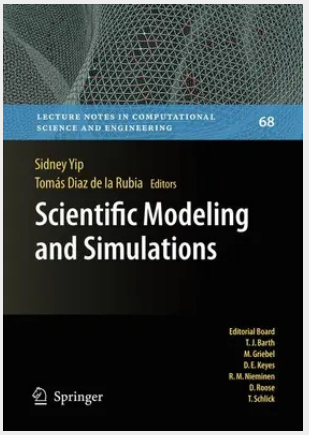
Yip / Rubia

Scientific Modeling and Simulations

Although computational modeling and simulation of material deformation was initiated with the study of structurally simple materials and inert environments, there is an increasing demand for predictive simulation of more realistic material structure and physical conditions. In particular, it is recognized that applied mechanical force can plausibly alter chemical reactions inside materials or at material interfaces, though the fundamental reasons for this chemomechanical coupling are studied in a material-speci c manner. Atomistic-level s- ulations can provide insight into the unit processes that facilitate kinetic reactions within complex materials, but the typical nanosecond timescales of such simulations are in contrast to the second-scale to hour-scale timescales of experimentally accessible or technologically relevant timescales. Further, in complex materials these key unit processes are “rare events” due to the high energy barriers associated with those processes. Examples of such rare events include unbinding between two proteins that tether biological cells to extracellular materials [1], unfolding of complex polymers, stiffness and bond breaking in amorphous glass bers and gels [2], and diffusive hops of point defects within crystalline alloys [3].

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