Nanoscale Oxidation

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Overview of Current Investigations

Scanned probe oxidation is a local surface oxidation induced by an electrically biased Atomic Force Microscope (AFM) tip. The AFM tip is typically a cone-shaped probe that is brought either close to or into direct contact with a substrate. The probe is attached to the end of a cantilever that bends as the tip moves across the substrate's surface. By increasing the voltage bias between the tip and the surface, the tip acts as an ion source that can be used to grow nanoscale oxide features on the substrate.

More specifically, the close proximity of the AFM tip to the substrate establishes an intense electric field. Water, due to condensation from the ambient air and transport from a thin film on the substrate surface, accumulates in the narrow gap capillary between the AFM tip and the substrate to form a liquid bridge (meniscus). The free surface of water contacts the AFM tip and the edge of the oxide or substrate. Hydroxyl ions are produced within the water and are directed by the electric field within the fluid; these ions subsequently react with the substrate to produce a thin oxide layer. Hereafter, we refer to this entire system as a nanocell.

Hence, the AFM tip acts as a pen ``writing'' oxide patterns on the substrate. These patterns have been employed successfully as an etch mask for wet and dry processes, as mechanisms for device isolation and for tunnel barrier formation, and as chemical and biological templates. Since most metals, semiconductors, and even insulating thin films such as silicon nitride can be oxidized within a nanocell, scanned probe oxidation is a very general method for prototyping nanoscale masks, templates, and devices. Hence, due to the generality of oxidation as chemical process, the simplicity of the tools and techniques required for producing nanometer-sized features, and the compatibility of the oxidation process with the techniques used by the semiconductor industry, scanned probe oxidation (SPO) using an atomic force microscope tip is a promising approach to nanostructure fabrication.

We develop continuum models of scanned probe oxidation. The models include equations describing the electric field, hydroxyl and hydrogen ion concentrations, and the free boundary of the oxide. The equations track ion transport in both the liquid and the oxide layers and incorporate the reaction mechanism at the substrate/oxide interface.

Further, the influence of the space charge trapped near the substrate/oxide interface is taken into account. The asymptotic limit in terms of a small aspect ratio of the oxide layer (height to width) and separation of time scales for the reaction and ion transport are used to reduce the governing system of partial differential equations to a one-dimensional system of ordinary differential equations. The solution of the reduced system of ordinary differential equations results in the evolution equation for the oxide thickness. Numerical solution of the evolution equation predicts features of oxide growth that qualitatively agree with the experimental observations. A parametric study is conducted to determine the influence of the key operating and material parameters on the thickness of the oxide, and the electric and ion concentration fields in the system.

We also developed an axisymmetric continuum model for oxide growth by the scanned probe oxidation technique. Two liquid configurations, semi-infinite layer and hemispherical drop of liquid, are examined to determine the potential in the liquid region. The AFM tip is modeled as either a point or ring source of charge. The asymptotic limit of a small aspect ratio oxide feature (height to width) is used to reduce the governing system of partial differential equations to a quasi-one-dimensional system to determine the ion transport in the nanocell system. The result of the model solution of the reduced system is an evolution equation for the oxide thickness and radius. Numerical solution of the evolution equation predicts features of oxide height and radial growth that qualitatively agree with experimental observations. A parametric study is conducted to determine the influence of key operating and material parameters on the thickness and radius of the oxide dot, and the electric and ion concentration fields in the system.

Publications

1. "One-Dimensional Dynamics of Nano-Scale Oxidation", A. Orians, C. B. Clemons, D. Golovaty, and G. W. Young, *Surface Science*, Vol. 600, (2006), pp. 3297-3312.

2. "Effects of the Electric Field Shape on Nano-Scale Oxidation", S. Djurkovic, C. B. Clemons, D. Golovaty and G. W. Young, *Surface Science*, Vol, 61 (2007), pp. 5340-5358.

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1. NSF Division of Mathematical Sciences - "Modeling and Analysis of an Electrochemical Nanocell" NSF Grant No. DMS-03-05577, (2003 - 2004): $100,000, G. W. Young – PI, C. B. Clemons, D. Golovaty, and S. I. Hariharan.