

Micro-structure of Portland Cement Paste and Time Evolution of Dynamic Properties of Its Hydration Water during the Curing Process

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Abstract

The major hydration product of commercial Portland cement paste, a construction material of the largest production and use in modern society, is the Calcium-Silicate-Hydrate (C-S-H) gel. Thus the detail knowledge of characteristic micro-structure of the C-S-H gel as a function of its hydration level is essential to the understanding of its ultimate mechanical strength when the cement paste eventually sets and becomes a concrete. The basic building block of the C-S-H is called a “globule” in Jennings’ Colloidal Model-II developed in 2006 [1]. The detailed nano-structure of the globule is so far not given quantitatively. We recently determined the structural parameters of the globule with good accuracy by an Extended-Q Small-Angle Neutron Scattering (EQ-SANS) technique probing a large interval of the scattering vector Q , from 0.015 \AA^{-1} to 1.0 \AA^{-1} . In this Q -range an inter-lamellar peak at 0.65 \AA^{-1} - 0.80 \AA^{-1} is present, shifting as a function of the water content present in the C-S-H gel. This additional feature enables us to confirm the presence of a lamellar structure and determine the thicknesses of both the water and the hydrated calcium silicate layers respectively proper of the C-S-H globules as a function of its hydration level [2].

The hydration kinetics of the four pure phases (C_3S , C_2S , C_3A , and C_4AF) present in the commercial Portland cement have been investigated by the incoherent Quasi-Elastic Neutron Scattering (QENS) technique, using Relaxing Cage Model (RCM), a method of analysis developed by Chen [3-12]. This model allows us to extract first the immobile fraction p of water, which gives the fraction, $1-p$, of the unreacted water during initial stage of hydration reaction in the cement paste. Furthermore, RCM gives also the average relaxation time $\langle\tau\rangle$, the self-diffusion constant D and the stretch exponent β of the relaxation function of hydration water. These parameters allow us to assess the average pore size and the pore size distribution inside a cement paste and their variations during the kinetic evolution of the hydration reaction.

References

- [1] J.J. Thomas and H.M. Jennings “A colloidal interpretation of chemical aging of the C-S-H gel and its effects on the properties of cement paste”, *Cement and concrete Research* (2006) **36**, 30-38.
- [2] W. -S. Chiang and S. -H. Chen, et al, “Microstructure Determination of Calcium-Silicate-Hydrate Globules by Small-Angle Neutron Scattering”, *J. Phys. Chem. C*, **116**, 5055 (2012).
- [3] E. Fratini, S.H. Chen, P. Baglioni, M. C. Bellissent-Funel, "Age-Dependent Dynamics of Water in Hydrated Cement Paste", *Phys. Rev. E*, **64**, 020201 (2001).
- [4] E. Fratini, S.H. Chen, P. Baglioni, M. C. Bellissent-Funel, "Quasi-Elastic Neutron

Scattering Study of Translational Dynamics of Hydration Water in Tricalcium Silicate", *J. Phys. Chem. B*, **106**, 158 (2002).

[5] E. Fratini, A. Faraone, P. Baglioni, M. C. Bellissent-Funel, S.H. Chen, "Dynamic Scaling of QENS Spectra of Glassy Water in Aging Cement Paste ", *Physica A*, **304**, 1 (2002).

[6] E. Fratini, S.H. Chen, P. Baglioni, J. C. Cook, J. R. D. Copley, "Dynamic Scaling of Quasi-Elastic Neutron Scattering Spectra From Interfacial Water", *Phys. Rev. E*, **65**, 010201(R) (2002).

[7] A. Faraone, S.H. Chen, E. Fratini, P. Baglioni, L. Liu, C. Brown, "Rotational Dynamics of Hydration Water in Dicalcium Silicate by Quasielastic Neutron Scattering", *Phys. Rev. E*, **65**, 040501 (2002).

[8] E. Fratini, S.H. Chen, P. Baglioni, "Investigation of the Temporal Evolution of Translational Dynamics of Water Molecules in Hydrated Calcium Aluminate Pastes", *J. Phys. Chem. B*, **107**, 10057 (2003).

[9] A. Faraone, E. Fratini, P. Baglioni, S.H. Chen, "Quasielastic and Inelastic Neutron Scattering on Hydrated Calcium Silicate Pastes", *J. Chem. Phys.*, **121**, 3212 (2004)

[10] E. Fratini, F. Ridi, S.H. Chen and P. Baglioni, "Hydration water and microstructure in calcium silicate and aluminate hydrates," *J. Phys. Condensed Matter* **18**, S2467-S2483 (2006).

[11] Y. Zhang, M. Lagi, F. Ridi, E. Fratini, P. Baglioni, E. Mamontov and S.H. Chen "Observation of dynamic crossover and dynamic heterogeneity in hydration water confined in aged cement paste", *J. Phys.: Condens. Matter* **20** 502101 (2008).

[12] Y. Zhang, M. Lagi, E. Fratini, P. Baglioni, E. Mamontov and S.H. Chen "Dynamic susceptibility of supercooled water and its relation to the dynamic crossover phenomenon", *Phys. Rev. E* **79**, 040201(R) (2009).

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