Quantitative Measurement of Adsorbed Metal Clusters by ncAFM

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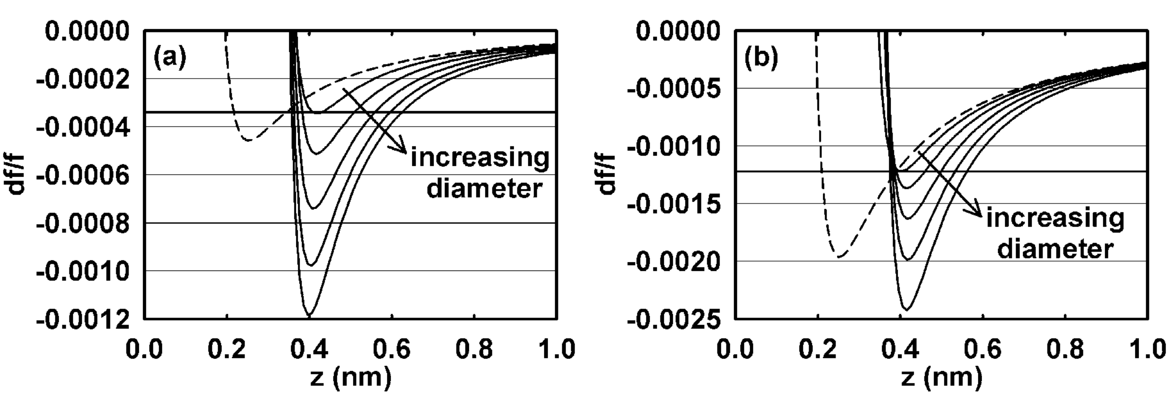
The apparent height and lateral extent of one-atomic-layer-high and larger metal clusters adsorbed on a flat substrate has been calculated for ncAFM imaging. Maximum accuracy in measuring metal clusters is obtained by choosing the most negative frequency-shift set-point possible that is consistent with a monotonic increase in frequency with distance. In the figures below, the frequency-shift vs. closest-approach distance curves are shown for spherical Si tips of radius 5 nm (a) and 20 nm (b) oscillating with a 10 nm amplitude. The substrate used in these figures was modelled as a Lennard-Jones continuum with parameters chosen to simulate alumina. To demonstrate the variation of the frequency-shift with the topography of the sample, the frequency-shift vs distance curve corresponding to a point above the substrate away from the particles (dashed line) is compared to those generated at points above the centers of quasi-circular 2D particles of increasing size: 7, 19, 37, 61, and 91 atoms (edge-to-edge diameters of 0.9, 1.1, 1.7, 2.2, and 2.8 nm). In order to attain stable imaging over an area that includes particles of this size range, the frequency shift set-point needs to be chosen at the horizontal line shown in each figure [$df/f = -0.34 \times 10^{-3}$ (a) and -1.22×10^{-3} (b)]. At this set-point, the apparent height of the smallest particles [0.09 nm (a) and 0.02 nm (b)] is much smaller than the real height of 0.28 nm, making them practically invisible with the larger tip diameter (b). If the Lennard-Jones type interaction is appropriate for ncAFM experiments done for Pd particles on alumina, these simulations explain the inability of ncAFM to detect small particles known to be present from low-energy ion scattering data [1].

Simulations for larger Pd particles modelled as continuum spheres on alumina indicate that the apparent height is much closer to the real height for particles of 2 nm radius and larger. These simulations also predict greater difficulty in detecting small metal particles in situations where the substrate had a larger polarizability, closer to that of the metal. The apparent lateral extent of the particles in this ncAFM simulation is comparable to what would be observed in a contact-mode AFM experiment. Supported by UW Mary Gates Fellowship (CP), the Joint Institute for Nanoscience funded by the University of Washington and Pacific Northwest National Laboratory (operated by Battelle for the U. S. Department of Energy) (SLT), and by DOE OBES Office of Chemical Sciences.



[1] S. L. Tait, L. T. Ngo, Q. Yu, et al., J. Chem. Phys. **122**, 064712 (2005)