Invited Article: VEDA: A web-based virtual environment for dynamic atomic force microscopy

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Invited Article: VEDA: A web-based virtual environment for dynamic atomic force microscopy

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We describe here the theory and applications of virtual environment dynamic atomic force microscopy (VEDA), a suite of state-of-the-art simulation tools deployed on nanoHUB (www.nanohub.org) for the accurate simulation of tip motion in dynamic atomic force microscopy (dAFM) over organic and inorganic samples. VEDA takes advantage of nanoHUB’s cyberinfrastructure to run high-fidelity dAFM tip dynamics computations on local clusters and the teragrid. Consequently, these tools are freely accessible and the dAFM simulations are run using standard web-based browsers without requiring additional software. A wide range of issues in dAFM ranging from optimal probe choice, probe stability, and tip-sample interaction forces, power dissipation, to material property extraction and scanning dynamics over heterogeneous samples can be addressed. © 2008 American Institute of Physics. [DOI: 10.1063/1.2938864]

I. INTRODUCTION

Dynamic atomic force microscopy (dAFM) has emerged as a powerful tool for imaging, measuring, and manipulating matter at the atomic and molecular scale. It consists of a oscillating nanoscale tip at the end of a resonant microcantilever that interacts with the sample via short and long range forces. At the same time, as a dAFM probe interrogates a sample, the resulting probe-tip dynamics may contribute to image artifacts and unreliable property measurements. Thus, the topographic images generated in dAFM scans are actually a cumulative result of nonlinear interaction forces between the probe tip and the sample, cantilever probe dynamics, tip-sample geometry convolution, and the dAFM feedback control system. Ultimately, the limits of dAFM nanometrology depend on the ability to correctly deconvolve these effects or eliminate them in some manner. This is one critical need than can be addressed via accurate mathematical simulations of the scanning process. Additionally, the measurement of material properties via dAFM requires model-based inversion of measured dynamics (amplitude, phase, higher harmonics, power dissipation) to nanoscale material properties (surface potential, sample viscosity, sample elasticity, adhesion, charge density, and magnetic moment). High-fidelity mathematical simulations are also critical for quantitative material property measurements using dAFM. Finally, due to a large parameter space and nonintuitive underlying nonlinear dynamics, the task of the dAFM experimentalist to choose an optimal cantilever, amplitude and set point for an application often includes much trial and error. Where intuition fails, simulations can provide valuable insight into the fundamental physics of this instrument.

Simulations of the oscillating probe-tip approaching and interacting with the sample have provided key insights into aspects of the probe dynamics that are also present while imaging. In addition, verification of analytical formulas in dAFM are often achieved through simulation of approaching the sample. Many authors have also chosen to study physical phenomena in dAFM with “virtual” microscopes where the feedback control effort is modeled in simulations of the cantilever interacting with the sample. By this approach, one can study the effect of the controller dynamics and various noise sources on topographic images, imaging forces, power dissipation, etc. However, these efforts have been largely concentrated on the noncontact (frequency modulated) community and have also not taken advantage of the unique capabilities of cyberinfrastructure.

In this article, we introduce virtual environment for dAFM (VEDA), a suite of high-powered, web-based simulation tools for dAFM under development on nanoHUB (Ref. 31). VEDA currently includes the dynamic approach curves (DACs) tool, which simulates a dAFM probe excited near resonance and introduced to a sample [Fig. 1(a)], and the amplitude modulated scanning (AMS) tool, which simulates an amplitude modulated scan over heterogeneous samples [Fig. 1(b)]. Both tools feature (a) accurate models of microcantilever dynamics, (b) realistic tip-sample interaction force models, and (c) accurate, high-speed, FORTRAN-based, numerical integration schemes that are well suited for nonsmooth, nonlinear differential equations. In addition, the AMS tool includes controller dynamics based on the lock-in amplifier amplitude error signal. Both tools allow users to investigate the contributions of different operating conditions and cantilever and sample properties and produce detailed information about the probe dynamics and nature of the tip-sample interaction. VEDA simulation tools are available on nanoHUB, which is a web-based interface for researchers, educators and students interested in science and technology at the nanoscale. NanoHUB is the web portal for the cyberinfrastructure to run high-fidelity dAFM tip dynamics computations on local clusters and the teragrid.
National Science Foundation funded Network for Computational Nanotechnology (NCN). NanoHUB allows its users an open access to research seminars, educational modules, and simulation tools such as VEDA.

In what follows, we describe the models for tip-sample interaction, cantilever dynamics and controller dynamics, and the numerical integration schemes which are implemented in VEDA and discuss the methodology behind the each tool. Finally, we present several example simulations for validation with prior work as well as demonstration of the insight gained through simulations in dAFM.

II. MODELING

VEDA simulations are based on accurate models of tip-sample interaction, cantilever probe dynamics and controller dynamics. These models ensure realistic predictions of the cantilever response as the dAFM probe vibrates in close vicinity of the sample.

A. Tip-sample interaction forces

The total tip-sample interaction force \( F_{ts}(d) = F_{tsc}(d) + F_{tc}(d) \) acting between the tip of the dAFM probe and the sample consists of a conservative component \( F_{tc}(d) \) and a nonconservative component \( F_{ts}(d) \). At present, in VEDA, the conservative interaction model is continuous but nonsmooth, consisting of a van der Waals force regime\(^{2,3} \) and a contact regime based on the Derjaguin–Müller–Toporov (DMT) model.\(^{33,34} \)

\[
F_{tc}(d) = \begin{cases} 
-HR/6d^2, & d > a_0, \\
-HR/6a_0^2 + 4E^* \sqrt{R(a_0 - d)^{3/2}}, & d \leq a_0, 
\end{cases}
\]  

(1)

where \( d \) is the gap between the tip and the sample, \( a_0 \) is the intermolecular distance, \( H \) is the Hamaker constant, \( R \) is the radius of the tip, and \( E^* = [(1 - \nu_2^2) / E_2] + (1 - \nu_{\text{sample}}^2) / E_{\text{sample}} \). \( E \) and \( \nu \) represent elastic moduli and Poisson’s ratios. The nonconservative interactions can be included as an option in a simulation based on the Kelvin–Voigt viscoelastic contact damping model\(^{19} \)

\[
F_{ts}(d) = -\eta \dot{d} \sqrt{R(a_0 - d)},
\]  

(2)

where \( \eta \) is the sample viscosity. Equation (1) is valid for stiff samples with low adhesion and probes with sharp tip radii.\(^{33} \) Viscoelastic contact damping [Eq. (2)] is a common feature on polymer surfaces\(^{19} \) and biological materials.\(^{35} \) In many instances, these models may be used outside their valid regimes to provide qualitative understanding.

B. Cantilever dynamics

The dynamics of the cantilever probe are modeled by a single degree of freedom (SDOF), point-mass model, which is derived from the continuous beam equation. We begin with the derivation of the acoustically (dither peizo) excited cantilever model for rectangular cantilevers in ambient conditions but later, we discuss how this model can be extended arbitrary geometry cantilevers, ultra high-vacuum (UHV) environments and other forms of excitation. From the classical Bernoulli–Euler beam theory, partial differential equation governing small deflections of the slender, rectangular dAFM cantilever in a ground-fixed (inertial) frame in the absence of tip-sample interactions can be written as

\[
\rho_c \ddot{w}(x,t) + \gamma_f w(x,t) + E_c I_c \frac{\partial^4 w(x,t)}{\partial x^4} = 0,
\]  

(3)

where \( x \) is the axial coordinate along the cantilever’s longitudinal axis, \( L_0 \) is the length, \( \gamma_f \) represent temporal derivatives, \( \gamma_i \) is the hydrodynamic damping coefficient, and \( \rho_c \), \( E_c \), and \( I_c \) are the linear density, elastic modulus, and area moment of inertia, respectively. The absolute deflection \( w(x,t) = Z(t) + y(t) + u(x,t) \) is composed of the separation from the sample \( Z(t) \), the base excitation \( y(t) = A_{\text{base}} \cos \omega t \), and the deflection in the noninertial frame attached to the base \( u(x,t) \) (Fig. 2).

Typically, in dAFM, a photodiode measures the bending angle \( \psi(L_0, t) \) and infers the deflection \( u(L_0, t) \) relative to the base, therefore, we proceed to model the dynamics of the cantilever in the noninertial, moving frame attached to the cantilever’s base. Translating Eq. (3) into a noninertial frame attached to the moving base of the cantilever leads to\(^{16} \)

\[
\rho_c \ddot{u}(x,t) + \gamma_f u(x,t) + E_c I_c \frac{\partial^4 u(x,t)}{\partial x^4} = -\rho_c \dot{y}(t) - \gamma_i \ddot{y}(t).
\]  

(4)

Our goal is to discretize Eq. (4) into a SDOF model describing the dynamics of the dAFM probe tip in the noninertial frame. In ambient environments, a single eigenmode of the cantilever beam \( \Phi(x) \) is typically sufficient to describe dynamics of the continuous probe.\(^{11} \) The appropriate discreti-
zation of Eq. (4) in terms of the generalized coordinate \( q(t) = \omega L(t) \), and including the tip-sample interaction force \( F_{ts} \) yields the equivalent point-mass model \(^{12}\)

\[
m_1 \ddot{q} + (m_1 \omega/L_1^2) \dot{q} + k_1 q = F_{ts}(d, \dot{d}) + F_i(t),
\]

where \( m_1 = \rho L_1 \), \( k_1 = E_1 I_1 a_1^2 / 4 L_1^3 \), and \( Q_i \) and \( \omega_i \) are the equivalent mass and stiffness, quality factor and natural frequency of the \( i \)th eigenmode, respectively (Fig. 2). \(^{37}\) \( \alpha_i \) is \( i \)th solution to the dispersion relation \( \cos \alpha \cosh \alpha + 1 = 0 \). Finally, for \( Q_i \gg 10 \), the excitation force \( F_i(t) \) may be expressed as \(^{38}\)

\[
F_i(t) = (\omega/\omega_i)^2 \bar{F}(t),
\]

where \( y_i(t) = B_i y(t) \) is the equivalent base excitation and \( B_i = f_{0i}^1 \Phi_i(x) dx / f_{0i}^1 \Phi_i^2(x) dx \) is a modal parameter. \(^{39}\)

For the purpose of the simulation, we choose to nondimensionalize the key spatial parameters by the initial amplitude, the precise value is not important as long as the quality factor is sufficiently large.

\[
\bar{F}(t) = \bar{y}_i(t) = (\omega/\omega_i)^2 \bar{F}(t).
\]

Finally, the nondimensional tip-sample interaction force \( \bar{F}_{ts} \) can be written as

\[
\bar{F}_{ts}(\bar{d}, \dot{\bar{d}}) = \begin{cases} 
-C_{vdw}/\dot{\bar{d}}^2, & \bar{d} > \bar{a}_0, \\
-C_{vdw}/\bar{a}_0^2 + C_{DMT}(\bar{a}_0 - \bar{d})^{3/2}, & \bar{d} = \bar{a}_0, \\
-D_a \bar{d}^2 / \sqrt{\bar{a}_0 - \bar{d}}, & \bar{d} = \bar{a}_0,
\end{cases}
\]

where \( \bar{a}_0 = a_0 / A_0 \), \( C_{vdw} = HR / 6 k_0 A_0 \), \( C_{DMT} = 4 \sqrt{RA_0 / 3k_e} \), and \( D_a = \eta_0 \sqrt{RA_0/k_e} \). At present, Eq. (7) is the model for cantilever dynamics implemented in both VEDA tools.

While Eq. (7) was formulated for acoustically (dither piezo) excited rectangular cantilevers oscillating in ambient conditions, coincidentally, it may be extended to a few additional scenarios. The key observation to note is that the quality factor in ambient conditions is typically quite large (on the order of 100). This had two important ramifications. For near resonant excitations, the base motion of cantilever \( y \) does not contribute substantially to instantaneous tip-sample gap \( d \) or its rate \( \dot{d} \). Second, for large quality factors, the bandwidth of the resonance peak is also very small. This means the factor of \((\omega/\omega_i)^2\) in the excitation force [Eq. (6)] can be considered constant for near resonant excitations. This allows the model for cantilever dynamics [Eq. (7)] to be extended to UVH environments and for magnetic excitations. \(^{40}\) Finally, experiments involving nonrectangular dAFM probes may also be simulated reasonably using Eq. (7) in VEDA if the correct probe stiffness is used. \(^{12}\) While the modal parameter \( B_i \) may be unknown for a particular nonrectangular cantilever, the precise value is not important as long as the quality factor is sufficiently large.

C. Lock-in amplifier and controller models

Scanning simulations also require reasonable models for the lock-in amplifier and controller dynamics as the dAFM probe scans the sample. The amplitude and phase of the deflection signal are determined by a lock-in amplifier. For a period of time referred to as the lock-in time constant, the amplitude and phase at the excitation frequency are determined by a Fourier transform of the deflection signal over a period of time \( \Delta t \). To avoid leakage in the frequency spectrum, \( \Delta t \) is adjusted according to the user specified lock-in time constant. The AMS tool additionally models shot noise according to a user specified signal-to-noise ratio in the deflection wave form.

While scanning, the controller objective is to maintain a constant tip amplitude as the cantilever probes the sample in the presence of tip-sample interaction forces. We choose a commonly used proportional-integral (PI) controller to maintain the desired amplitude. More specifically, the feedback parameter is the amplitude error \( e \), which is defined as

\[
e = A/A_0 - A_{sp},
\]

where \( A \) and \( A_{sp} \) are the current amplitude and the set-point amplitude ratio, respectively. Based on the amplitude error, the \( Z \) distance from the sample is adjusted according to

\[
\Delta Z(t) = -K_p e(t) - K_i \Delta t \sum_{i=1}^{\text{run}} e(t),
\]

where \( K_p \) and \( K_i \) are the proportional and integral gain constants, respectively, and \( t_i = i \Delta t \).

D. Tip-sample convolution

Scanning simulations also include the option to simulate image artifacts due to the finite size of the tip probe. However, we stress that such approximations consider only geometry \(^{14}\) and do not account for differences in the tip-sample interaction potential itself or any resulting nonconservative interactions. Figure 3 illustrates the actual tip-sample surface \( h \) and geometrically convolved surface \( h^* \). For continuous functions, \( h^* \) may be determined algebraically, however, since the scanning tool includes the option of a sharp discontinuous step, the convolved surface is found by itera-
E. Numerical integration

Next, we discuss the numerical integration routine implemented in VEDA and why it is particularly well suited for dAFM simulations. The DMT tip-sample interaction model described above and other modes, such as Johnson–Kendall–Roberts (JKR) and the capillary force model, involve nonsmooth and even discontinuous tip-sample interactions. Numerical integration of nonsmooth and discontinuous differential equations requires careful consideration to ensure accurate results. Accordingly, the DDASKR routine with a root finding algorithm based on DASPK differential algebraic equation (DAE) software package is used.

Figure 4 illustrates the key advantage of the DDASKR routine over conventional routines. For simplicity of argument, first consider explicit integration routines, such as the explicit Euler method, where \( y' = F(t, y) \) are solved explicitly by \( y_{n+1} = y_n + h \cdot F(t_n, y_n) \) for an initial condition \( y(t_0) = y_0 \) and time step \( h \). As shown in Fig. 4, explicit fixed-step routines will integrate from the initial position at \( A \) across the sample surface to \( C \) based on the noncontact forces at \( A \). Similarly, explicit adaptive time steps will also pass through the sample surface to \( C \) before realizing the presence of stiff contact forces. In reality, more advanced techniques, such as fourth order Runge–Kutta routines, implicit backward differentiation formulas, and numerical differentiation formulas are often used for stiff differential equations; however, these techniques generally do not solve for the intersection of the tip and the sample boundary.

The DDASKR routine is particularly well suited for such equations because of a root finding algorithm that solves for the precise intersection of the tip with the sample surface and creates the appropriate intermediates thereafter. This is a key advantage in simulation of dAFM probe dynamics where the tip-sample interaction forces change drastically when crossing the boundary between noncontact and contact force regimes. Additionally, the DDASKR routine is FORTRAN based and is around two orders faster than MATLAB solvers such as ODE45 and ODE15S.

III. OVERVIEW

In this section we provide a brief overview of the DAC and AMS simulation tools. We describe the graphical user interface (GUI) in terms of the input parameters and output data available. We also discuss the general methodology followed in the simulations.

A. Graphical user interface

The GUI allows the user to specify input parameters for a simulation as well as view the results. Rapture, an open-source toolkit, is used to construct each GUI. To provide flexibility, the GUI contains several input parameters which are sorted into the panels. Input panels for the DAC tool are shown in Figs. 5(a)–5(c) and for the AMS tool in Figs. 5(d)–5(f). Each panel contains a group of related parameters required for the simulation. Default values and limits are imposed on each parameter, however, some knowledge of what is practical may be required.

Once a simulation has concluded, the results are plotted in the GUI. Some manipulation of these plots is possible within the GUI, however, users are encouraged to download the data for postprocessing. Subsequent simulations may be performed (and plotted together) simply by returning to the input panels of GUI and changing one or more parameters.

B. Dynamic approach curves tool

The DAC tool simulates a dAFM cantilever excited and approaching a sample [Fig. 1(a)]. The simulation is performed over some range of the approach distance \( Z \) from \( Z_0 \) to \( Z_f \). The \( Z \) datum is consistent with the \( Z \) datum defined for the tip-sample interaction models, i.e., the sample surface is located at \( Z = a_0 \). Choosing \( Z_0 > Z_f \) causes the cantilever to approach the sample, while choosing \( Z_0 < Z_f \) results in a retraction curve. The default \( Z \) range is \( Z_0 = A_0 + 5 \text{ nm} \) and \( Z_f = 0 \).

The initial conditions of the dAFM probe are chosen to be close to the steady state solution to minimize transients. For \( Z - a_0 \gg A_0 \), the initial conditions \( [\tilde{q}(0) = \cos \phi, \tilde{q}'(0) = \tilde{\Omega} \sin \phi] \), where, \( \tan \phi = \tilde{\Omega}/[Q_1(1 - \tilde{\Omega}^2)] \) are approximated by the unconstrained, linear vibrations. For \( Z - a_0 \ll A_0 \), the magnitudes of \( \tilde{q}(0) \) and \( \tilde{q}'(0) \) are reduced by a factor of \( (Z_0 - a_0)/A_0 \).

Prior to approaching the sample, at \( Z = Z_0 \), 100 transient excitation cycles are allowed to pass. Users are discouraged from choosing \( Z_0 \) in the bistable region where two amplitude solutions are possible.

C. Amplitude modulated scanning tool

The AMS tool simulates a dAFM cantilever scanning over a sample controlled by amplitude modulation feedback [Fig. 1(b)]. For the simulation the probe is placed at \( Z = A_0 \), and is around two orders faster than MATLAB solvers such as ODE45 and ODE15S.

FIG. 4. (Color) A simplified comparison between the DDASKR routine and conventional integration routines. Both fixed and adaptive time step routines integrate from \( A \) to \( C \) without detecting the boundary between contact and noncontact regimes. The DDASKR routine solves for the intersection with the sample surface and creates an intermediate \( B' \) and appropriate subsequent intermediates until reaching point \( B \).
simulation with the same relevant parameters to determine a set-point amplitude which is in the monostable repulsive regime of oscillation.

IV. EXAMPLE SIMULATIONS

In this section, we present several example simulations which were performed on VEDA according to parameter values listed in the corresponding table. For brevity, we have only presented select results in each example. The full set of output data available for the user to download in the DACs tool includes amplitude and phase of oscillation, mean time averaged, peak attractive and repulsive interaction forces, power dissipated by nonconservative interactions, and indentation all versus the \( Z \) separation of the base of the cantilever. In addition, there is the option of including the option of displaying and recording the tip deflection waveform and accompanying tip-sample interaction history for a specified \( Z \) location and duration. The AMS tool provides the user with plots of the measured topography, measurement error, amplitude error, mean, peak attractive and peak repulsive interaction forces, power dissipated by nonconservative forces, and indentation versus the displacement in the scan direction. For each plot, the data are available for download in user specified formats.

A. Attractive and repulsive regimes of oscillation

The first example examines jumps in amplitude due to the coexistence of attractive and repulsive regimes of oscillation and provides a comparison between simulations in \(^2\) and a DAC simulation using the input parameter values in Table I. The results are consistent for the large amplitude simulations, however, for \( A_0 = 10 \text{ nm} \) VEDA does not predict the jump to repulsive oscillations (Fig. 6).

As previously mentioned, conventional integration routines will tend to overpredict indentations and corresponding interaction forces. Under certain circumstances, this overpre-

Table I. Simulation parameter values for the attractive and repulsive regimes of oscillation example (Sec. IV A).

<table>
<thead>
<tr>
<th>Operating conditions and cantilever properties</th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>Initial amplitude (nm)</td>
<td>10, 30, 60</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cantilever stiffness (N/m)</td>
<td>40</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cantilever oscillation mode</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Quality factor</td>
<td>400</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Resonance frequency (kHz)</td>
<td>350</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Excitation frequency (kHz)</td>
<td>350</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sampling frequency (MHz)</td>
<td>10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Scanning velocity (nm/s)</td>
<td>2000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Set point ratio</td>
<td>0.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Signal/Noise ratio (dB)</td>
<td>0.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Proportional gain</td>
<td>0.00001</td>
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<td></td>
</tr>
<tr>
<td>Integral gain</td>
<td>0.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lock-in time constant (us)</td>
<td>500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number of points plotted</td>
<td>500</td>
<td></td>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>Tip-sample interaction properties</th>
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<tbody>
<tr>
<td>Hamaker constant ( (J) )</td>
<td>( 7.1 \times 10^{-20} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tip radius (nm)</td>
<td>20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sample viscosity (Pa-s)</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Elastic modulus (tip) (GPa)</td>
<td>130</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Elastic modulus (sample) (GPa)</td>
<td>1.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Poisson’s ratio (tip)</td>
<td>0.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Poisson’s ratio (sample)</td>
<td>0.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Adhesion force (nN)</td>
<td>8.8</td>
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<table>
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<tr>
<th>Simulation parameters</th>
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<tbody>
<tr>
<td>Number of points plotted</td>
<td>500</td>
<td></td>
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</tr>
<tr>
<td>Deflection points per cycle</td>
<td>500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Specify Z Range</td>
<td>No</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIG. 5. (Color) Screenshots from the GUIs of the DAC and AMS tools showing the input panels. The input panels of DAC are (a) operating conditions and cantilever properties, (b) tip-sample interaction properties, and (c) simulation parameters. The input panels of AMS include (e) operating conditions, cantilever, simulation, (f) tip and substrate properties, and (g) feature properties. Additional information about an individual input parameter can be found in the GUI itself or in the comprehensive online manual.
diction of tip-sample interaction forces may lead to false amplitude jumps. However, the jump predicted in Ref. 2 for \( A_0 \) is most likely due to the choice of initial conditions in, which must be imposed at each data point. A subsequent DAC simulation of retracting from the sample revealed a large bistable region for \( A_0 = 10 \) nm. When performing simulations at discrete Z positions, initial conditions must be specified for each Z position, which becomes problematic in the bistable regime. Therefore, it is necessary to have Z changing continuously and initial position Z \( Z_0 \) to be in a monostable regime.

**B. Viscoelastic dissipation identification**

The second example demonstrates the power dissipation curve for viscoelastic interactions shown in Ref. 19. Although simulations in Ref. 19 considered only Hertzian contact with van der Waals forces, DMT contact simulations are similar for the cases where the effect of attractive regime is small (i.e., small adhesion forces or large energy oscillations). Choosing a sharp tip radius (5 nm) results in a small adhesion force since \( F_{ad} = 4 \pi R \gamma \), where \( \gamma \) is the surface energy. Parameter values required to reproduce this example are given in Table II.

Figure 7 contains the key results from the simulation. The curves in Fig. 7 were constructed by downloading the amplitude and power dissipation data from DAC and post-processing, such as computing \( A/A_0 \) and \( P'_{ts} = \partial P_{ts}/\partial A \). The results are plotted in MATLAB. The trend of \( P'_{ts} \) versus \( A/A_0 \) is clearly indicative of viscoelastic energy dissipation.

**C. Q-control simulations**

Active feedback control has been used to modify the quality factor of dAFM cantilevers either enhance the probe sensitivity48 or improve imaging speeds.49 Such feedback schemes, commonly referred to as Q control, can be reasonably simulated in VEDA for near resonant excitations and high quality factors20 simply by taking the quality factor to be the effective quality factor modified in the feedback scheme.

A recent publication by Holscher and Schwarz20 demonstrates the improved sensitivity to tip-sample interaction achieved by increasing the effective quality factor of the dAFM cantilever. Simulations performed with VEDA using parameters from Ref. 20 (listed in Table III) show good agreement (Fig. 8). For the effective quality factor of 1500, the probe remains in the attractive regime without tapping on the sample for the entire range of approach.

**D. Material properties in heterogeneous samples**

In this example, we investigate the phase contrast observed while scanning heterogeneous samples using the
TABLE III. Simulation parameter values for the Q-control example (see Sec. IV C)

<table>
<thead>
<tr>
<th>Operating conditions and cantilever properties</th>
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<tbody>
<tr>
<td>Initial amplitude (nm)</td>
<td>10</td>
</tr>
<tr>
<td>Cantilever stiffness (N/m)</td>
<td>40</td>
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<tr>
<td>Cantilever oscillation mode</td>
<td>1</td>
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<tr>
<td>Quality factor</td>
<td>1500</td>
</tr>
<tr>
<td>Resonance frequency (kHz)</td>
<td>300</td>
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<tr>
<td>Excitation frequency (kHz)</td>
<td>300</td>
</tr>
<tr>
<td>Z approach velocity (nm/s)</td>
<td>20</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Tip-sample interaction properties</th>
<th></th>
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</thead>
<tbody>
<tr>
<td>Hamaker constant (J)</td>
<td>$2 \times 10^{-19}$</td>
</tr>
<tr>
<td>Tip radius (nm)</td>
<td>10</td>
</tr>
<tr>
<td>Sample viscosity (Pa s)</td>
<td>0</td>
</tr>
<tr>
<td>Elastic modulus (tip) (GPa)</td>
<td>130</td>
</tr>
<tr>
<td>Elastic modulus (sample) (GPa)</td>
<td>1</td>
</tr>
<tr>
<td>Poisson’s ratio (tip)</td>
<td>0.3</td>
</tr>
<tr>
<td>Poisson’s ratio (sample)</td>
<td>0.3</td>
</tr>
<tr>
<td>Adhesion force (nN)</td>
<td>3.7</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Simulation parameters</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of points plotted</td>
<td>1000</td>
</tr>
<tr>
<td>Deflection points per cycle</td>
<td>500</td>
</tr>
<tr>
<td>Specify Z Range</td>
<td>Yes</td>
</tr>
<tr>
<td>Initial Z separation</td>
<td>12(0)</td>
</tr>
<tr>
<td>Final Z separation</td>
<td>0(12)</td>
</tr>
</tbody>
</table>

Shown in parentheses are the parameter values for a second simulation in which the cantilever retracts from the sample.

AMS tool. From previous work,\textsuperscript{50} we know that the power dissipated by nonconservative tip-sample interactions is strongly related to the phase of the probe oscillation. In this example, we show that phase contrast can result from either variation in sample viscosity or elasticity. Table IV lists the input parameter values used in the simulation. The sample consists of a hypothetically flat surface with 30 nm length, with contrasting material properties (either elasticity or viscosity) specified for the center 10 nm. This is achieved by selecting the “step” feature in the GUI, entering a height of 0 nm and choosing to specify separate properties for the feature.

From the simulation results (Fig. 9), we find that the scan involving contrast in sample viscosity results in negligible measurement error (within the 20 dB noise) but yields a non-negligible phase contrast. For a second scanning simulation involving contrast in sample elasticity, we see a small measurement error due an increased indentation over the soft material. The larger indentations result in an increase in power dissipation (corresponding to the phase) even though viscosity of the sample has not changed. Interestingly, the larger of the two phase contrasts corresponds to the simulation with varying elasticity, even though phase contrast is usually associated with viscosity contrast alone.

E. Strong and weak controller parameters

A second scanning simulation is presented here to show the effect controller settings on scanned images. One simulation is performed with strong control parameters (large proportional and integral gains) while a second simulation is performed with weak controller settings (small proportional gains).
and integral gains. The parameters used for the simulation are listed in Table V. A sinusoidal feature type with a 50 nm length and 30 nm height with homogeneous properties is chosen for the simulation. Finally, our goal in this simulation is to isolate the effects of the controller parameters. To do so, we reduced the noise in deflection signal by choosing a 50 dB signal-to-noise ratio. In addition, we choose not to include the effects of tip-sample geometry convolution (Sec. II D).

The measured topography observed with the strong controller settings well approximates the true sample surface (Fig. 10). The subsequent simulation performed with weak controller settings allows a small error in the measured topography. A larger deviation is seen in the phase of oscillation as the weakly controlled dAFM scans over the feature. The gradual drift in phase is a result of the small integral gain while the change in phase seen while scanning over the sample is a result of the small proportional gain. Also, the phase exhibits a striking resemblance with the amplitude error signal, which confirms that the phase contrast did not result from variation in sample properties. Interestingly, for the weak controller settings, the amplitude error strongly resembles the first derivative of the sample height with respect to the scanning distance $X$, while for the strong controller settings, the amplitude error follows the general trend of the second derivative of the sample height. Finally, we note that...
peak interaction forces may be influenced significantly by the amplitude transients, which means the controller settings play some role in the peak interaction forces. This implies that beyond the amplitude setpoint, scanning feedback parameters also need to be fine tuned to minimize imaging forces while scanning a sample.

V. SUPPORTING MATERIALS

Additional supporting materials for VEDA simulation tools are available on the nanoHUB website. Selecting a simulation tool on nanoHUB first leads to the tool’s information site where information about the tool, its contributors and other related resources can be found. Information pages
TABLE V. Input parameters for the strong and weak controller parameters example (Sec. IV E).

<table>
<thead>
<tr>
<th>Operating conditions, cantilever, simulation</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial amplitude (nm)</td>
<td>30</td>
</tr>
<tr>
<td>Cantilever stiffness (N/m)</td>
<td>40</td>
</tr>
<tr>
<td>Cantilever oscillation mode</td>
<td>1</td>
</tr>
<tr>
<td>Quality factor</td>
<td>400</td>
</tr>
<tr>
<td>Resonance frequency (kHz)</td>
<td>350</td>
</tr>
<tr>
<td>Excitation frequency (kHz)</td>
<td>350</td>
</tr>
<tr>
<td>Sampling frequency (MHz)</td>
<td>10</td>
</tr>
<tr>
<td>Scanning velocity (nm/s)</td>
<td>2000</td>
</tr>
<tr>
<td>Set point ratio</td>
<td>0.9</td>
</tr>
<tr>
<td>Signal/Noise ratio (dB)</td>
<td>50</td>
</tr>
<tr>
<td>Proportional gain</td>
<td>0.15(0.05)</td>
</tr>
<tr>
<td>Integral gain (kHz)</td>
<td>$1 \times 10^{-7}(1 \times 10^{-6}$</td>
</tr>
<tr>
<td>Lock-in time constant ($\mu$s)</td>
<td>30</td>
</tr>
<tr>
<td>Number of points plotted</td>
<td>500</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Tip and substrate properties</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Hamaker constant ($J$)</td>
<td>$5 \times 10^{-20}$</td>
</tr>
<tr>
<td>Tip radius (nm)</td>
<td>10</td>
</tr>
<tr>
<td>Elastic modulus (tip) (GPa)</td>
<td>130</td>
</tr>
<tr>
<td>Elastic modulus (sample) (GPa)</td>
<td>1.2</td>
</tr>
<tr>
<td>Poisson’s ratio (tip)</td>
<td>0.3</td>
</tr>
<tr>
<td>Poisson’s ratio (sample)</td>
<td>0.3</td>
</tr>
<tr>
<td>Sample viscosity (Pa s)</td>
<td>500</td>
</tr>
<tr>
<td>Adhesion force (nN)</td>
<td>5</td>
</tr>
<tr>
<td>Length of substrate (nm)</td>
<td>100</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Feature properties</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Select geometric feature</td>
<td>Sinusoid</td>
</tr>
<tr>
<td>Feature height (nm)</td>
<td>30</td>
</tr>
<tr>
<td>Feature Length (nm)</td>
<td>50</td>
</tr>
<tr>
<td>Specify material properties</td>
<td>No</td>
</tr>
</tbody>
</table>

Shown in parentheses are the parameter values for a second simulation with weak controller settings, i.e., small proportional and integral gains.

for VEDA currently include links to a comprehensive user’s manual, learning modules for each simulation tool (downloadable in breeze format), and other resources for dAFM.

VI. UPCOMING FEATURES AND CONCLUSIONS

In this article, we have introduced two VEDA simulation tools for dAFM that are part of a suite being developed on nanoHUB. We have demonstrated a good agreement with prior work as well as provided some new insight into dAFM operation and interpretation.

There are many possibilities for future developments in VEDA. An expansion to the DAC with capabilities in liquid environments and multiple frequency excitations is currently underway and is slated for release in late summer 2008. Eventually, VEDA is likely to include additional tip-sample interaction force models and eventually ab initio molecular dynamics. Finally, we may include filter models in the lock-in amplifier and additional realistic noise sources.

Accurate simulations of dAFM can have a profound effect on our understanding of what is really a deceptively complex instrument. While the versatility of dAFM has attracted researchers from a variety fields, accurate simulation software is not accessible to most experimentalists. Through the aid of a web-based infrastructure, NCN’s nanoHUB provides dAFM experimentalists with ready access via desktop, laptop/handheld web-enabled device to research-grade simulation software, lectures, and learning modules for dAFM. High-fidelity simulation tools for dAFM offer both qualitative and quantitative insight into the nonintuitive, underlying physics of dAFM. Such an understanding is a critical for effective use of the instrument, accurate interpretation of data and the overall development of dAFM.

ACKNOWLEDGMENTS

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36 While $\dot{Z}$ is nonzero when approaching/retracting from the sample and $\ddot{Z}$ is additionally nonzero while scanning, it is reasonable to assume $\dot{Z} \equiv \ddot{y}$ and $\dddot{Z} \equiv \ddot{y}$, therefore, we can neglect corresponding hydrodynamic and inertial forces due to $Z(t)$.

37 Equation (5) is intended for the range of $Z$ where $(\partial F_{\text{ex}} / \partial t)|_{Z=0} \leq 3E_{\text{I}}/1$. In general, the excitation force may be expressed as $F(t) = A_{\text{exc}} k B_{\text{r}} (\omega / \omega_0)^2 \left( 1 + (\omega / \omega_0) Q_0 \right)^2 \cos(\omega t + \phi_0)$, where $\phi_0 = \omega_0 / \omega Q_0$. For rare instances when $Q_0 \ll 1$ and/or $\omega \ll \omega_0$, this form may be needed. Otherwise, Eq. (6) is adequate.

39 We had previously included a factor $(\omega / \omega_0)^2$ in $y_1$ (Ref. 12), however, this factor arises because of the moving frame and not because of the nature of the continuous beam.

40 W. H. Han, S. M. Lindsay, and T. W. Jing, Appl. Phys. Lett. 69, 4111 (1996).


47 See www.rappture.org.


