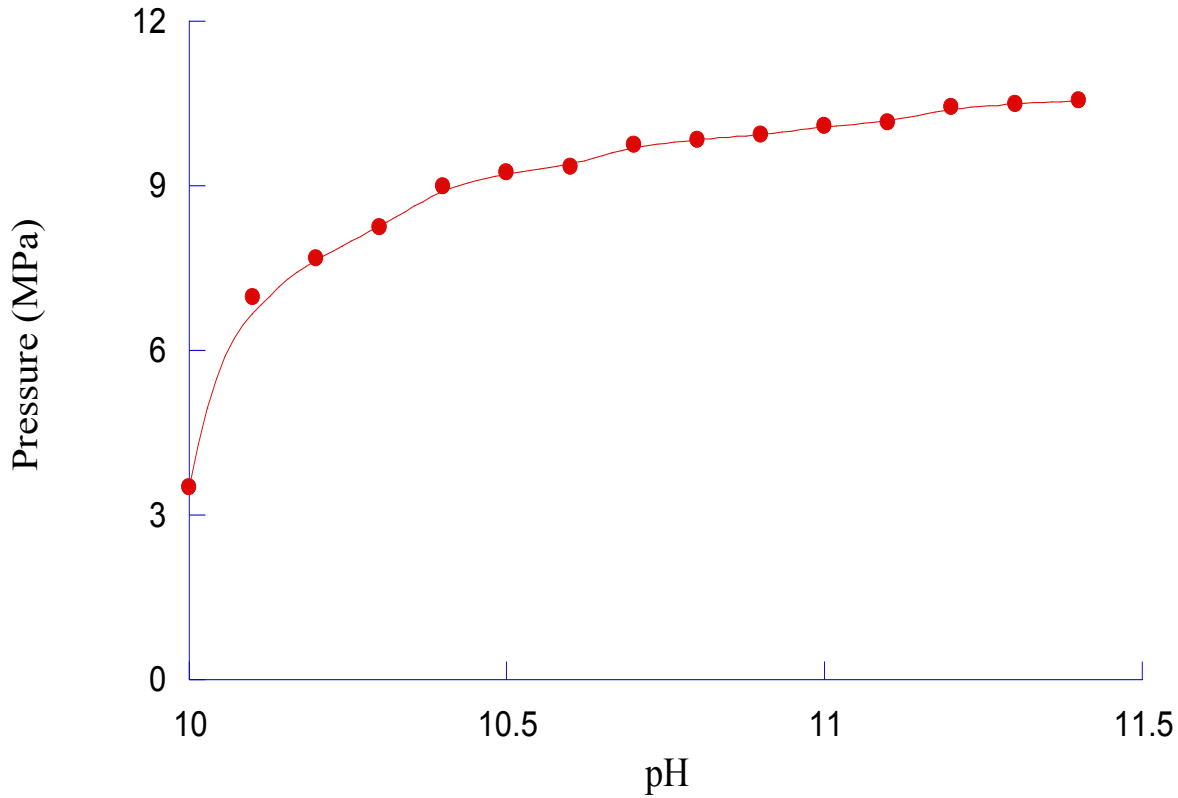
Surface charge



An Important Result



Computation of stress



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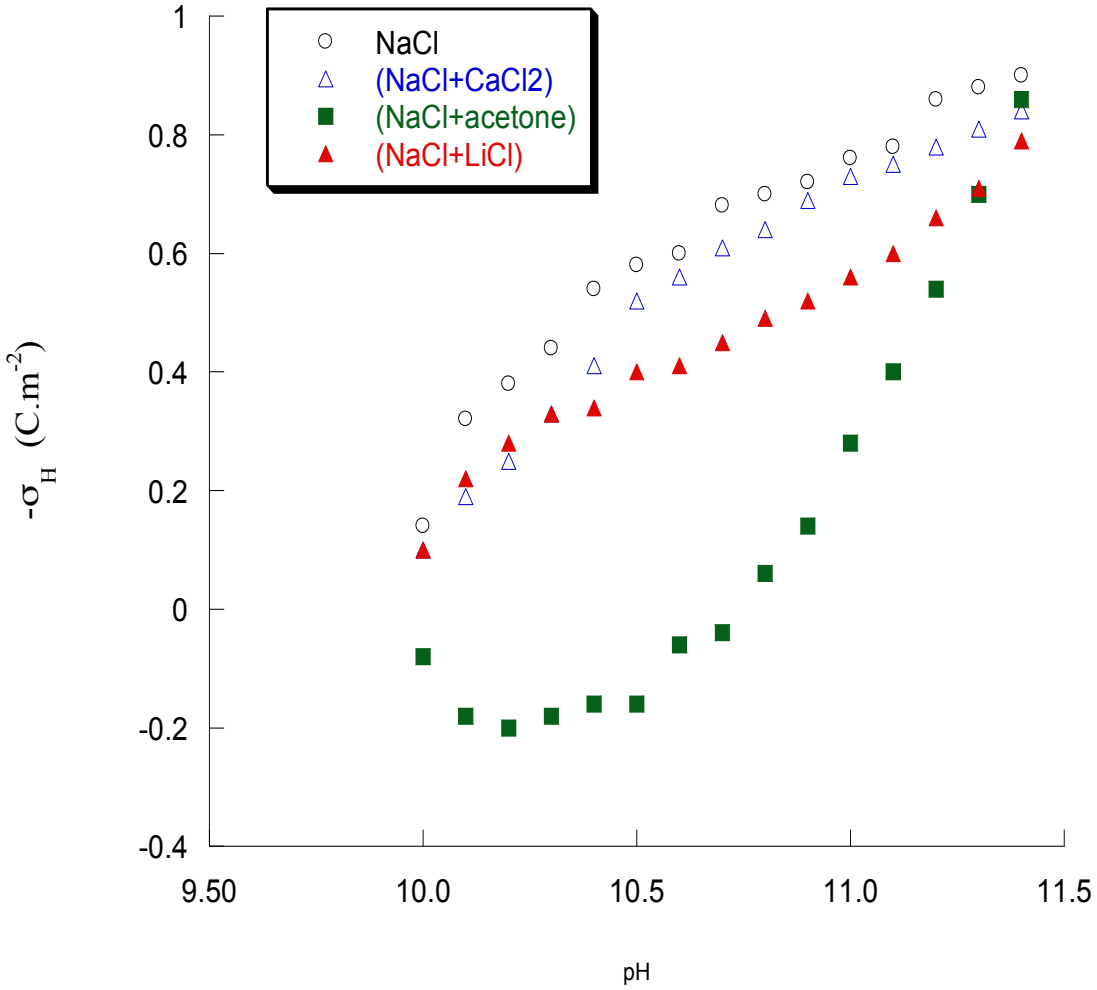
- Rodrigues, F. A., P.J.M. Monteiro, and G. Sposito, “The alkali-silica reaction: the Effect of monovalent and bivalent cations on the surface charge of opal,” Cement and Concrete Research, V31, 1549-1552, 2001.

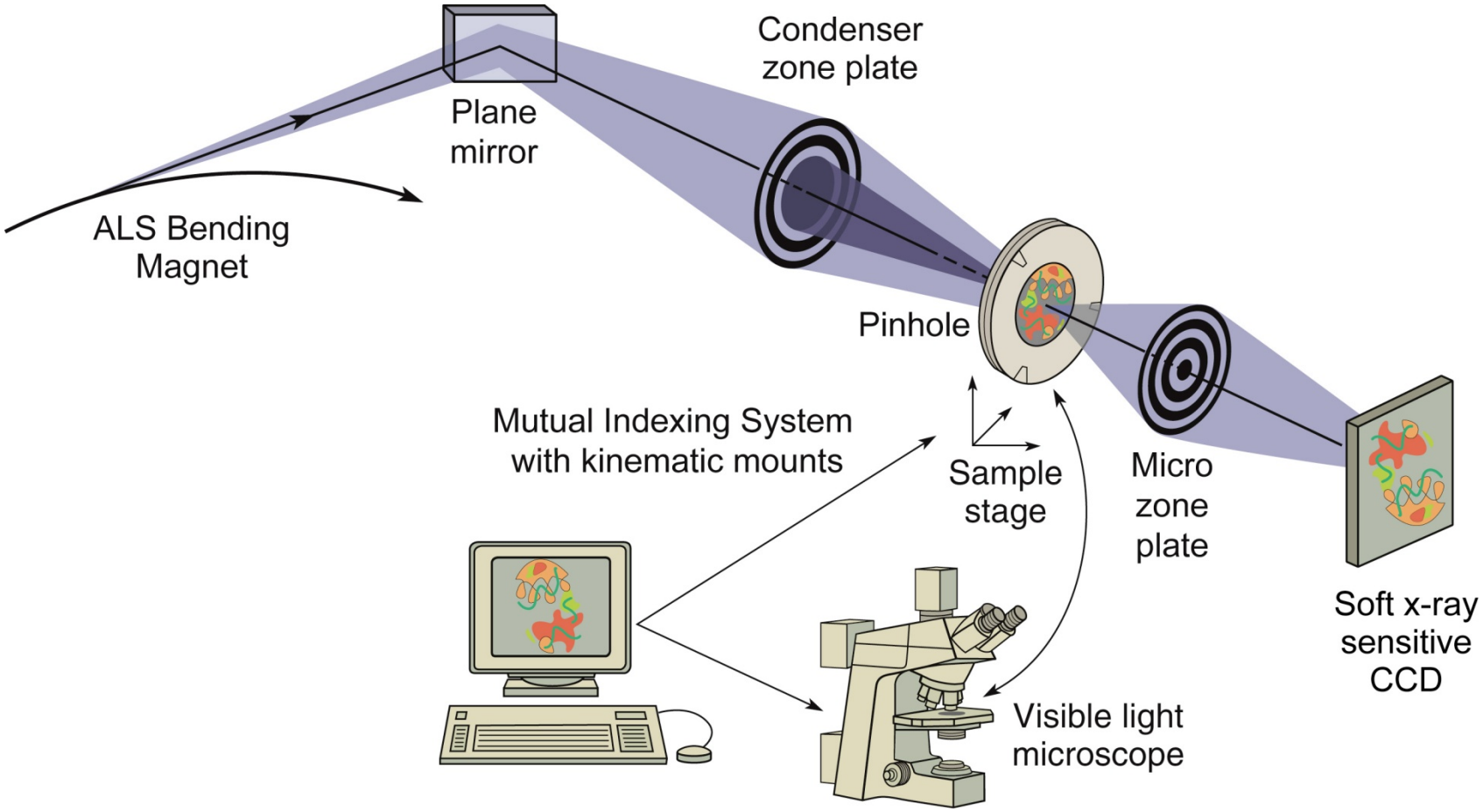
- F. A. Rodrigues, , P. J. M. Monteiro, and G. Sposito A Reply to Discussion of the Paper “The Alkali-silica Reaction: The Effect Of Monovalent And Bivalent Cations On The Surface Charge Of Opal, Cement and Concrete Research, 933-934, 2003.

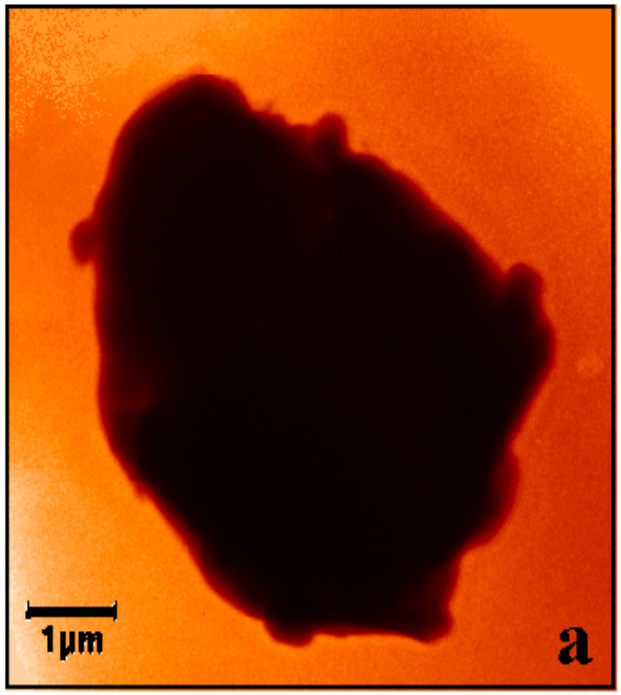
- K. Shomglin, L. Turanli, H. -R. Wenk, P. J. M. Monteiro and G. Sposito The effects of potassium and rubidium hydroxide on the alkali–silica reaction, *Cement and Concrete Research, Volume 33, Issue 11, November 2003, Pages 1825-1830*

Phase III: Effect of admixtures



Microstructure: X-ray microscopy

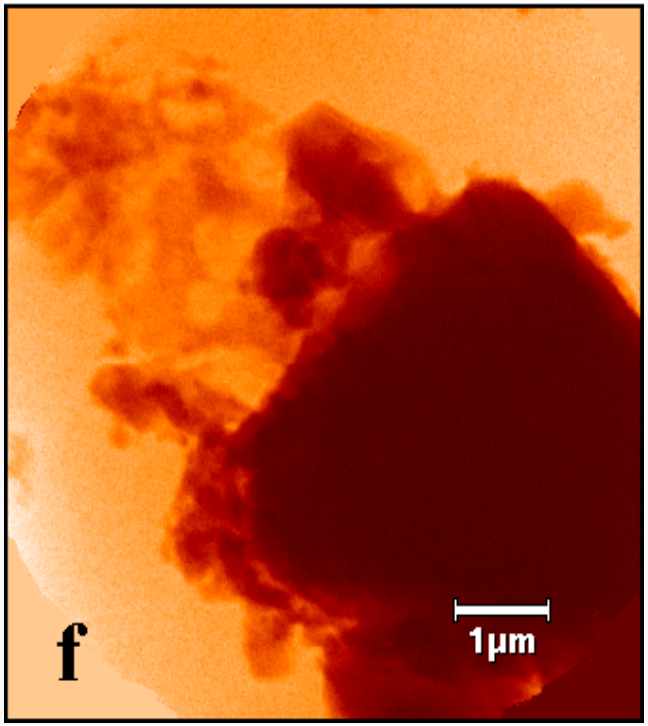




Microstructure: X-ray microscopy

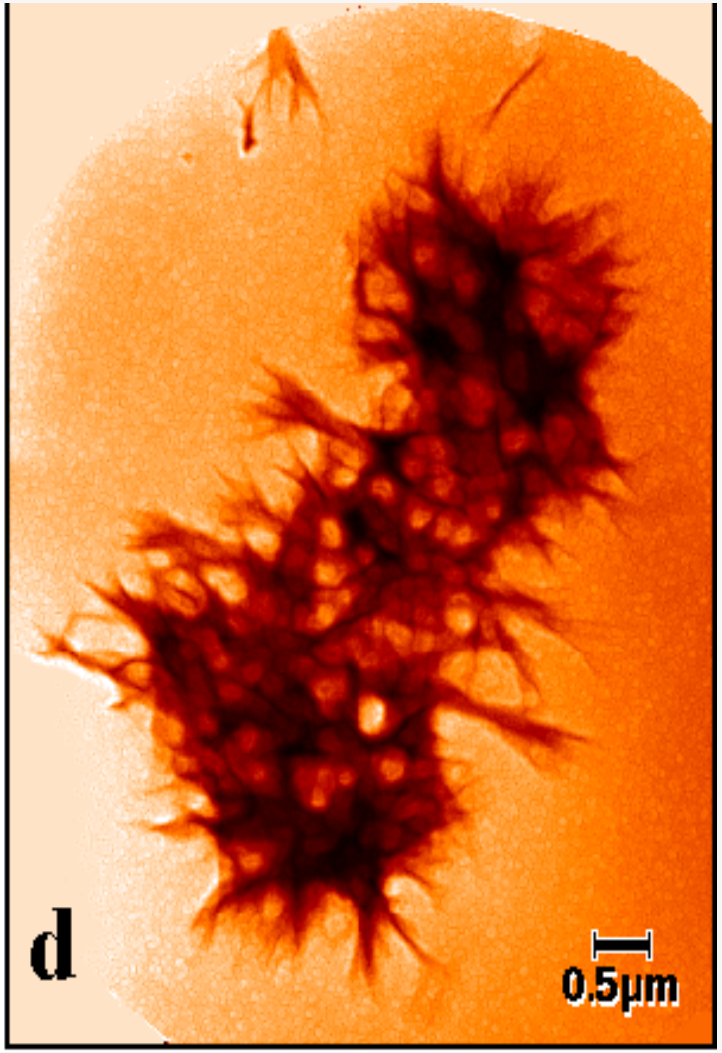
Dissolution in Na(OH)

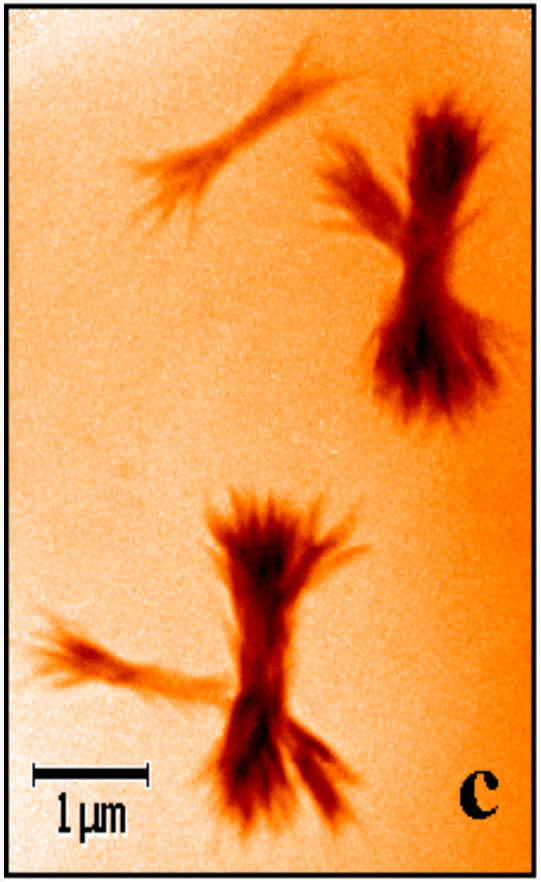
ASR Gel



E. Kurtis, Monteiro, P. J. M., J. Brown, and W. Meyer-Ilse, "Imaging of ASR Gel by Soft X-ray Microscopy," *CCR journal*, V28 N3:411-421, (1998).

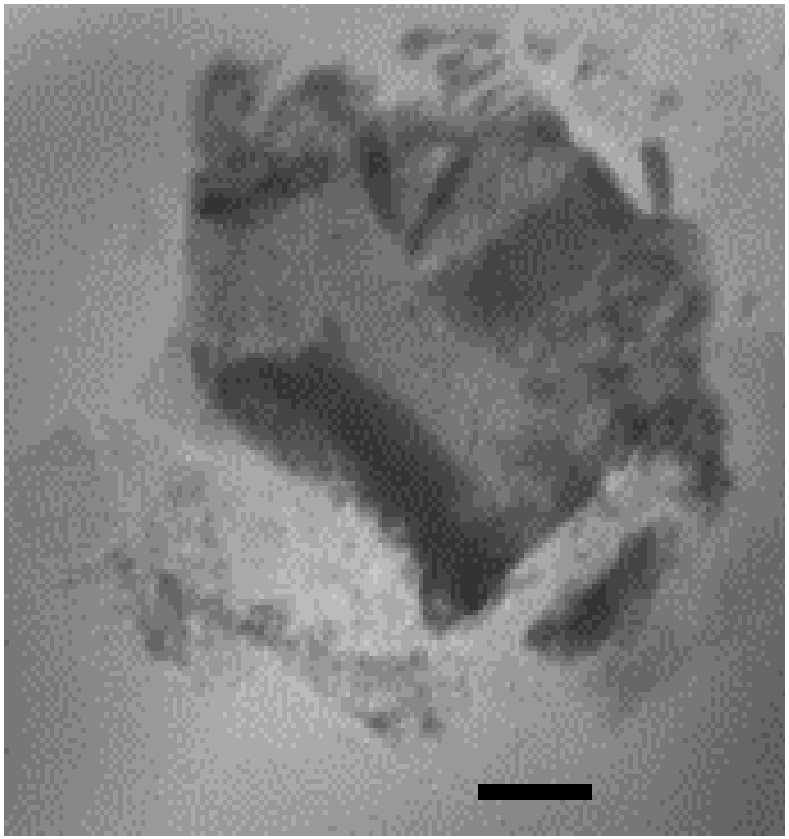
In presence of saturated Ca(OH)2 solution





E. Kurtis, Monteiro, P. J. M., J. Brown, and W. Meyer-Ilse, “Imaging of ASR Gel by Soft X-ray Microscopy,” *CCR journal*, V28 N3:411-421, (1998).

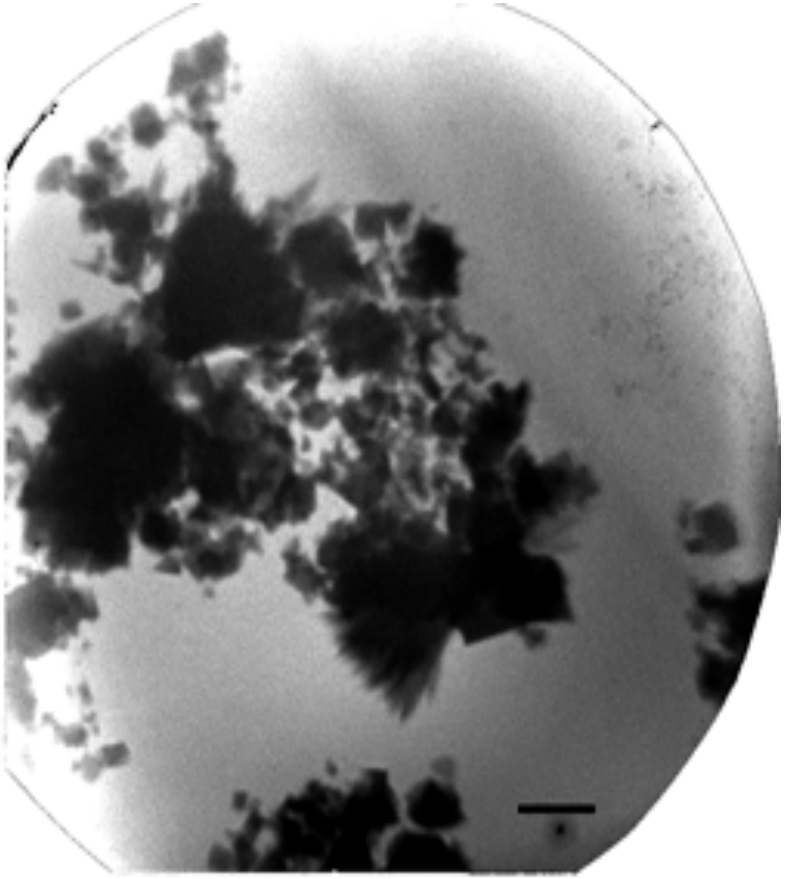
Effect of LiCl



0.7M NaOH + 0.1M LiCl solution
scalebar = 1μm

Dissolution and the formation of a relatively small amount of repolymerized gel
Lithium is known to stabilize colloids and to prevent gelling

Effect of LiCl



lithium may promote the aggregation of relatively larger (but still colloidal) silicate particles

Alkali-Aggregate Reaction

- Problematic siliceous aggregate are easy to identify but it is very challenging to characterize reactive silicate aggregates.
- The use of extinction angle is not reliable test

Scientific question:

How does amount of deformation in the aggregate affect its reactivity?

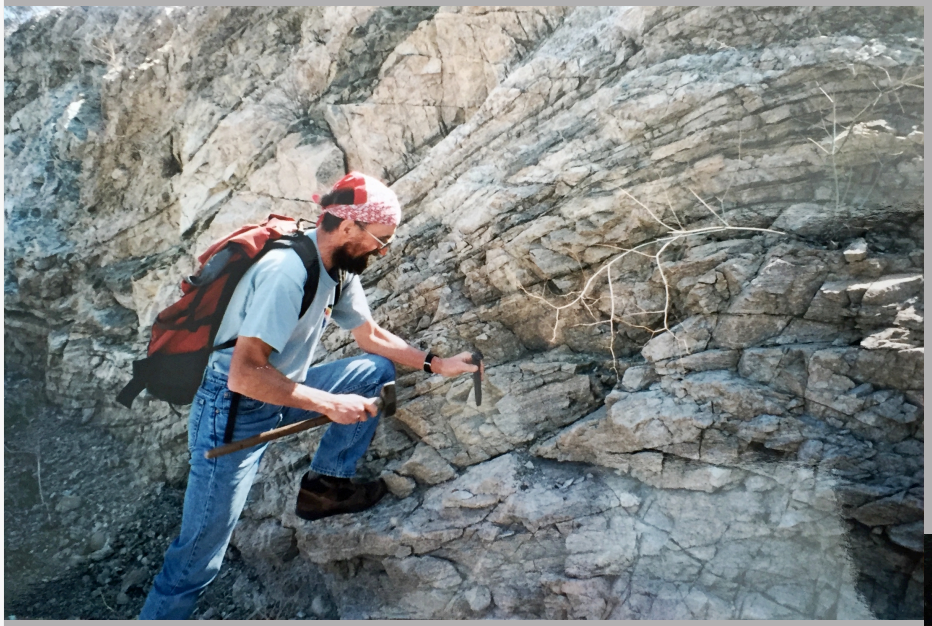
Our approach:

Use neutron diffraction experiments

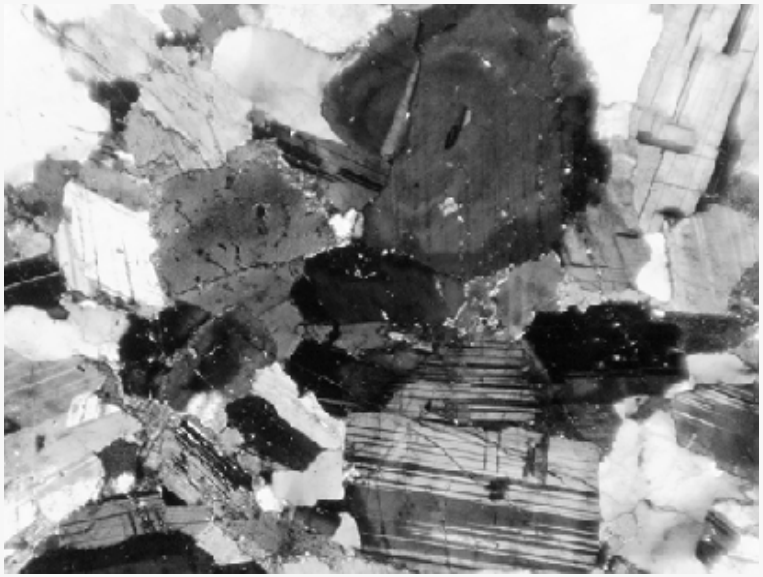
Materials

In an interesting location in the earthquake zone of Santa Rosa near Los Angeles, we collected granodiorite, mylonite, phylonite, and ultramylonite with the same chemistry but different amount of deformation.

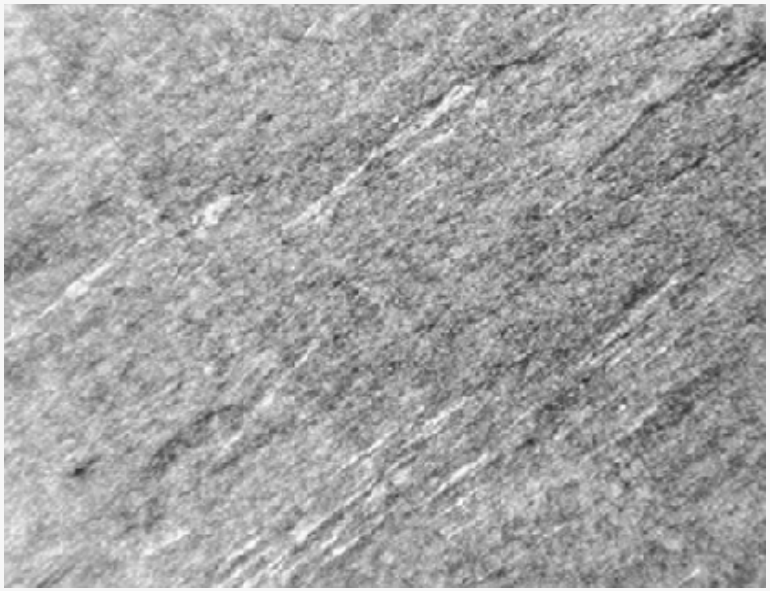
- Prof. Rudy Wenk and I collecting the rocks



Deformation



Granite

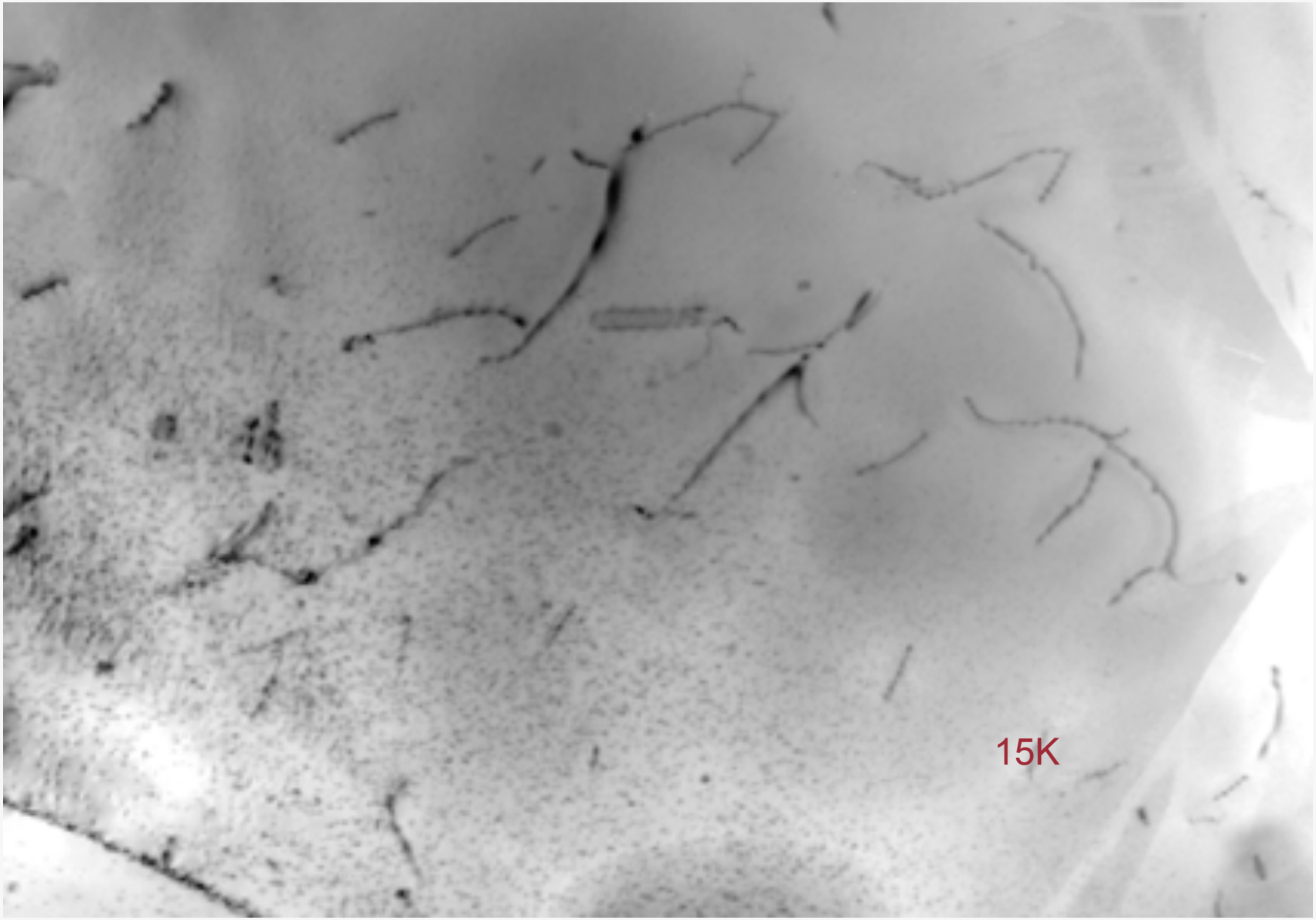


Pyllonite

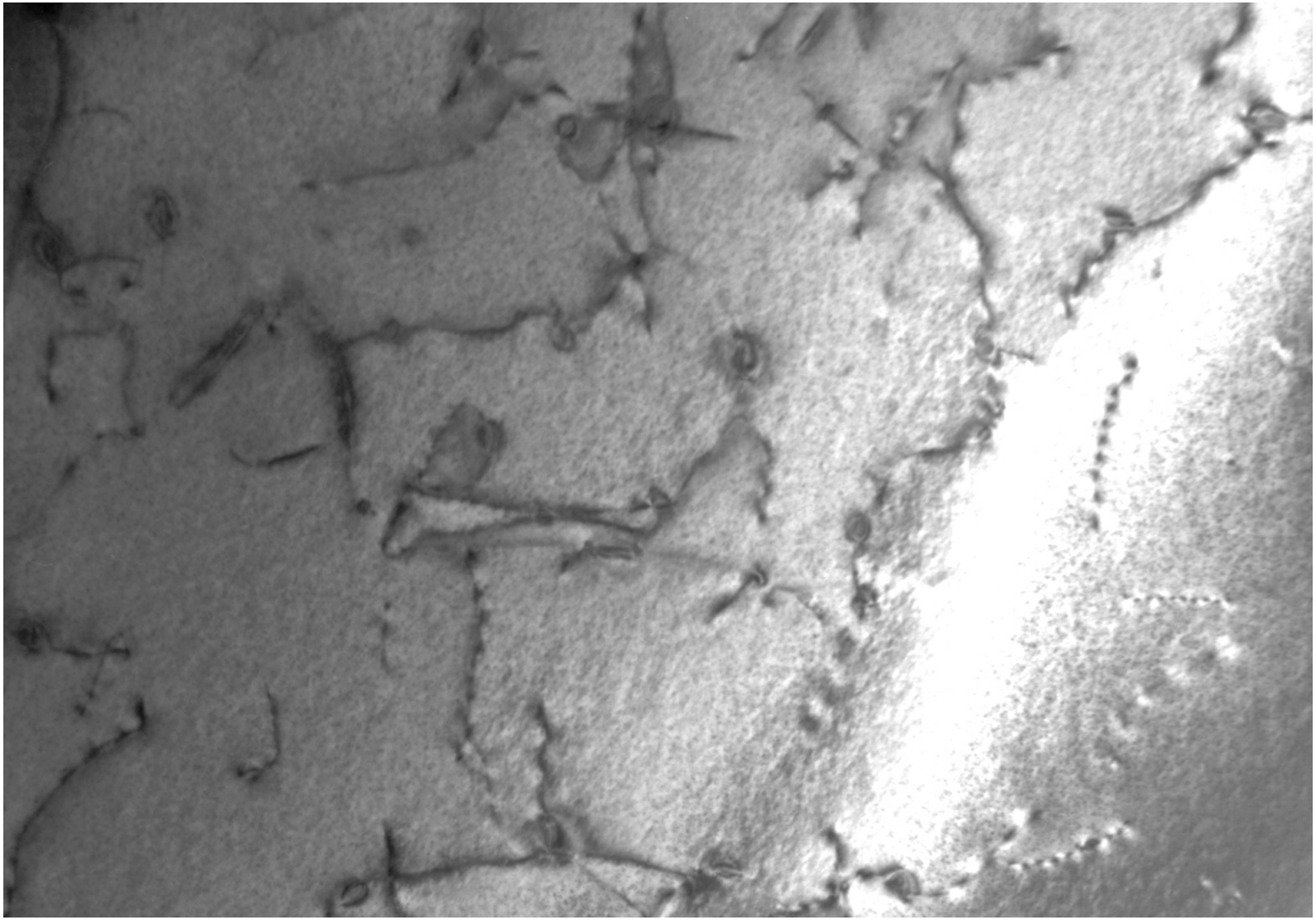
Deformation

Ultramylonite

TEM: granite

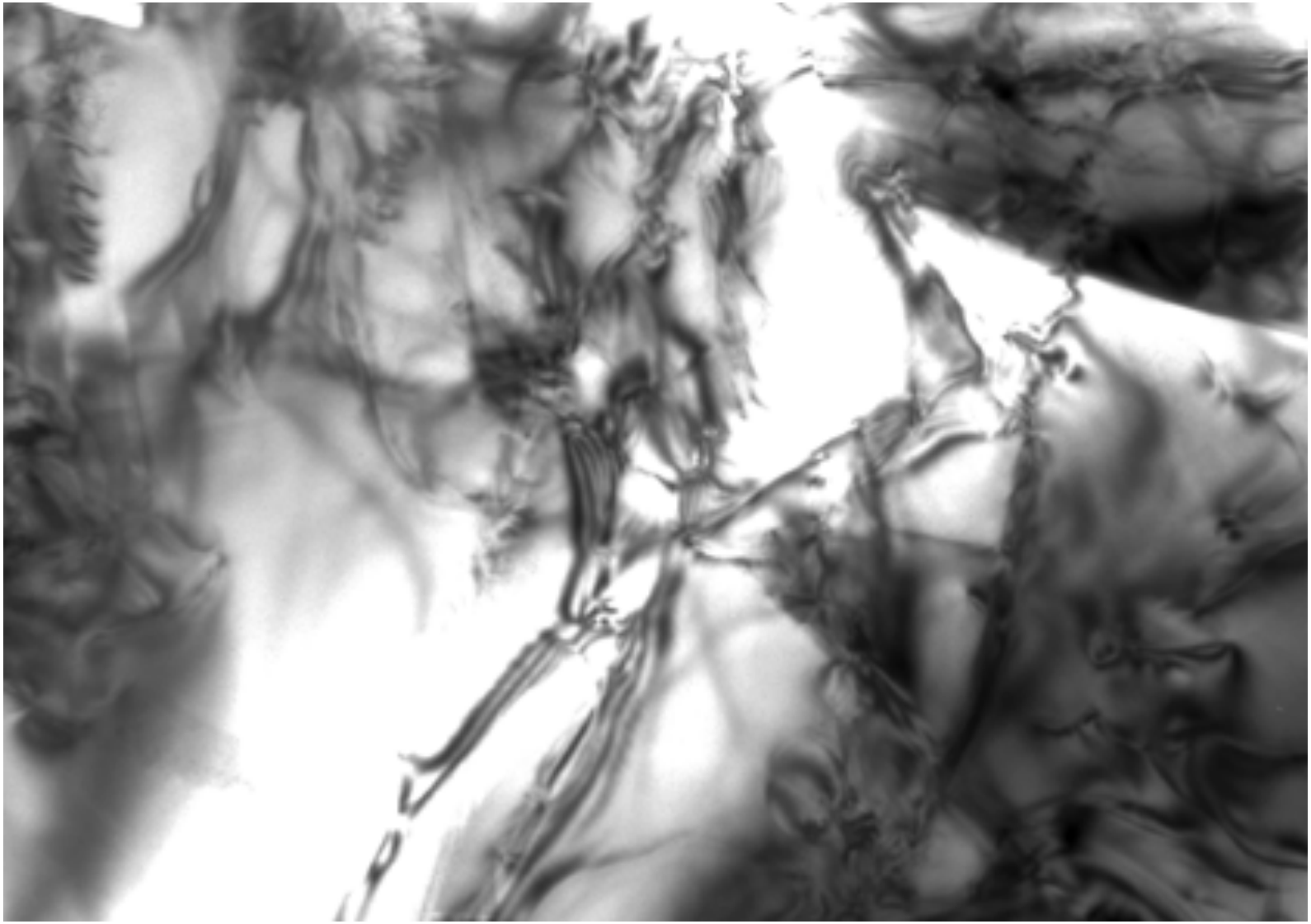


TEM: Mylonite



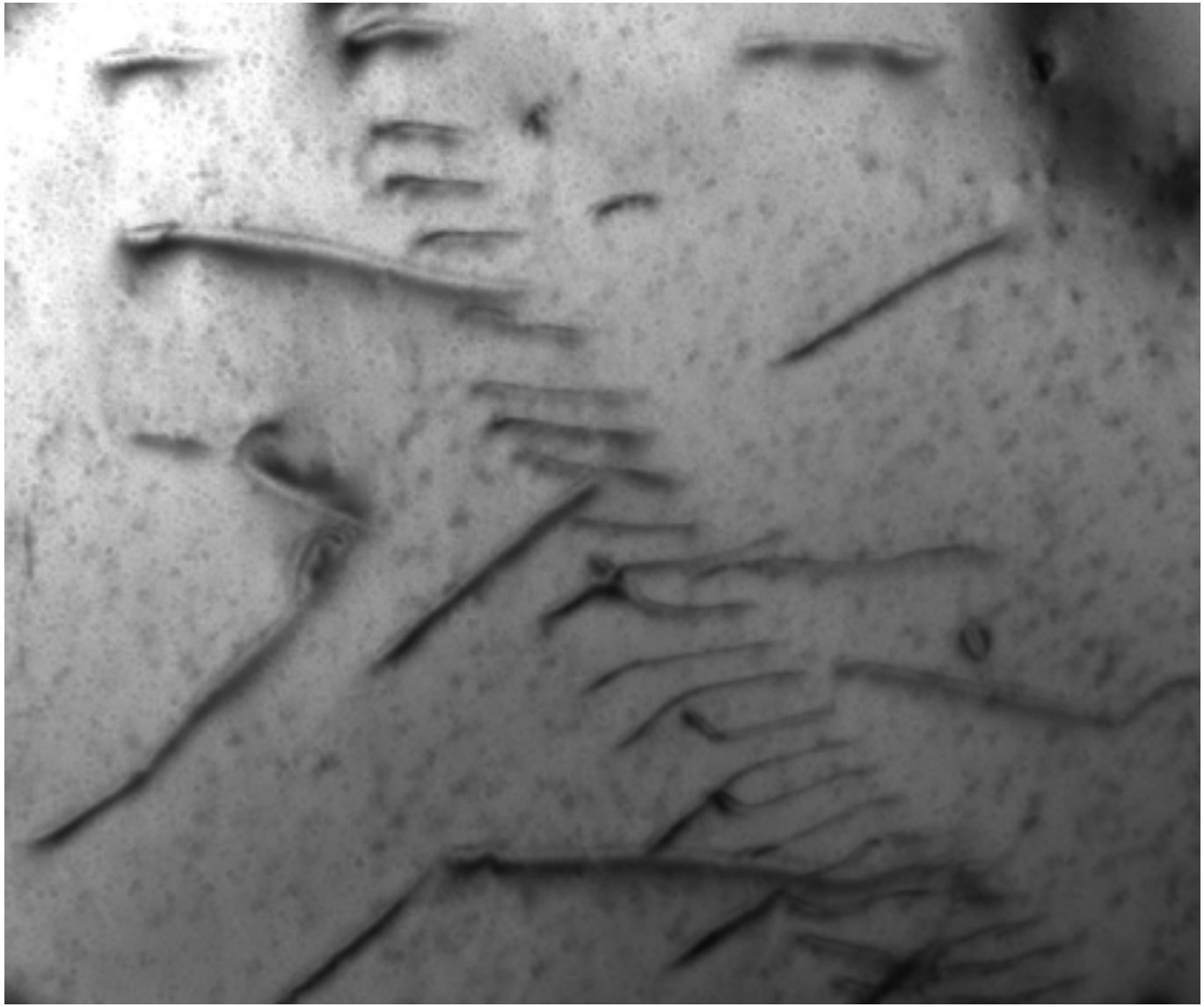
H.-R. Wenk, P.J.M. Monteiro and K. Shomglin, Relationship between aggregate microstructure and concrete expansion. A case study of deformed granitic rocks from the Santa Rosa Mylonite Zone, JOURNAL OF MATERIALS SCIENCE, Volume: 43, 1278-1285, 2008.

TEM: Phyllonite



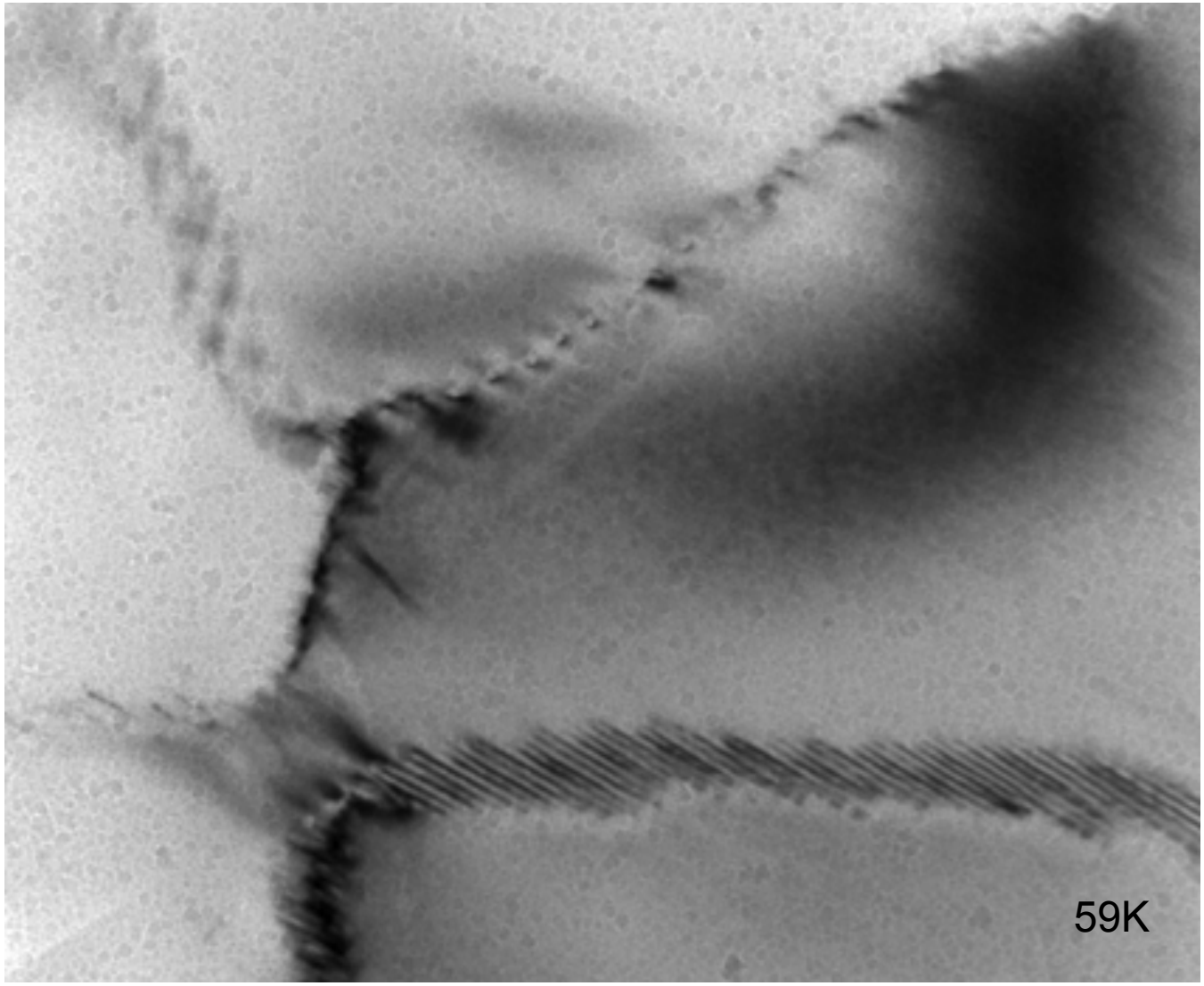
20K

TEM: Formation of sub-grains

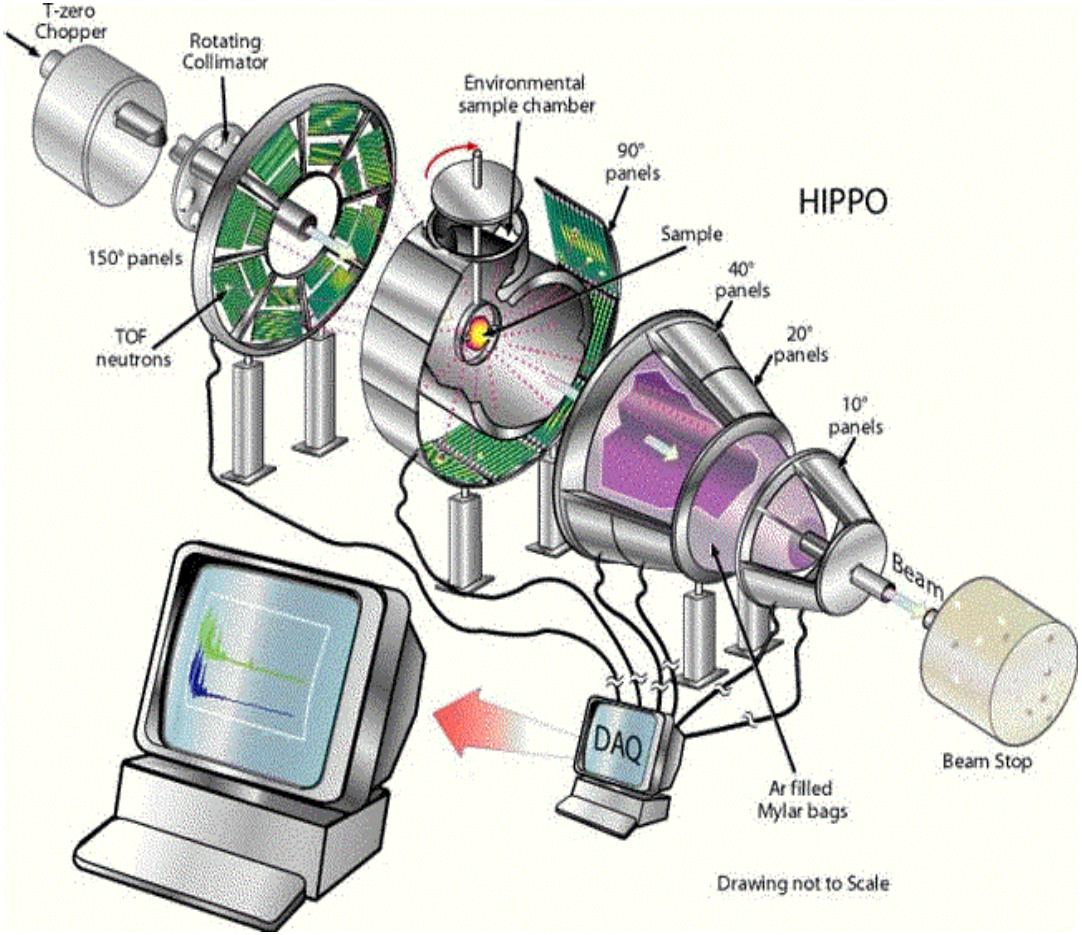


37K

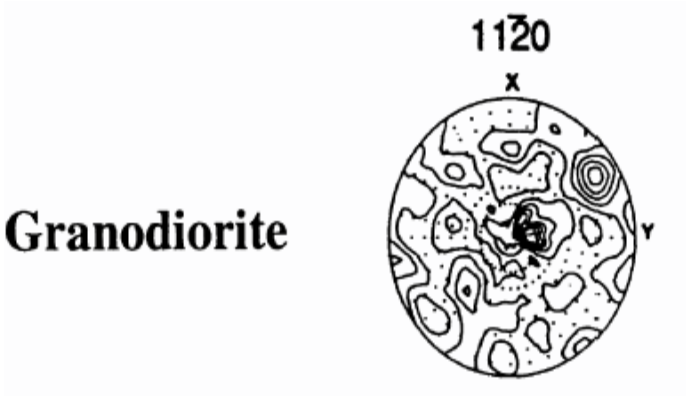
TEM: Formation of sub-grains



Determination of deformation in reactive aggregate

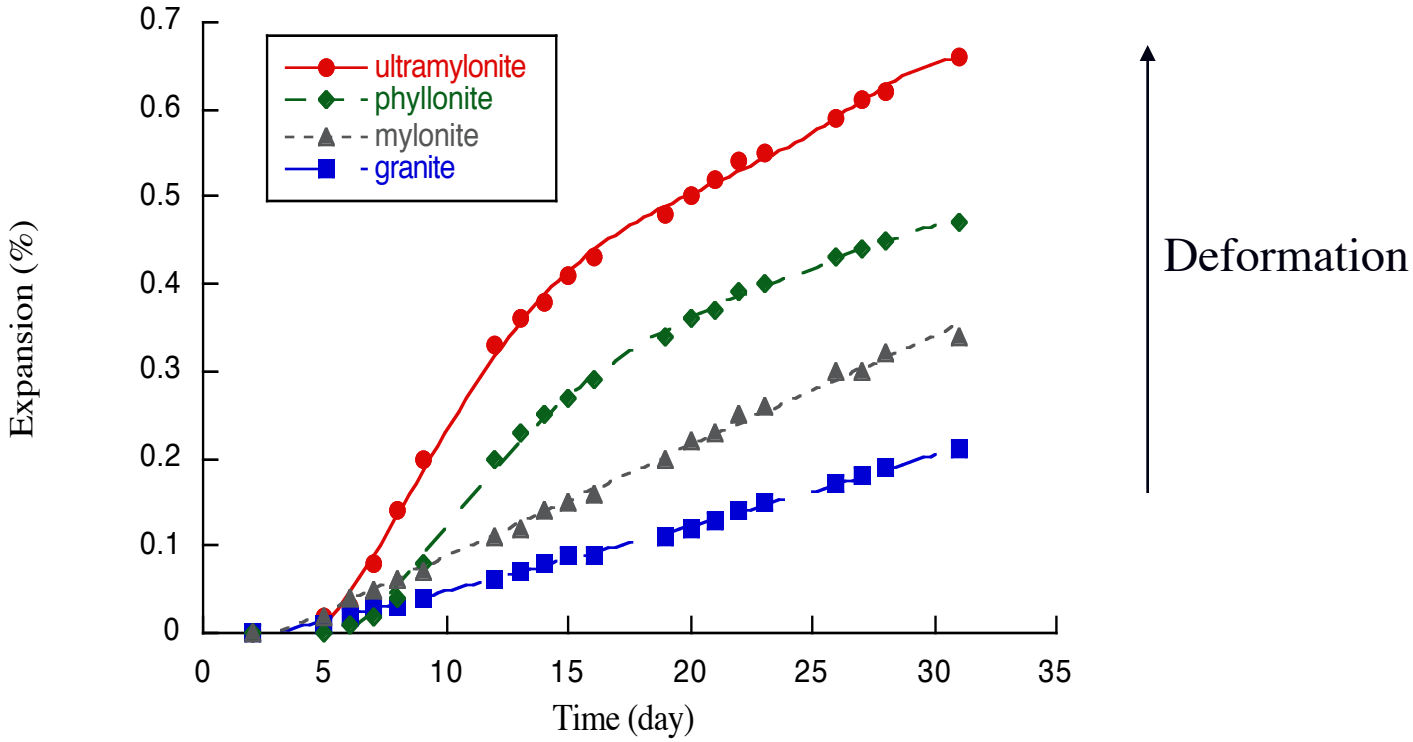


Texture Analysis – Quartz



Monteiro, P.J.M., K. Shomglin, H.R. Wenk and Nicole P. Hasparyk, “Effect of Aggregate Deformation on the Alkali-Silica Reaction,” *ACI Materials Journal*, **V98** (N2): 179-183, Mar-Apr 2001.

Expansion

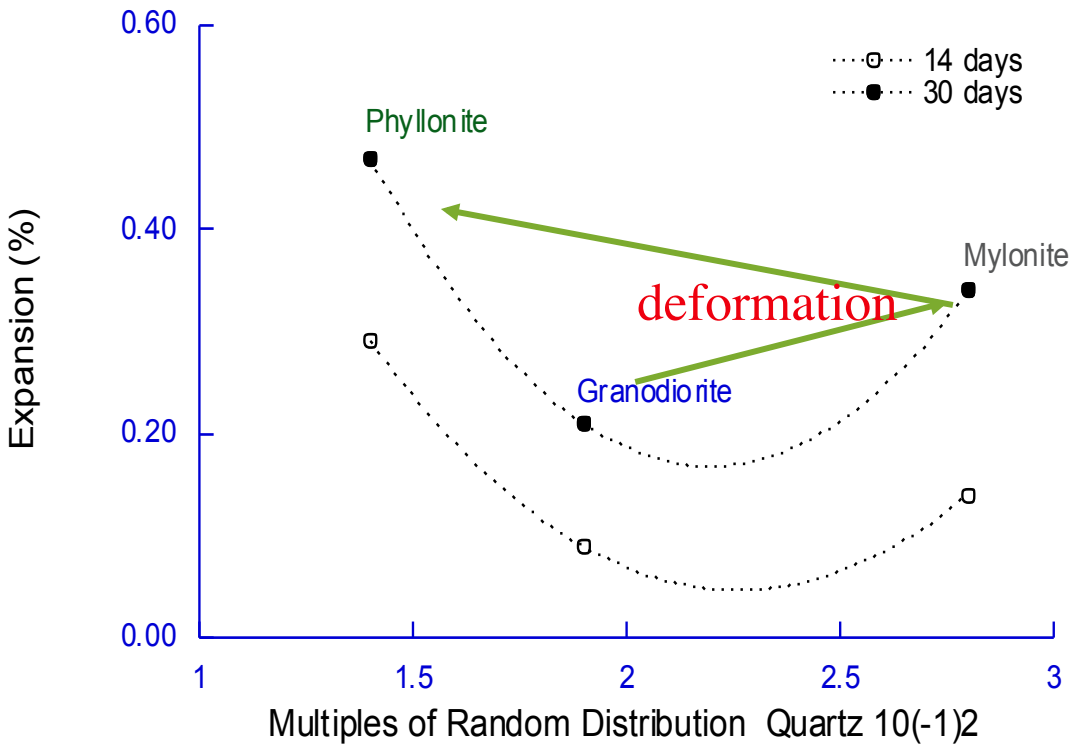


Note: all rocks had the same chemical composition

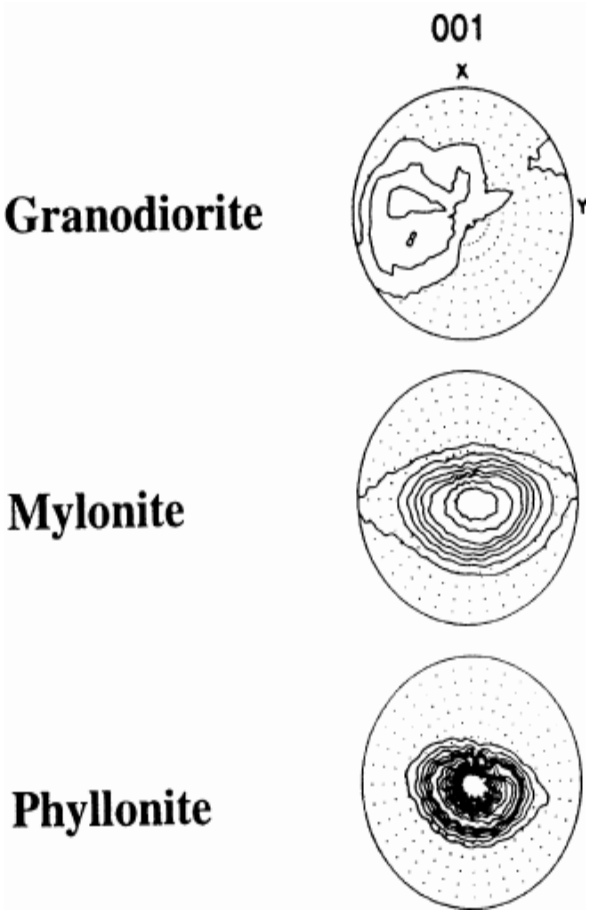
Expansion tests

- The ASTM C 1260 expansion tests indicate that mortar expands increasingly when made with granite, mylonite, phyllonite, and ultramylonite respectively

Mortar Bar Expansion



Texture Analysis – Biotite



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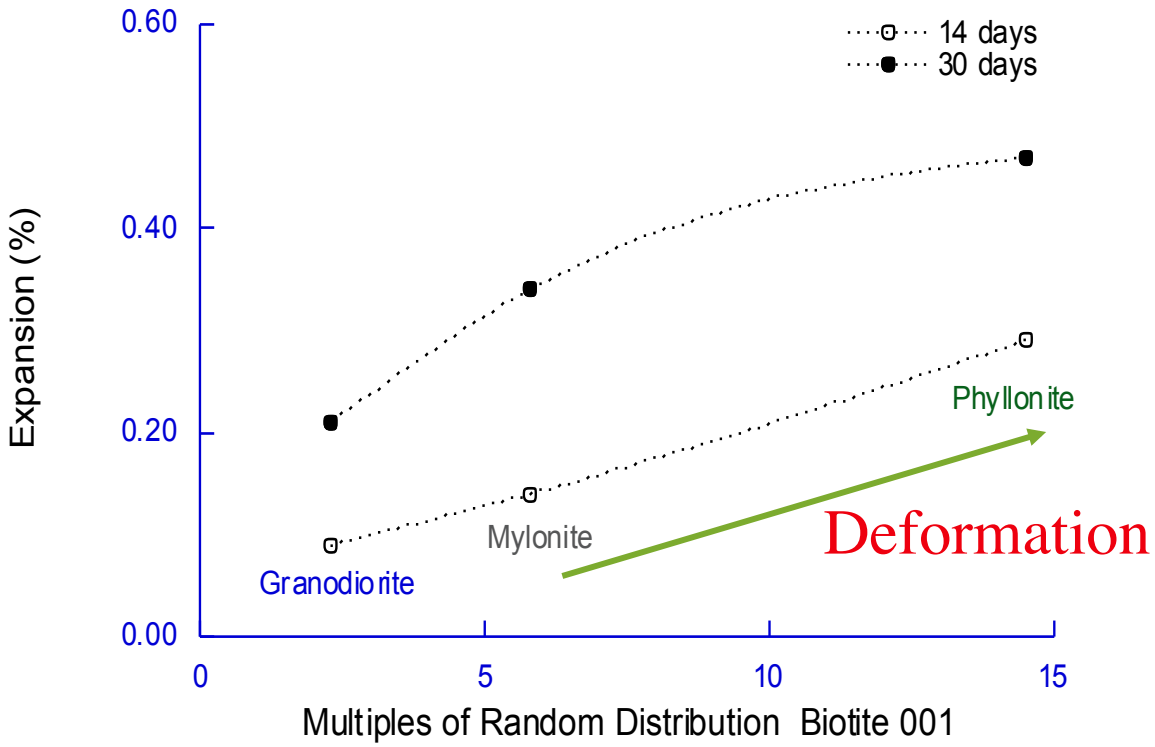
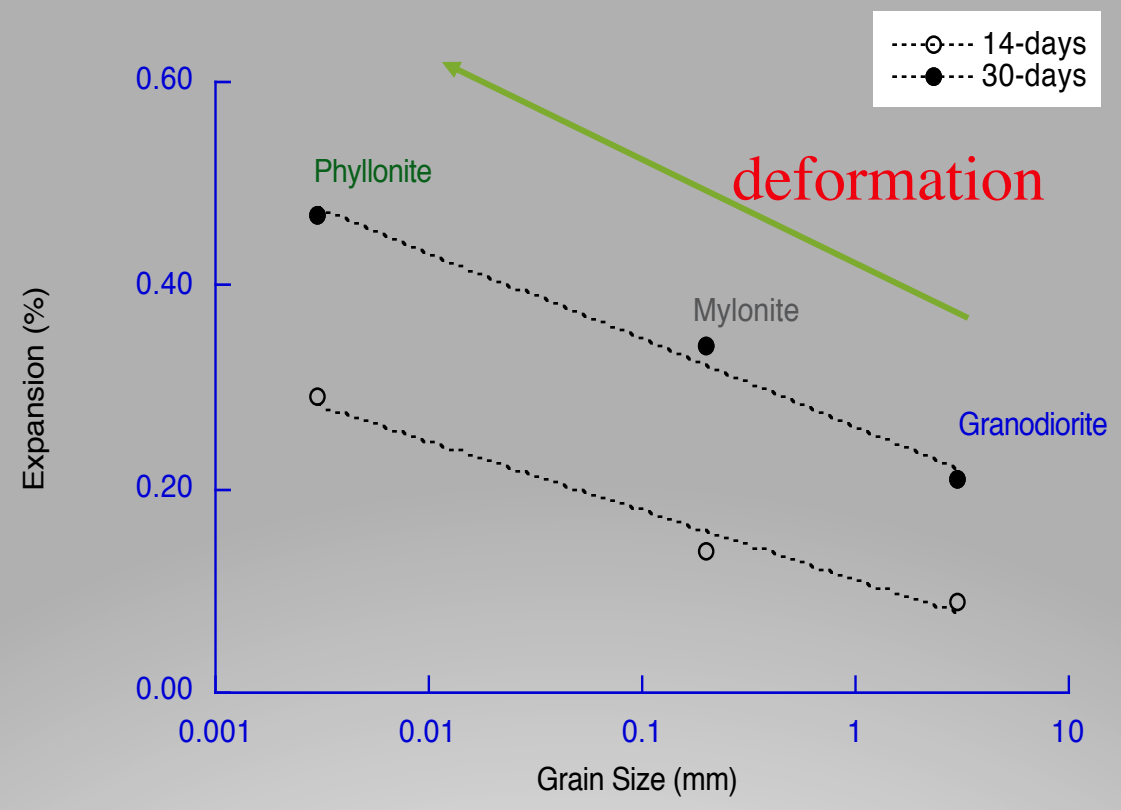
Mortar Bar Expansion



Effect of Grain Size



Conclusions

- There is a significant correlation between expansion and the development of foliation, and accompanying reduction in grain size.
- The results suggest that the alkali-silica reaction depends on more factors than simply the crystallinity of quartz.

Conclusions

- Deformed granitic rocks provide a good system to quantify these parameters.
- Texture analysis of these rocks indicated that there is a quantitative relationship between the degree of deformation and reactivity

- STRUCTURE OF ALKALI SILICATE GEL BY TOTAL SCATTERING METHODS

Pair distribution function

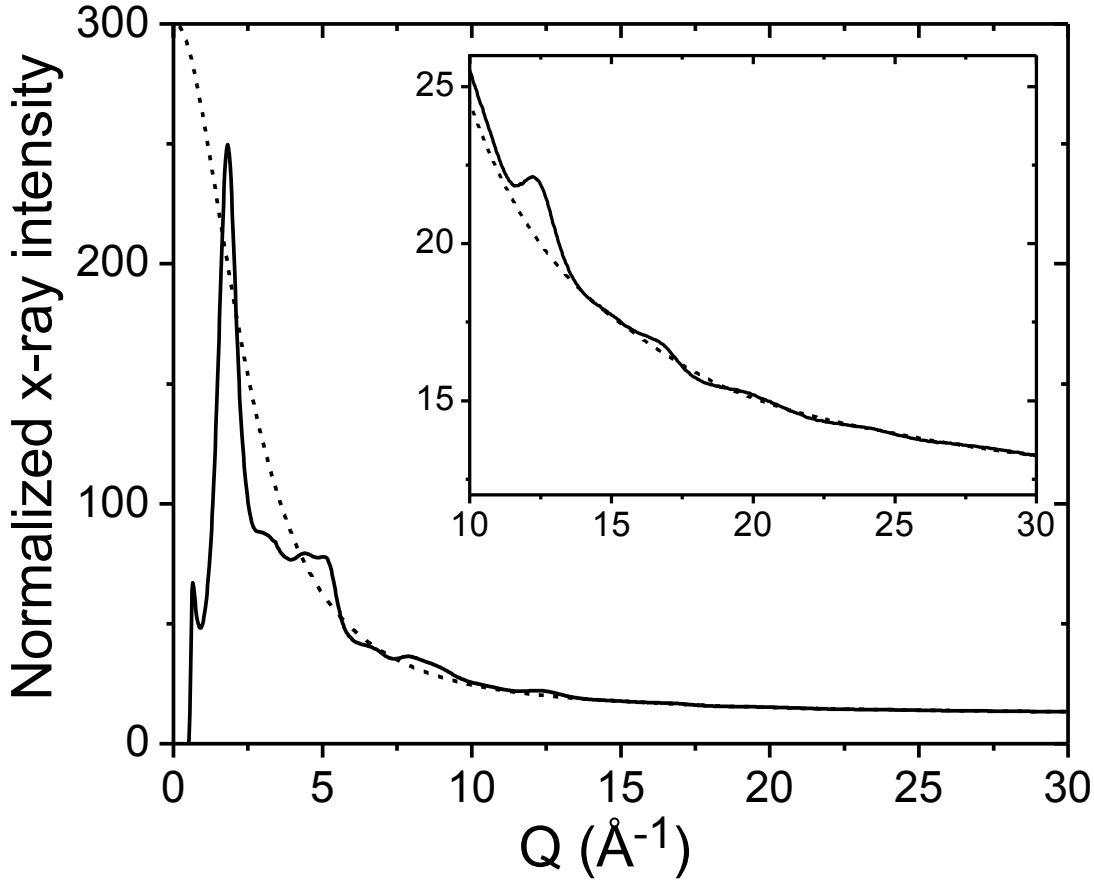
$$G_X(r) = \frac{f_i(Q) f_j(Q)}{(2\pi)^3 \rho_o} \int_0^\infty 4\pi Q^2 S_X(Q) \frac{\sin Qr}{Qr} dQ$$

Where $S_X(Q)$ the structure factor and ρ_o=N/V is the atomic number density

Testing Methods

- High-energy x-ray diffraction measurements on beamline 1-ID at the Advanced Photon Source, Argonne National Laboratory.
- Incident beam energy of 100.0 keV.
- Two-dimensional GE amorphous silicon area detector

The measured and background corrected x-ray intensity



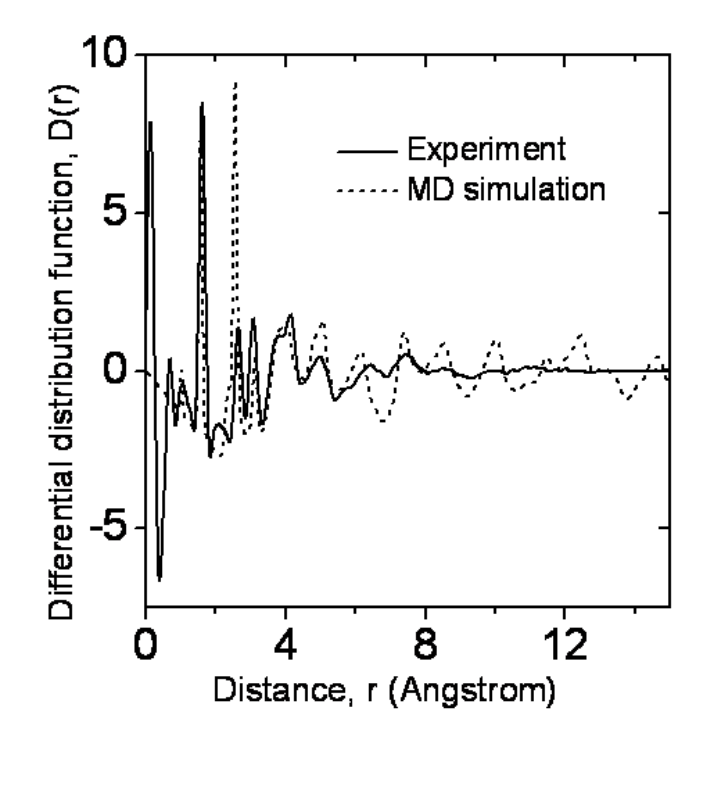
C. Benmore and Monteiro P.J.M., The structure of alkali silicate gel by total scattering methods, Cement and Concrete Research, Volume 40, Issue 6, 2010, Pages 892-897.

Comparisons with MD (I)

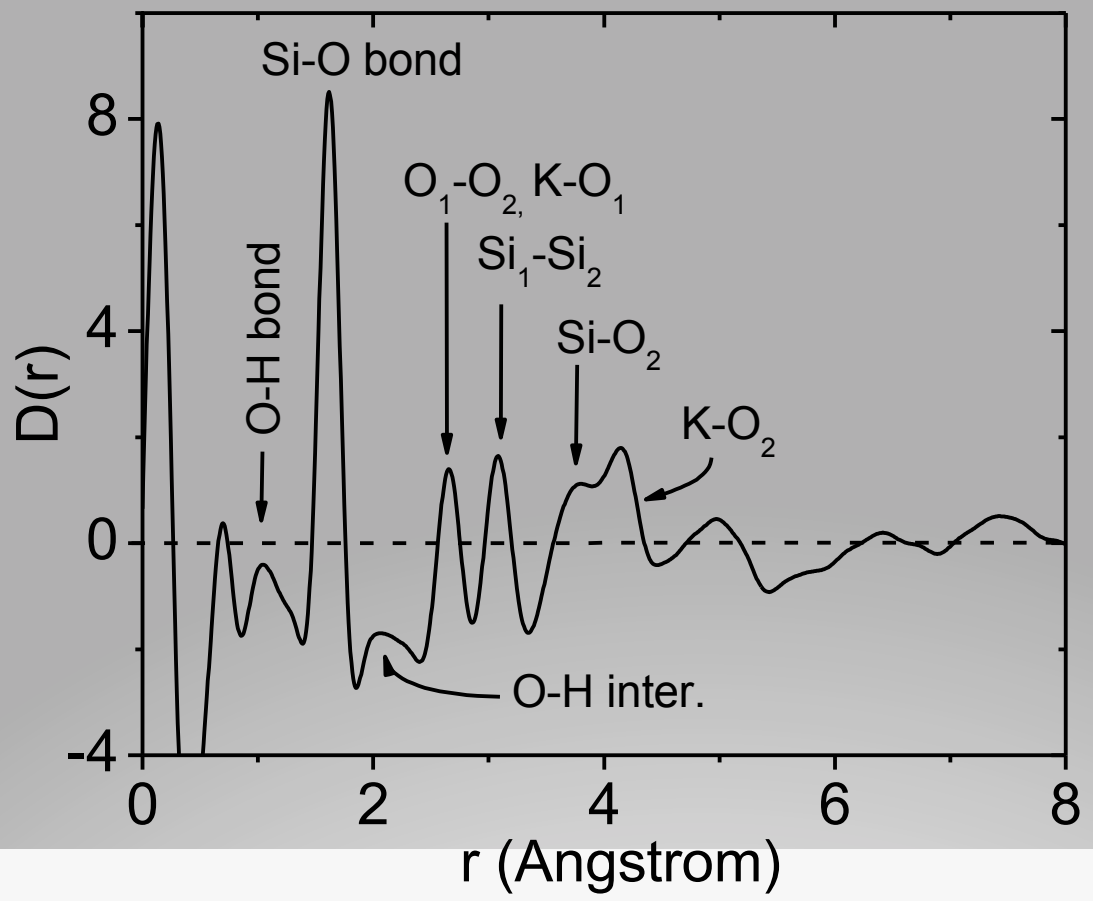
- Thanks to Profs. Kirkpatrick and Kalinichev for sharing their data.
- The persistence of a distorted kanemite-like structure is in good agreement with the MD simulation.
- The PDF measurements are consistent with MD predictions that it is energetically unfavourable for the water to penetrate the interlayer volume in significant quantity.

Comparisons with MD (II)

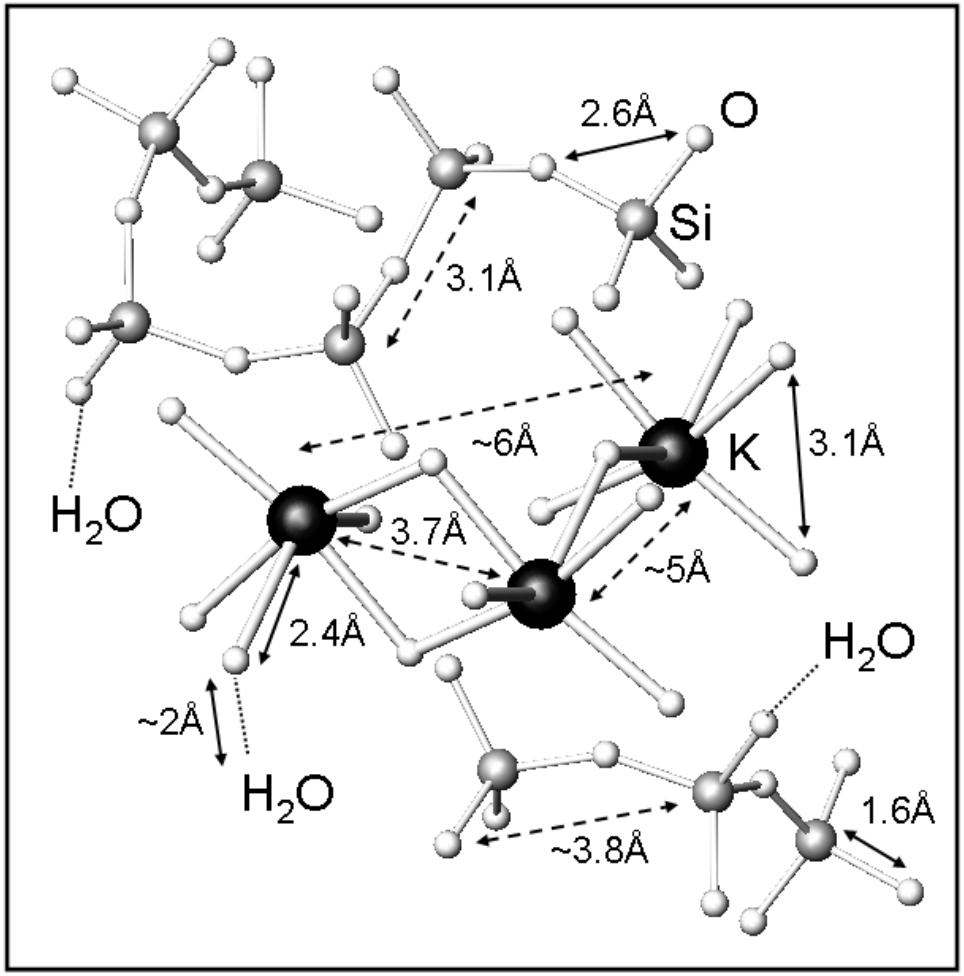
- Our results show no distinct preferred orientational correlations beyond ~10Å



X-ray differential distribution function D(r)



A local structural model of the amorphous alkali silicate gel



C. Benmore and Monteiro P.J.M., The structure of alkali silicate gel by total scattering methods, Cement and Concrete Research, Volume 40, Issue 6, 2010, Pages 892-897.

Where is the water?

- Due to the lack of long range ordering in this material we suggest that water molecules probably reside in pores surrounding these kanemite-like fragments as well as within the layers themselves.