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Decoding the chemomechanics of friction and scratch in complex granular hydrated oxides

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ABSTRACT

Calcium-Silicate-Hydrate (C–S-–H) is a structurally complex material that is the primary binding phase of all Portland cement concrete materials. C–S-–H is typically considered as an assemblage of discrete nanoscale particles whose interactions are governed by nanoscale friction and interfacial cohesion. Despite the critical role of interparticle forces on mechanics of granular materials, such as C–S-–H, there is currently no unified understanding on the atomistic mechanisms governing the nanoscale friction, scratch, and cohesion in C–S-–H; a lack of knowledge, which presents a major barrier to decode the interplay between chemistry, structure, and mechanics of various C–S-–H systems. Here, we develop a molecular dynamics framework, coupled to a set of redefined classical continuum relations, aimed at filling this gap. The normal force is calculated by relaxation of two C–S-–H particles at various distances and crystallographic orientations. The effect of watery environment is studied by immersing the particles in water molecules, and the friction and scratch forces are calculated by sliding the tip over the substrate in various directions. Our study identifies the distinct contribution of van der Waals and electrostatic forces to the interfacial behavior of C–S-–H particles. Although the electrostatic forces govern the interaction of particles at short and large distances, the van der Waals forces are responsible for variations in the normal force at intermediate distances. We find that normal force varies sublinearly with nanoscale contact area between the tip and substrate, whereas the friction force shows a linear trend. Our results demonstrate to what extent atoms of particular type contribute to the total interfacial forces. Because of large electronegativity, Si atoms (vs. Ca, O, and H) contribute most to the friction and normal forces. Finally, we probe the effect of pile-up and show that the nanoscale scratch test does not follow the classical laws of size-effect in fracture of quasi-brittle materials. Our findings, for the first time, provide an “atomistic lens” on nanoscale friction and contact phenomena in particulate C–S-–H systems. This has a significant impact on fundamental understating of C–S-–H and modulation of its behavior, thus impacting the mechanics of granular cementitious materials