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MODELLING NANOSCALE DEFORMATIONS IN CEMENT PASTES: IMPLICATIONS FOR STRENGTH AND DURABILITY

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The macroscopic behavior of cement pastes is largely determined by the mesoporous calcium-silicate-hydrate (C-S-H) gel, which is normally the main binding phase. Recent advances from atomistic simulations provide information regarding the elastic response and the failure of non-porous C-S-H at nanometer scale. We upscale this information and construct a model of the mesoporous C-S-H gel at the scale above, between 1 and 100 nm. Our model is based on densely packed nanoparticles with different sizes. The particles stick to each other due to strong and size-dependent cohesive interactions. The mechanical properties of a set of such model gel structures is probed. In the elastic regime, our results agree well with instrumented nanoindentation experiments. In the large deformation regime, we predict mechanisms of local deformation due to particles sliding on each other. The size of these mechanisms and their relation with the packing density and morphology of the model structures, are analyzed. Finally, we discuss the implications of our findings to the understanding and control of the macroscopic strength and creep of the cement paste.