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Failure of cement hydrates: freeze-thaw and fracture KATERINA IOANNIDOU, Massachusetts Institute of Technology, EMANUELA DEL GADO, Georgetown University, FRANZ-JOSEF ULM, ROLAND PELLENQ, Massachusetts Institute of Technology — Mechanical and viscoelastic behavior of concrete crucially depends on cement hydrates, the "glue" of cement. Even more than the atomistic structure, the mesoscale amorphous texture of cement hydrates over hundreds of nanometers plays a crucial role for material properties. We use simulations that combine information of the nano-scale building units of cement hydrates and on their effective interactions, obtained from atomistic simulations and experiments, into a statistical physics framework for aggregating nanoparticles.Our mesoscale model was able to reconcile different experimental results ranging from small-angle neutron scattering, SEM, adsorption/desorption of N_2, and water to nanoindentation and gain the new fundamental insights into the microscopic origin of the properties measured [1]. Our results suggest that heterogeneities developed during the early stages of hydration persist in the structure of C-S-H, impacting the rheological and mechanical performance of the hardened cement paste. In this talk I discuss recent investigation on failure mechanism at the mesoscale of hardened cement paste such as freeze-thaw and fracture. Using correlations between local volume fractions and local stress we provide a link between structural and mechanical heterogeneities during the failure mechanisms. 1. Ioannidou K. et al, The mesoscale texture of cement hydrates, Proceedings of National Academy of Science USA, 113 (8), 2029-2034 (2016)

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