## Simulation of Silicon Nanopatterning Using nc-AFM

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During the last decades, it has been shown that nc-AFM can be used as an efficient lithographic technique capable of manufacturing nanometer sized devices on the surface of a silicon wafer [1]. Other AFM techniques have also shown the potential for nanooxidation, but nc-AFM proved to be the best candidate due to the soft interaction between the surface and the needle tip. The nanooxidation approach is based on generating a potential difference between the AFM needle tip and the silicon wafer. A water bridge builds up between the tip and the wafer, resulting in a medium for oxyions to move due to the high electric field in the region. The oxyions interact with the silicon surface, resulting in an oxidation process. A simulator for nanooxidation with nc-AFM tools, implemented in a Level Set environment, was developed. The simulator uses physical and empirical models from recent publications in order to deduce the shape (height and width) of a desired oxide nanodot based on the applied voltage, pulse time, and ambient humidity. Previously available simulators generate a nanodot using a Monte Carlo rejection technique, which is undesirable for large aspect ratio problems. Alternatives are nanodots with a shape following a desired particle distribution (Gaussian or Lorentzian) [2]. The model presented here is a physics-based nanodot model using a particle distribution directly derived from the surface charge density equation. The tip of the AFM needle is seen as a charged source whose charge depends on the applied voltage, while the silicon wafer is seen as a grounded infinitely long plane. Based on the equation describing the distribution of charges on the wafer surface, a quantile function is derived in order to generate a two-dimensional particle distribution. The generated particles are then accelerated towards the surface along the surface normal, where their impact with the wafer is detected and the surface is advanced using a Level Set technique. The shape of an AFM-formed nanowire depends on the same factors as the shape of the nanodot in addition to the wire's orientation with respect to the (010) direction. The width of the wire is determined by impacting particles, which are accelerated as the result of a one-dimensional surface charge density distribution. An added advantage of our approach is the ease with which further processing steps, such as etching or deposition, can be integrated within the same simulation environment. Sample oxide nanodots and nanowires are analyzed, showing the ability of the process to generate nanometer sized structures. The figures below show a sample nanowire and a nanodot generated with particles using a random distribution based on the surface charge density distribution. Both geometries have a height of approximately 1nm, but the vertical axis for each figure has been scaled for improved visualization.

**References**

[1] J. Dagata et al., "Modification of Hydrogen-Passivated Silicon by a Scanning Tunneling Microscope Operating in Air," *Applied Physics Letters*, vol.56, pp.2001–2003, May 1990.
[2] L. Filipovic and S. Selberherr, "A Level Set Simulator for Nanooxidation Using Non-Contact Atomic Force Microscopy," *Intl.Conf. on Simulation of Semiconductor Processes and Devices (SISPAD)*, pp.307-310, 8-10 Sept. 2011.