Full-wave broadband modeling of near field scanning microwave microscopy

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Abstract: Near field microscopy breaks the diffraction limit and probes the image at subwave-length resolution by exploiting the properties of evanescent wave near the sample under study. Its implementation in the microwave frequency range, scanning microwave microscopy (SMM) has recently attracted more attention as it brings radio frequency and microwave measurements down to the molecular and atomic scale. Currently, the modeling of SMM and quantification of local material properties of samples usually neglects radiation and scattering losses of the nano-sized probe based on low frequency assumptions. To improve numerical accuracy of SMM modeling and evaluate existing models, we have applied a rigorous full wave numerical model with all wave components in the near field taken into consideration. In virtue of the proposed full wave model, several approximations presented in previous studies are validated, and we conclude that the SMM has potential for use as a broadband dielectric spectroscopy operating at even higher frequencies.

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References and links
1. Introduction

Near field scanning microwave microscopy (SMM) is a new paradigm of microwave measurement of local material properties, and it has found various applications in super-resolution imaging and characterization of inorganic and organic substances [1–10], as well as in the development of functional materials and devices at nanoscale such as molecular electronics [11]. Encouraged by the success of near field scanning optical microscopy (NSOM) [12, 13], SMM has also been applied to biological imaging for single bacterial [14], live cells in situ [15], muscle cells [16]. Comparing to light waves used in NSOM, microwaves have larger penetration depths, thus the SMM provides high resolution mapping of both surface and internal properties of material samples.

A typical SMM consists of a nanosized sharp probe (of atomic force microscope, AFM [17] or scanning tunneling microscope, STM [18]) connected to a microwave source through an impedance matching circuit. Comparing to other near field microwave microscopy techniques [19–21, 21–25], SMM provides an excellent spatial resolution down to the molecular and atomic scales with the help of the nanosized probe tip and controlling the probe-sample distance developed in the scanning probe microscopy (SPM). SMM generally measures the S-parameter [1, 4, 8, 16, 26] or directly the complex impedance [5, 9, 27] of tip-sample electrodynamic interaction, and then the capacitance or conductance of the tip-sample system can be simply derived. However, it is not trivial to map these quantities with local material properties such as complex permittivity or permeability of samples. These quantities represent complex convolutions between the probe geometry and electromagnetic response including real material properties and surface topography [19, 27]. Since current SMMs operate largely in the reflection mode, and reflected signals from the highly-localized tip-sample interaction are extremely small, an exceptionally sensitive and stable signal detection system is required. Thus, a good estimation of the tip-sample impedance is also of great significance in the design of the impedance matching circuit, especially for future implementation of broadband SMMs. Full-wave modeling also allows the study of SMM integrated with additional metamaterial component, such as a flat lens with negative refraction index that amplifies evanescent waves. Such lenses have been fully-studied and demonstrated at microwave frequencies [28, 29], and its integration with SMM would further improve the spatial resolution and may enhance the ability on detecting buried features.

Ideally, the complex impedance of probe tip-sample interaction should be modeled rigorously by solving Maxwell-equations without any approximation to establish an accurate mapping between SMM measured quantities and local material properties. Since the probe size of AFM is much smaller than the operating wavelength, and it barely radiates electromagnetic waves, thus the radiation or scattering and the magnetic field is neglected. In the local near field region, the electric field is nearly irrational and Maxwell equations are reduced to Poisson’s equation of electrostatic potential. Solving this quasistatic model numerically, the complex tip impedance then can be calculated for both probe and sample with arbitrary geometry and material constitutions. This approach has been widely used in modeling scanning probe devices utilizing low frequencies (30–300kHz) such as nanoscale capacitance microscopy [30], electrostatic force microscopy (EFM) [31, 32], as well as SMM based applications [2, 3, 5, 9, 14, 27]. The accuracy of this method has been verified by comparing the results with those obtained from analytical method for particular shaped probes at low frequencies [30, 31]. Besides the quasistatic model, some researchers used equivalent circuit models for profiling doped semiconductors and measuring material conductivity [1, 3, 8]. Although these models have been proved useful for devices operating at low frequencies and some specific applications, the question is, however, for a given SMM setup, at which frequencies are these models valid, and to which level of accuracy?

Local material properties at microwave frequencies (X band or higher) are also of tremendous interest in various applications, such as high-speed micro/nano electronics [11], nanoscale mate-
rial characterization from L-band to K-band [1,3,6,8,14,26]. Evanescent fields are embedded in the solutions to the Maxwell equations, thus a full-wave approach is always preferred to model the near field microscopy, which accounts for all wavenumbers both real and imaginary. However, there exist significant challenges in numerical modeling of nanostructures and nano-materials at microwave frequencies. Unlike near field imaging in the optical regime for NOSM applications where the nanosized tip is around $1/100\lambda$ at visible or infrared range [12,13], or probes at millimeter scale for microwave applications [23–25], SMMs use AFM or STM probes with tip dimensions can be less than $1/10^6\lambda$ at millimeter frequency band [10]. This leads to a challenging problem, so-called low frequency breakdown [33,34], in full wave numerical modeling of SMM, as the numerically discretized Maxwell equation ends up with an ill-conditioned matrix and inaccurate solutions due to the finite machine precision in computing.

2. Theory and method

Consider the near field probe tip as a two-terminal connected to its detection system (e.g., antennas), it stores reactive energy through exponentially decayed evanescent fields, which can be expressed as reactance in the equivalent circuit model. Meanwhile, the material loss can be included in the equivalent circuit as resistive components, and, at the high frequency range, radiation and scattering losses must be also taken into account. Thus the tip-sample interaction is modeled by a complex impedance $Z = R + jX$ consisted of lumped elements. The resistance and reactance impedance generally depends on the tip-sample geometry and material properties [19] and are given by

$$R = \frac{\omega}{|I_0|^2} \iiint_V \varepsilon_r^\prime |E|^2 + \mu_0 \mu_r^\prime |H|^2 dV + \frac{1}{|I_0|^2} \iint_S \text{Re} [E \times H^*] \cdot ds$$  \hspace{1cm} (1)

$$X = \frac{\omega}{|I_0|^2} \iiint_V \mu_0 \mu_r^\prime |H|^2 - \varepsilon_r^\prime |E|^2 dV$$  \hspace{1cm} (2)

where $\omega$ is the angular frequency, $I_0$ is input current intensity to the probe terminal, and $\varepsilon_r^\prime$ and $\varepsilon_r^\prime$ are real and imaginary part of relative complex permittivity, $\mu_r^\prime$ and $\mu_r^\prime$ are real and imaginary part of relative complex permeability. In quasistatic models, for electrical probes the magnetic field in (1) and (2) as well as the radiation impedance (second term in (1)) are neglected based on low-frequency assumption.

To find electrodynamic quantification of tip-sample interaction rigorously at microwave frequencies, we solve the following wave equation derived from the Maxwell’s equation

$$\nabla \times (\mu_r^\prime - j\mu_r^\prime) \nabla \times E - \omega^2 \varepsilon_0 \mu_0 (\varepsilon_r^\prime - j\varepsilon_r^\prime) E = J$$  \hspace{1cm} (3)

where the excitation on the right-hand side is a current source $J$ located between the probe and the substrate which holds the sample under study. To simplify the simulation, we use a delta-gap source as the excitation current which is a common treatment for antenna simulation using the Method of Moment(MOM) [35]. Namely, we use an infinite thin line current connecting the tip probe and substrate, and the current have a constant intensity $I_0$ along the line as its length is much smaller than a wavelength. The complex impedance of tip-sample can then be calculated by

$$Z = \frac{V}{I_0} = \frac{\int_L E \cdot dI}{I_0}$$  \hspace{1cm} (4)

after solving the wave equation (3) and $L$ is the path of the line current. Alternatively, the complex impedance can be calculated by its definition using equation (1) and (2). Similar to the solution of quasistatic model, we use the finite element method to solve equation (3) because of its flexibility in handling complex geometry and material constitutions [36]. At microwave
frequencies, a metallic probe tip can be treated as perfect conductor, and we have the perfect conducting condition (PEC) on the internal boundary
\[ \hat{n} \times \mathbf{E} = 0 \quad \mathbf{r} \in \Omega_{probe} \]  
where \( \Omega_{probe} \) is the probe surface. To truncate the simulation domain, we use the Sommerfeld boundary condition [37]
\[ \hat{n} \times (\nabla \times \mathbf{E}) - j k_0 \hat{n} \times (\mathbf{E} \times \hat{n}) = 0 \quad \mathbf{r} \in \Omega_S \]  
where \( \Omega_S \) is the truncation boundary enclosing the tip and sample.

Following the standard FEM procedure, the discretized equation becomes to a matrix equation
\[ \begin{bmatrix} A & \mathbf{b} \end{bmatrix} \begin{bmatrix} \mathbf{E} \end{bmatrix} = 0 \]  
and the matrix \( A \) is the sum of
\[ A(\omega) = S - \omega^2 T + j \omega R \]  
where \( S \) is the stiffness matrix, \( T \) and \( R \) are the mass matrices. They are assembled by the elemental contributions
\[ S_{ij}^e = \int_{V_e} \left( \mu_r' - j \mu_r'' \right)^{-1} (\nabla \times \mathbf{N}_i) \cdot (\nabla \times \mathbf{N}_j) dV \]
\[ T_{ij}^e = \int_{V_e} \frac{\epsilon_r' - j \epsilon_r''}{c^2} \mathbf{N}_i \cdot \mathbf{N}_j dV \]
\[ R_{ij}^e = \frac{1}{c} \int_{\Omega_{Som}} (\hat{n} \times \mathbf{N}_i) \cdot (\hat{n} \times \mathbf{N}_j) dS \]
and the right-hand side of (7) are assembled by
\[ b_i^e = -j \omega \mu_0 \int_{V_e} \mathbf{N}_i \cdot \mathbf{J} dV \]  
where \( \mathbf{N} \) is the normalized vector basis function for electric field. For a fine mesh representing a nanosized tip, the average length of \( l \) of the mesh can be as small as 1nm to 20nm. Since the norm of \( \nabla \times \mathbf{N} \) is proportional to \( l \), the value of \( S_{ij} \) is the order of \( l \) and \( T_{ij} \) is the order of \( 10^{-17} l^3 \) [34]. Hence, at microwave ranges \( \omega^2 T \) may \( 10^{15} \) times smaller than \( S \), even using double-precision computing, the contribution of some entries in \( \omega^2 T \) is treated as zeros in the FEM system matrix \( A \). Then matrix \( A(\omega) \) becomes ill-conditioned or singular at low-frequency, and the full wave FEM solution breaks down.

To eliminate the low-frequency breakdown of SMM full wave simulation due to the finite machine precision, we first find the inverse of the nearly ill-condition component of matrix \( A \) by transforming it from frequency dependent problem to a frequency independent generalized eigenvalue problem [34]. Specifically, we first divide matrix \( A \) into
\[ A(\omega) = \begin{bmatrix} A_{ss}(\omega) & A_{sr}(\omega) \\ A_{rs}(\omega) & A_{rr}(\omega) \end{bmatrix} \]  
where \( A_{ss} \) represent the ill-conditioned or singular submatrix, and associated with the mesh region of the probe tip apex, \( A_{rr} \) is the regular component in \( A \). Correspondingly, the unknowns \( E \) in (7) are also divided into two categories \( E_S \) and \( E_R \). \( A_{sr} = A_{rs}^T \) represent the coupling between these two sets of unknowns.

According to the Schur-complement lemma, the inverse of \( A \) can be written as
\[ A(\omega)^{-1} = \begin{bmatrix} A_{ss}^{-1} + A_{ss}^{-1} A_{sr} B_{rr}^{-1} A_{rs} A_{ss}^{-1} & -A_{ss}^{-1} A_{sr} B_{rr}^{-1} \\ -B_{rr}^{-1} A_{rs} A_{ss}^{-1} & B_{rr}^{-1} \end{bmatrix} \]  
where
where
\[ B_{rr} = A_{rr} - A_{rs}A_{ss}^{-1}A_{sr} \] (13)

here we omit the \( \omega \) for simplicity. Since the singular submatrix \( A_{ss} \) is associated with the tip apex because of the nanoscale geometric feature and extremely small mesh length, the frequency dependency of \( A_{ss} \) can be written as
\[ A_{ss}(\omega) = S_{ss} - \omega^2 T_{ss} \] (14)

Especially, for SMM operating in non-contact mode where the tip apex and sample are separated, and surrounding media assumed to be lossless, then the both \( S_{ss} \) and \( T_{ss} \) are real and symmetric. To solving the following generalized eigenvalue problem
\[ S_{ss}\lambda = T_{ss} \] (15)

where \( \lambda \) is the eigenvalue and \( \nu \) is the associated eigenvector, we have the frequency dependent inverse of \( A_{ss}(\omega) \) [34]
\[ A_{ss}(\omega)^{-1} = (V_0 V_h) \begin{bmatrix} -\omega^2 I & 0 \\ 0 & \Lambda_h - \omega^2 I \end{bmatrix}^{-1} (V_0 V_h)^T = \frac{1}{\omega^2} V_0 V_h^T + V_h \begin{bmatrix} \Lambda_h - \omega^2 I \end{bmatrix}^{-1} V_h^T \] (16)

where \( V_0 \) is the set of eigenvectors associated with zero eigenvalues, and represents the DC modes near the tip apex area, and \( V_h \) is the set of eigenvectors associates with non-zero eigenvalues \( \Lambda_h \). For SMM operating in contact mode where tip touching the sample surface or in lossy media, the inverse of \( A_{ss} \) can be found in a similar way [38]. Matrix \( B_{rr} \) usually is non-singular, and its inverse can be found normally or using eigenvalue decomposition again for a frequency dependent inversion as introduced in reference [34]. The electrical field in the simulation domain then can be calculated using the solved unknowns \( E \) and basis functions \( N \).

3. Result

**Full wave FEM modeling of SMM**

The tip-sample capacitance \( C \) and conductance \( G \) related its admittance by \( Y_S = 1/Z = G + j \omega C \), which are quantities often used to determine dielectric constant and loss tangent of material or samples under study. As shown in Fig.1.(a), a metallic SMM probe is placed on a conducting substrate illustrated by gray colored grid for simplicity. The difference of capacitance \( \Delta C \) with respect to the value at a distance between tip and substrate of \( z_{Lift} = 1050nm \) is given in Fig.1.(b), the capacitance is obtained from the full wave FEM method and the electrostatic model using COMSOL (AC/DC electrostatic module), as well as those from the measurement data [14] were used to validate the model. The theoretical value of capacitance calculated by the full wave FEM method and the electrostatic method shows a very good agreement with measurement data. In Fig.1.(b)-(e), we sweep both the real and
imagery part of permittivity and the calculated capacitance and conductance curves from the tip-sample impedance are presented. As shown in these figures, calculations obtained from the quasistatic model agree very with those based on the full wave method below 1.0GHz. The capacitance values at different frequencies are almost constant across the whole frequency range as shown in Fig.2(b) and(d), while conductance curves are gradually varied as frequencies increase as shown in Fig.2(c) and (e).

The discrepancy is due to the fact that the value of radiation admittance becomes significant in the calculation of total conductance, which is neglected in the quasistatic model. Although the resistive impedance $R$ is not accurate at 20GHz, the calculated capacitance from both the quasistatic model and full wave model still agrees very well as $R$ is much more smaller than reactive impedance $X$, and the error in $R$ has a very limited effect on the capacitance calculation. Intuitively, the tip-sample system only stores electric energy due to the fact that the size of the tip is still much smaller than the operating wavelength, and the capacitance which is the ability to store the electrical charges only dependent on dielectric properties of materials. Generally, for a sub-micron sized metallic tip operating below K-band, the real part of the permittivity can be quantified from the SMM capacitance without considering the radiation resistance of the probe tip. Otherwise, full wave modeling is necessary for the characterization of dielectric property of materials under test. The radiation resistance is usually affected by the sample surface during the scanning procedure and it cannot be removed or calibrated, yet specially designed experiment setup might be available for measurement calibration, such as using a flat and ultrathin membrane to separate the sample and probe tip [15].

Fig. 1. Illustration and capacitance results of SMM:(a)Schematic representation of the 3D geometry of SMM probe tip on the conducting substrate, the substrate is represented by gray grids; (b) the difference capacitance of tip-substrate system obtain by different models and measurement.

**High Frequency Properties**

One increasing trend for SMM development is to push its operating frequency to higher frequency bands, in order to achieve broadband characterization of local material properties [6] or to enable future studies in molecular electronic engineering [10,11]. For example, the complex permittivity of water changes dramatically in the millimeter frequency band, and it provides stark contrast in biological imaging techniques since the water is ubiquitous in biological tissues. Furthermore, terahertz imaging and spectroscopy has become very popular in applications related to, for example, skin cancer detection [39] in the last few years. In this study, we applied the proposed numerical technique to investigate a micron-size pure water droplet under SMM operating from 30GHz to 60GHz, the simulated intrinsic capacitance and dissipation loss conductance images are shown in Fig.3. The spherical cap shape water droplet has height 0.6µm and radius 1.0µm,
Fig. 2. Theoretic study of a parabolic shaped sample under SMM using quasistatic model and full-wave method under difference frequencies: (a) Schematic representation of the 3D geometry of SMM probe tip on a parabolic sample with diameter $D_w$ and height $C_w$; the dielectric properties of this sample assumed to be $\varepsilon_{\text{Sample}} = \varepsilon_0(\varepsilon_r' - j\varepsilon_r'') = \varepsilon_0\varepsilon_r'(1 - j\tan\delta)$. (b-c) the difference of capacitance $\Delta C$ with respect to $\varepsilon_r' = 1$ and total conductance for different dielectric loss values and $\varepsilon_r'' = 5.0$. (d-e) the difference of capacitance $\Delta C$ with respect to loss tangent $\tan\delta = 0$ and total conductance for different loss tangent values and $\varepsilon_r' = 5$. The metallic tip apex has a radius 217nm and the scanning surface is 100nm above the sample and the substrate surface. The dielectric constant of pure water is described by the modified Klein-Swift model with two Debye relaxations \cite{40, 41}. Although relative dielectric constant $\varepsilon_r'$ of the sample decreases from around 27 at 30GHz to 12 at 60GHz, the intrinsic capacitance of image does not change significantly as we can see from the colorbars in Fig. 3(a)-(d). The dissipation conductance images shown in Fig. 3(e)-(g) are obtained by extracting radiation admittance from the total conductance. The image contrasts are gradually enhanced as the frequency increases despite the fact that imaginary part of relative permittivity varies from -33 to -21. This suggests that increasing SMM operation frequencies would help to improve the image contrast in relation to conductance or absorption of samples under test.

Fig. 3. $4\mu m \times 4\mu m$ SMM capacitance and conductance images of a water droplet at $25^\circ$: (a)-(d) intrinsic capacitance images at 30GHz, 40GHz, 50GHz and 60GHz, (e)-(g) sample dissipation loss conductance images at 30GHz, 40GHz, 50GHz and 60GHz.
**Skin effect**

In the SMM measurement, samples are usually placed on a conducting surface such as metals, and the probe tip of AFMs is also made of or coated with metals as titanium, aluminum, or tungsten [42, 43]. At any non-zero operating frequencies, current flowing in a conductor distributed towards the boundary due to the skin effect. At microwave frequency range, the skin depth of metal ranges from hundreds of nanometers to several micrometers which is comparable to the probe tip apex radius. In previous modeling of SMM and similar devices at low frequency such as EFM, metallic components are treated as perfect conductors with zero skin depth, and modeled as a terminal applied to a constant AC voltage on their boundaries. To assess the accuracy of this approach, we modeled the metallic tip as a lossy medium and compared the result with that of PEC boundary approximation. The conducting substrate is treated as impedance boundary since its thickness is much larger than skin depth and electromagnetic waves cannot penetrate the substrate [37]. Normalized local electric field profile near a titanium tip when it is modeled by PEC boundary and a lossy medium are presented respectively in Fig.4.(a) and (b). At 5GHz, the skin depth of titanium is 5.23μm which is several times larger than the radius of the tip apex (517nm). As we can see from the figures, the local electric field profiles are almost identical, and the field intensity inside the titanium tip when it is modelled as a lossy medium is almost zero. The electric field intensity along the red dash lines in Fig.4(a) and (b) applying respective PEC boundary and lossy media is shown in Fig. 4(d), they also have a very good agreement below the tip apex. We also consider the case of metallic tip made of aluminum, which has higher conductivity and hence smaller skin depth comparing to titanium, the local electric field intensity inside and below the tip apex is also presented in this figure, and agree very well with the result of using PEC boundary. Numerical results of a metal tip placed on a micron-sized high purity silicon block using PEC boundary and lossy media with a conductivity of aluminum and titanium from 5GHz to 60GHz are shown in Fig.5 (b) and (c). The complex permittivity of high-purity silicon is reported in [44], and the loss tangent fit to experimental data is shown in Fig.5(a). The sample loss resistance over this frequency band is shown in Fig.5(b), which is obtained by extracting the radiation resistance from the total port resistance $R$. The capacitance of the tip-sample interaction is nearly a constant value due to the small variance of the dielectric constant of the high-purity silicon. Although, the loss tangent becomes smaller at high frequencies as shown in Fig.5(a), and so is the dissipation loss resistance, its reciprocal conductance increases rapidly as frequency increase due to the fast decay of $X \sim 1/\omega C$. From these comparisons, we can see that the simplification of metallic tip to a PEC boundary is a good approximation to improve SMM modeling efficiency at frequencies up to 60GHz.

**Metallic tip versus dielectric tip**

SMM in some applications uses dielectric probes instead of metallic tips, such as silicon(Si) or silicon nitride ($Si_3N_4$) tip, which are commonly used in AFM [4]. The difference between metallic tip and dielectric tip is qualitatively compared in this section. The normalized electric field near and inside of a silicon tip is shown in Fig.4(c), unlike a metallic tip, the dielectric tip acting like a tapped dielectric waveguide in NSOM, the electric field intensity along the red line is shown in Fig.4.(d). Comparing to the metallic probe, the electric field near the silicon tip is less localized, and the maximum field intensity is much lower. The electric field on a bare conducting substrate illuminated by a titanium tip and a same-sized silicon tip is shown in Fig.6(a) and (b), the electric field under the metallic tip is more concentrated than that under the silicon tip, and this indicates the SMM with a metal tip has a better lateral resolution, while the silicon tip has a wider scope. The strong local electric field of the metal tip may however induce nonlinear behavior of samples under the test, which have to be avoided in some application scenarios, and it makes the using of dielectric probe a better choice.
Fig. 4. Electrical field of different types of probe tips at 5GHz: (a) normalized field profile near the PEC boundary tip, (b) normalized field profile near the titanium tip with skin depth 5.32μm, (c) normalized field profile near and inside the silicon tip, (d) electric field intensity along the red dash lines in (a) and (b), (e) electric field intensity along the red line in (c).

Fig. 5. A 4μm × 4μm × 1.5μm high-purity semi-insulating silicon sample under SMM. (a) Loss tangent of high-purity semi-insulating silicon [44], (b) silicon sample dissipation loss resistance; (c) conductance corresponded to sample dissipation loss.

4. Conclusion

In this work, we perform a rigorous modeling of various nanosized SMM probes and their electrodynamic interaction with material samples at microwave frequencies by fixing the low-frequency breakdown problem in numerical implementation. We found that the quasistatic model provides good accuracy in terms of calculating the tip-sample interaction, while the calculation of losses of sample materials becomes less accurate as the frequency goes higher. Our simulation results show that SMMs operating at high frequency provide better sensitivity on dielectric loss measurement while radiation losses also increase as the operating frequency increases. The proposed full wave modeling of SMM will provide some physical insights for the development of broadband near field microwave scanning spectroscopy with high imaging precision by taking both propagation and evanescent wave components into consideration. This work will present a complete modal picture of SMM, in line with illumination or collection mode used in NSOM,
Fig. 6. Normalized electric field on a conducting substrate plane 1.55\mu m below the SMM probe tip (a) titanium tip, (b) silicon tip.

which determine local material properties by applying evanescent-scattering field to propagating field conversion and it may therefore open up new frontiers of SMM research at high frequencies up to THz.

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