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Nanoelectronics: Metrology and Computation

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Abstract. Research in nanoelectronics poses new challenges for metrology, but advances in theory, simulation and computing and networking technology provide new opportunities to couple simulation and metrology. This paper begins with a brief overview of current work in computational nanoelectronics. Three examples of how computation can assist metrology will then be discussed. The paper concludes with a discussion of how cyberinfrastructure can help connect computing and metrology using the nanoHUB (www.nanoHUB.org) as a specific example.

Keywords: modeling, simulation, cyberinfrastructure, scanning probe, NEMS, heterostructures.

INTRODUCTION

Research in nanoelectronics is driving the development of a new class of simulation methods that comprehend atomistic structure and quantum transport [1]. Although we can now simulate electronics at the atomistic scale, these technologies demand new capabilities for metrology at the nanoscale. At the same time, advances in computing and network technology are leading to the increased use of so-called cyberinfrastructure are changing the way people access and use simulation programs. Our objective in this talk is to illustrate with three examples how computation can support metrology. The paper will conclude with some brief thoughts about the role that cyberinfrastructure may play to facilitate the connection of computation to metrology.

ANALYSIS OF DYNAMIC AFM

The Atomic Force Microscope (AFM) [2] has become one of the most important tools for nanotechnology with its remarkable ability to measure nanoscale forces and image and manipulate atoms and molecules with nanometer resolution. It is evolving rapidly from a tool for nanoscale metrology to a versatile platform with multi-functional nanoprobes for the measurement of mechanical, chemical, electronic and magnetic properties of nanostructures with unprecedented accuracy and nanometer spatial resolution.

The most common implementation of AFM is the so-called dynamic AFM [3], which uses a micromechanical force sensor - a microcantilever with a nanoscale tip that is driven at resonance, to detect nanoscale forces between the atoms on the tip and sample (Fig. 1). The dynamics of the microcantilever (amplitude, phase, resonance frequency) change as it is brought closer to the sample due to the influence of nonlinear short and long-range forces between the tip and sample. These data are called dynamic approach curves and they provide invaluable information about tip-sample interaction physics including: local...
elasticity, viscoelasticity, nanoscale friction, van der Waals, electrostatic and specific chemical forces.

Besides these force spectroscopy applications, dynamic AFM is the most commonly used tool for nanoscale metrology and imaging. In this case, the amplitude or phase of the probe is maintained approximately constant while scanning the sample topography. This is achieved by means of an imaging feedback control system. Because the probe dynamics depend strongly on the nonlinear tip-sample interaction forces [4], the scanned image is strongly influenced by tip-sample interactions and the feedback control dynamics. As a consequence, even for an infinitely sharp tip (hypothetical), the scanned image can be quite different from the real topography.

Currently under VEDA, two tools have been developed: (1.) Dynamic approach curve simulations, and (2.) Dynamic scanning simulations. Both tools are sophisticated, state-of-the-art simulations for dynamic AFM that include (a) accurate microcantilever models, (b) realistic tip-sample interaction force models, (c) and accurate FORTRAN based numerical integration schemes that are well-suited for stiff, nonlinear differential equations. Using VEDA, users can explore how probe, sample and operating parameters influence the "images" generated in AFM.

The theoretical modeling behind the simulations is rigorous. Briefly, the tip-sample interaction models are based on the Derjaguin-Müller-Toporov contact mechanics model that includes van der Waals forces and elastic contact mechanics [5]. Provision is also made for possibly visco-elastic sample surfaces. The model is valid for low adhesive contacts in either ambient or ultrahigh vacuum (UHV) conditions. The tip dynamics are represented rigorously by a mathematically equivalent point mass model (Fig. 2) of the continuum elastic AFM probe [6]. This together with special numerical integration schemes from FORTRAN libraries ensures high fidelity simulations. The code simulates the tip displacement history that is converted into interaction force history, or amplitude, phase, or tip-sample power dissipation. The output of the tools have been compared extensively with previously published numerical and experimental results and found to be in excellent agreement.

**FIGURE 2.** A schematic of a continuous elastic AFM probe driven at resonance at a specific mode and oscillating near a sample surface. On the right is an equivalent point mass model that possesses exactly the same kinetic, elastic, and tip-sample interaction energies as the original continuum elastic probe.

**FIGURE 3.** Dynamic scanning simulation of a Si trench structure using a Si tip using a 350 kHz, 40 N/m, Q = 400 lever operating at 30 nm initial amplitude and 90% setpoint amplitude, at a very high scan speed of 5 microns/second with reasonable feedback control parameters (a) the trench topography to be measured (b) the measured profile, and (c) the peak tip-sample repulsive (blue) and attractive (red) forces (nN).
The dynamic simulation tool is concerned with nanometrology using AFM. Coupled to the basic dynamic equations now are the equations describing the feedback controller (proportional/integral) commonly used in AFM scans. The key observation (Fig. 3) is that tip dynamics and feedback control loop can significantly perturb the measured topography near the edges of features. Large interaction forces are exerted on the sample near the edges of features. Most AFM users assume steady state operating conditions, but the transient oscillations and associated peak forces are often revealing to experimentalists.

Moving forward, plans are underway to extend these simulation tools for dynamic AFM in liquids for the nanometrology of soft biological samples. Eventually, such tools could be merged with existing programs that deal with tip geometry de-convolution. Ready access to a suite of such computational tools in the future could lead to significant improvements in nanometrology using AFM.

**ELECTRO-MICRO-METROLOGY**

Determining the fundamental properties of microdevices has been a longstanding problem. Properties vary from lab to lab, from run to run at the same lab, and from chip to chip across a single wafer. For instance, in Fig. 4, layout geometry is superimposed onto the actual geometry of a microdevice. The modified support beams and electrostatic gaps significantly affect the ability to predict performance before it is fabricated. It is also difficult to numerically match performance after it is fabricated because conventional metrology techniques yield large uncertainties. There is a need to build consensus on terminology, on best practices for measuring properties of nanodevices and on reporting those properties. Such a consensus would contribute to reducing uncertainties and make comparisons easier for both researchers and manufacturers.

Electro-Micro-Metrology (EMM) involves determining what geometric and material properties of an effective model are required to match the performance of the true device. Full details of this theory are given in [7]. These effective properties of the model are assumed to be the effective properties of the true device. Since electronic measurands are the most precise measurands to date, reformulating these properties as functions of electrical measurands may significantly reduce uncertainties in geometry and material properties. For example, J. Green reports deflecting a microstructure $10^{-13}$ meters due to changes in comb drive capacitance of $10^{-21}$ farads [8]. Preliminary analysis predicts similar orders of precision in the extraction of geometry, dynamics, and material properties [7]. In essence, uncertainty in measurement has the form $\delta X = \left(\frac{\partial X}{\partial E} \right) \delta E$, where $E$ is an electrical measurand (i.e. change in capacitance); $X$ is a geometric, dynamic, or material quantity (i.e. force, displacement, etc.) expressed as a function of $E \pm \delta E$; $\delta X$ and $\delta E$ are the uncertainties of these measurements; and the ratio $\partial X / \partial E$ is the sensitivity of the measured quantity to the error in the electrical measurand. Although the sensitivity $\partial X / \partial E$ may be quite large, e.g. $O\left(10^6\right)$, the error in the electronic measurand $\delta E$ (correlated noise floor) can be made to be much, much smaller, such that the uncertainty in measurement $\delta X$ can be reduced.

Electro Micro-Metrology (EMM) techniques have the potential to increase the sensitivity and precision of nanoscale metrology by extracting geometric, dynamic, and material properties using electronic measurands. The technique leverages the sensitive electrical-mechanical coupling of microsystems to measure and characterize themselves.

**INVERSE MODELING**

Most experimental characterization and metrology tools are invasive and destructive. Quantitatively exact inverse modeling may be able to provide insights into nanoelectronic structural information from externally measured device performance. One can view this as a form of EMM, but on structures designed as devices rather than for metrology.

Klimeck et al. [9,10] have demonstrated such quantitative, exact inverse modeling with the GENES (Genetically Engineered NanoElectronic Structures) software package. GENES has three key ingredients: 1) a physics-based quantitatively exact modeling tool (NEMO 1-D) [11-15], 2) a generalized parallel genetic

![FIGURE 4. Layout vs. fabricated dimensions.](image.png)
algorithm package (PGAPACK) [16], and 3) a flexible fitness function management software.

NEMO 1-D was developed as a general-purpose quantum mechanics-based 1-D device design and analysis tool. It is based on the non-equilibrium Green function approach (NEGF), which allows a fundamentally sound inclusion of the required physics: bandstructure, scattering, and charge self-consistency. The primary simulation target was the quantitative, experimentally verified modeling of Resonant Tunneling Diodes. The theory and representative results are documented in references [10-15].

A set of fitness functions need to evaluate the numerical results and compare them to desired performance criteria. For a tool to be useful, the access of the fitness function parameters must be flexible and not involve a constant recompilation of the software. A table-oriented fitness function design based on least square evaluation with different weights has been implemented in GENES that enables the modification of the fitness function from one run to the next.

Details of the GENES packages and its application to the inverse modeling of resonant tunneling diodes and the design of empirical tight binding parameters for the atomistic modeling of materials are documented in [9,10]. Here a few highlights are repeated. Figure 5 shows a sketch of the parallel arrangement of statistical evaluations of design candidates, where the NEMO code is driven through Genes generated from PGAPACK with a fitness function.

Figure 6 shows the numerical experiment set-up for the variation of five structural RTD properties, layer thicknesses and doping profiles. Starting from a random distribution of initial guesses the genetic algorithm did identify a device topology close to experimental data. In the NEMO project it was identified that indeed the barriers were thicker than originally experimentally specified. The GENES package finds this deviation and also identifies the no intentional central device doping to be larger than specified.

Reference [10] provides more details about the operation of genetic algorithms and it explores the use of GENES for the generation of empirical tight binding parameters. The optimization of these tight binding parameters to properly represent the bulk properties of semiconductors amounts to a very large dimensional optimization problem. Optimization spaces involving some 30 to 150 parameters have been successfully explored with the GENES package, resulting in advancements of tight binding models [17] and in a variety of new parameterizations for III-V and Si/Ge parameters [18, 19].

**CYBERINFRASTRUCTURE**

The creative integration of high-speed networks, high-performance computing, and data storage (so-called cyberinfrastructure) is beginning to change the way scientific research is conducted. The National Science Foundation funded Network for Computational Nanotechnology (NCN) is one example of how communities are organizing around resources and services that are shared through cyberinfrastructure. The NCN’s mission is to lower barriers to the use of simulations in emerging fields of study. Towards that goal, the NCN has created a unique science gateway, the nanoHUB, (www.nanoHUB.org) where users log on, access state-
of-the-art simulation software, run interactive graphical or batch simulations, and view the results online, with no need to download, install, support, and maintain sophisticated software. Computing resources are provided transparently without the need to worry about accounts or how to access specific machines.

The NCN’s nanoHUB has also become a resource for cross-disciplinary education. It hosts online tutorials, short courses, and full courses. Efficient production processes, easy ways for users to locate and access materials, a delivery mechanism that works at low bandwidth, and processes to collect and analyze usage statistics have all been developed. Over 20,000 people now make use of the nanoHUB each year, and the number is doubling annually.

FIGURE 7. The nanoHUB (www.nanoHUB.org), a science gateway that provides services for online simulation, collaboration, and education.

The NCN created the nanoHUB to share computational tools in emerging fields of research. The use of computation as an integral component of metrology is one such emerging field. The nanoHUB software development platform, Rappture, (www.rappture.org) facilitates the rapidly development of new simulation codes with friendly user interfaces. The nanoHUB middleware accepts Rappture applications and delivers simulation services to the user’s desktop. If complemented by online tutorials and open-source software, we believe that this kind of infrastructure could play a useful role is assisting the development of the field of computational metrology.

SUMMARY

Nanotechnology is placing increased demands on metrology. We have discussed three examples of how computation can assist metrology along with some ideas on how novel cyberinfrastructure could promote the development of a community of developers and users of such tools.

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