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Abstracts

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Exploring the Future of Nanotechnology
Using SPM and Related Techniques

Modeling and Simulation of Nanobubbles on Material Substrates

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Tapping mode Atomic Force Microscopy (AFM) of hydrophobic material surfaces in water shows that they are covered with closely spaced soft domains. The radii of curvature of these features are of the order of 100 nm and their heights above the substrate are in the range 20-30 nm. The consensus in the interpretation of these features is that they are nanosized gas bubbles that are formed on the substrate after immersion. However, there still remains the difficulty of explaining their apparent stability with conventional thermodynamics. Particularly the fact that they are expected to rapidly dissolve because of their high predicted internal pressure. It is still not known deterministically how hydrophobic a surface needs to be before nanobubbles appear in AFM images. The predicted number of molecules inside a nanobubble is small. For this reason a simulation of the dynamics of molecules inside a nanobubble is feasible, and can also provide insight into its formation and stability. We will present our preliminary results relating to modeling and molecular dynamics simulation of nanobubble formation on hydrophobic material substrates. A simple model for nanobubbles formation and stability has been developed that relates the contact angle to the surface tension and the water-solid potential. The contact angle is finite and therefore the nanobubble is a spherical cap when the temperature (T) is lower than the "wetting temperature" (T_w). For $T > T_w$, the nanobubble is a full sphere (with zero contact angle). For example, a spherical bubble that forms on the water-graphite interface at $T \sim 500$ K would evolve to a semispherical shape when it cools down to room temperature, while the system is maintained at the liquid-vapor equilibrium pressure. We have also explored the use of the Molecular Dynamics Simulator software LAMMPS developed by Sandia Laboratory in this regard. Results from both approaches will be presented.