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From STM Images to Chemical Understanding: Kinetic Monte Carlo Simulations of Si(100) Etching ANKUSH GUPTA, IAN T. CLARK, BRANDON S. ALDINGER, MELISSA A. HINES, Cornell University, Ithaca NY — Etching reactions literally write a record of their chemical reactivity in the morphology of the etched surface – a record that can be read using scanning tunneling microscopy (STM) and decoded with the help of simulation. We have developed a fully atomistic kinetic Monte Carlo simulation of Si(100) etching that is appropriate for aqueous etchants that produce fully H-terminated surfaces [e. g., NH_4F(aq), KOH(aq) and even H_2O]. The model assumes that the reactivity of individual surface sites is determined by the local geometry. As an example, we simulate the production of near-atomically flat Si(100) surfaces, recently observed experimentally, and show that interadsorbate stress plays a crucial role in determining the steady-state etch morphology. The simulated morphologies are in good agreement with experimental observations.

Ankush Gupta
Cornell University, Ithaca NY

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