Simple models for efficient simulation of AFM

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Even with recent advances in computational power the simulation of AFM imaging remains challenging. The problem is that it has been found that in almost all cases the atomically sharp tip must be included explicitly in the simulation at each lateral and vertical position above the surface: this can easily lead to 10,000s of simulations needed to be carried out to construct and image of a complex surface, molecule or defect. Our recent work suggests two classes of problem when this difficulty can be alleviated, and images constructed from a single simulation leading to 3-4 orders of magnitude speed-up in image simulation: (i) Ionic materials, such as NaCl or NiO, when imaged using a carefully prepared metallic tip at large tip-surface separations. (ii) AFM in liquid when a sharp tip with a closely bound water molecule or hydroxyl group is primarily responsible for imaging. In the first case we find we can obtain quantitative agreement with experiment by considering only the electrostatic contributions from the tip and the surface [1]. In the second class of problems we show that an argument based on statistical mechanical properties of the adsorbed liquid above a surface can be used to construct approximate images of the surface [2].