

An Open-Source Framework for Quantitative Electrostatic Simulations in Kelvin Probe Force Microscopy

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We developed an open-source numerical code for calculating electrostatic interactions between a hyperbolic metallic tip and a conducting surface under Kelvin probe force microscopy (KPFM)-relevant conditions. The code solves the electrostatic potential in the tip-sample vacuum gap under an applied bias by imposing Dirichlet boundary conditions on the tip and sample surfaces, and evaluates electrostatic force observables from the calculated potential. In addition to laterally homogeneous samples, the full three-dimensional implementation treats spatially inhomogeneous surfaces and reproduces contact potential difference profiles. Quantitative comparison with experiments is achieved without arbitrary scale factors or other ad hoc proportionality constants. The method provides a practical framework for experimental-parameter extraction, quantitative KPFM data analysis, and future investigations of contrast formation and other measurement aspects in KPFM.

I. INTRODUCTION

Kelvin probe force microscopy (KPFM) is a powerful technique for visualizing nanoscale surface-potential distributions [1–3] across a wide range of materials under realistic device-operating conditions [4–9]. However, because the KPFM signal originates from electrostatic interactions, it inevitably includes long-range contributions. As a result, the measured potential does not necessarily correspond directly to the local value immediately beneath the tip apex, but rather reflects a weighted average of the surrounding electrostatic environment. Consequently, a consistent framework that relates probe geometry and measurement conditions to the resulting electrostatic field and force is essential not only for the quantitative interpretation of KPFM data, but also for the continued improvement of KPFM methodology.

To date, numerous studies have evaluated electrostatic tip-sample interactions using numerical and semi-analytical approaches to discuss the mechanisms of signal formation in electrostatic force microscopy (EFM) and KPFM [10–14]. The nonlocal response of KPFM has also motivated complementary inverse-analysis approaches, including point-spread-function/deconvolution methods, Green’s-function methods, and finite-element/KPFM-hybrid approaches for reconstructing surface-potential or charge-density distributions from measured KPFM images [15–20]. Most of the forward-modelling studies focused on cantilever-based force sensors and examined, for example, the differences in contrast formation between amplitude-modulation (AM) and frequency-modulation (FM) EFM/KPFM [21–23], as well as how different parts of the probe assembly, including the tip apex, the shank, and the cantilever, contribute to the electrostatic interaction [11–13, 23, 24]. By contrast, relatively few studies have explicitly considered AFM configurations employ-

ing a sharp metallic tip mounted on a self-sensing force sensor and operated under ultrahigh-vacuum (UHV) conditions, where very small tip radii and tip-sample separations are typically assumed for high-spatial-resolution measurements [25, 26].

Representative studies by Belaidi *et al.* [27] and Shen *et al.* [22] examined how the probe-sample geometry affects the apparent spatial resolution, showing that, in the regime $s \ll R$, it scales as $(Rs)^{1/2}$, where R and s denote the tip radius of curvature and the tip-sample separation, respectively. However, these studies were primarily concerned with forward analyses of contrast formation and resolution limits, rather than with rigorous comparison to experimental observables or the establishment of a practical framework for quantitative data analysis. As a result, a general approach for extracting physically meaningful probe parameters from measured data has not yet been fully established. One likely reason is that the tip radius, opening angle, and tip-sample separation can be mutually correlated, making it difficult to impose physically meaningful constraints on the fitting parameters. Moreover, the accuracy of existing models and the precision of experimental calibration have not always been sufficient to support fully quantitative fitting capable of reliably identifying physical parameters from experimental data.

In this study, we developed a numerical software package, METALTIP, to compute the electrostatic response of a hyperbolic metallic tip above a conducting surface. For user-defined parameters such as the tip radius, opening angle, and tip-sample separation, the code solves the electrostatic potential in the tip-sample vacuum gap under an applied bias and computes the resulting electrostatic force. This enables direct simulation of the bias (U) dependences of the electrostatic force, $F(U)$, and frequency shift, $\Delta f(U)$. The full three-dimensional (3D) implementation further treats laterally varying surface potentials and reproduces contact potential difference (CPD) profiles across inhomogeneous interfaces. We validated the numerical accuracy by benchmarking against established theoretical models and demonstrated quanti-

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tative fitting of experimental data without ad hoc tuning parameters. This quantitative accuracy enables *in situ* extraction of key experimental parameters, including the tip-sample separation and the effective tip radius. These capabilities establish METALTIP as a practical framework for the quantitative interpretation of KPFM data and for the development of new measurement and analysis approaches.

II. NUMERICAL METHODS

To quantitatively calculate the electrostatic interaction between a metallic tip and a conducting sample surface, METALTIP builds on the potential-solver framework of SEMITIP developed by Feenstra [28–33] and largely follows its numerical implementation. SEMITIP was originally developed to model scanning tunneling microscopy (STM) measurements on semiconductor surfaces by calculating the tunneling current, which requires solving the electrostatic potential and charge distribution inside semiconductors. In contrast, METALTIP is designed for atomic force microscopy (AFM)/KPFM measurements, where the relevant observable is the electrostatic force acting on a metallic tip. The code addresses the electrostatic boundary-value problem of an ideal metallic tip above a sample surface whose potential is specified as a Dirichlet boundary condition. Thus, the electrostatic potential is solved only in the tip-sample vacuum gap.

This formulation does not describe electrostatic responses inside the sample, such as finite screening, dielectric polarization, charge redistribution, or band bending. Therefore, it is not directly applicable to general semiconductor surfaces where electric-field penetration into the sample plays an essential role. However, semiconductor surfaces that behave approximately as equipotential boundaries owing to strong screening or a high density of surface states may still be treated within the same effective-boundary framework.

In the following, we outline only the essential computational workflow and key equations; full numerical details and implementation-specific procedures are provided in Supplementary Note I.

In the vacuum region, the electrostatic potential ϕ satisfies the Laplace equation, $\nabla^2\phi = 0$. In the two-dimensional (2D) case, corresponding to a laterally homogeneous sample, axial symmetry is assumed, and the potential is written as $\phi(r, z)$ in cylindrical coordinates, where r is the radial coordinate and z is the surface-normal coordinate. The (r, z) domain is discretized using a generalized prolate spheroidal coordinate system (ξ, η) , which enables a compact grid that captures both the apex curvature and the shank opening. The sample surface ($z = 0$) corresponds to $\eta = 0$, and the tip surface is aligned with $\eta = \eta_T$, where η_T is determined by the full shank opening angle α (see Supplementary Fig. S1).

After solving the Laplace equation numerically to obtain the electrostatic potential ϕ , we evaluate the elec-

trostatic force from the electrostatic pressure on the tip and sample surfaces. The surface pressure is obtained from the electric field at the conductor surfaces using the Maxwell-stress expression. In vacuum, the pressure is given by [34]

$$p = \frac{1}{2}\varepsilon_0 E_n^2, \quad (1)$$

where ε_0 is the vacuum permittivity and E_n is the surface-normal component of the electric field. Because the electric field at a conductor surface is normal to the surface, E_n can be evaluated from $\mathbf{E} = -\nabla\phi$ at the boundary.

The vertical force component is then obtained by integrating the pressure over the surface,

$$F_z = \iint p n_z dS, \quad (2)$$

where n_z is the z component of the unit normal vector and dS is the surface area element. In practice, we evaluate F_z from the pressure on the planar sample surface, which is numerically more stable, especially for sharp tips. We verified that the sample-side and tip-side force evaluations agree to within a few percent after mesh refinement; details of the implementation and convergence tests are provided in Supplementary Note I.

The 3D solver introduces the azimuthal angle θ and solves $\phi(\xi, \eta, \theta)$ with periodic boundary conditions in θ . An arbitrary surface-potential distribution can be prescribed on the sample surface as $\phi(\xi, \eta = 0, \theta) = V_s(\xi, \theta)$, enabling laterally varying potentials (and corresponding CPD variations), such as interface steps and patch-like inhomogeneities. In contrast to the laterally uniform 2D case, such spatially varying surface potentials generally produce not only a normal electric-field component but also lateral field components on the sample surface. Accordingly, the vertical force component in the 3D calculations is evaluated from the Maxwell stress using the full surface traction, so that the contributions of both the normal and lateral electric-field components are properly taken into account. The explicit expression used for this evaluation is given in Supplementary Note I.

III. EXPERIMENTAL METHODS

To obtain experimental data suitable for direct comparison with the simulations, we prepared a Cu(111) surface partially covered with an ultrathin NaCl overlayer [35, 36]. The coexistence of bare Cu(111) terraces and NaCl islands on the same substrate provides a well-defined lateral boundary across which the surface potential changes abruptly [36]. Details of the sample preparation are provided in Supplementary Note II.

All KPFM measurements were performed at 78 K under ultrahigh-vacuum (UHV) conditions (base pressure $< 1 \times 10^{-8}$ Pa) using a low-temperature scanning probe

microscopy (SPM) system (Unisoku USM-1400). qPlus sensors [37, 38] equipped with electrochemically etched tungsten (W) tips (P-100WS, Unisoku) were used as probes. The resonance frequencies of the sensors ranged from 27 to 31 kHz, and the quality factors ranged from 18,000 to 25,000 at 78 K. The W tips were subjected to Ar^+ -ion sputtering for 20 min to remove the oxide layer and sharpen the tip apex. Tip-sample forces were measured in FM mode [39] after calibration of the oscillation amplitude [40]. The tip-sample separation was regulated in STM mode, that is, using the cycle-averaged tunneling current as the feedback signal. Bias voltages are defined as the sample voltage with respect to the tip. CPD signals were acquired by Kelvin probe force spectroscopy (KPFS) [41–43], in which $\Delta f-U$ spectra were recorded at each measurement position and fitted to a parabola.

IV. RESULTS AND DISCUSSION

A. Potential and electric-field distributions near the tip apex

Figure 1(a,b) shows the calculated electrostatic potential distribution and the corresponding electric-field-magnitude map for a representative tip-sample geometry with a tip radius $R = 10$ nm, a full shank opening angle $\alpha = 10^\circ$, a tip-sample separation $s = 1.5$ nm, and a bias voltage $U = 1$ V. The computational domain spans $\sim 20 \mu\text{m}$ in the radial direction and $\sim 18 \mu\text{m}$ in the z direction, ensuring that the outer boundaries are sufficiently far from the tip-sample junction. To clearly visualize the strong-field region near the apex, only a magnified view around the tip apex is presented in Fig. 1. The electric field was calculated from the potential distribution as $\mathbf{E} = -\nabla\phi$, and the color scale in Fig. 1(b) represents its magnitude, $|\mathbf{E}|$. The $|\mathbf{E}|$ map indicates pronounced localization of the electric field in the immediate vicinity of the apex. In the following section, this localization is analyzed more quantitatively through the radial distribution of the electrostatic pressure.

B. Radial distribution of electrostatic pressure and validation against the sphere-plane model

Using the same numerical data as in Fig. 1, we evaluate the radial dependence of the electrostatic pressure on the tip and sample surfaces, as shown in Fig. 2. In both evaluations, the pressure decreases steeply with increasing r over a length scale comparable to the tip radius R (10 nm), indicating that the dominant contribution arises from the near-apex region. A weak long-range tail, which is not readily visible on a linear scale but becomes evident on a logarithmic plot (Supplementary Fig. S2), nevertheless contributes to the total force because the surface integral is area-weighted ($\propto r dr$). Accordingly, a sufficiently large radial integration range is

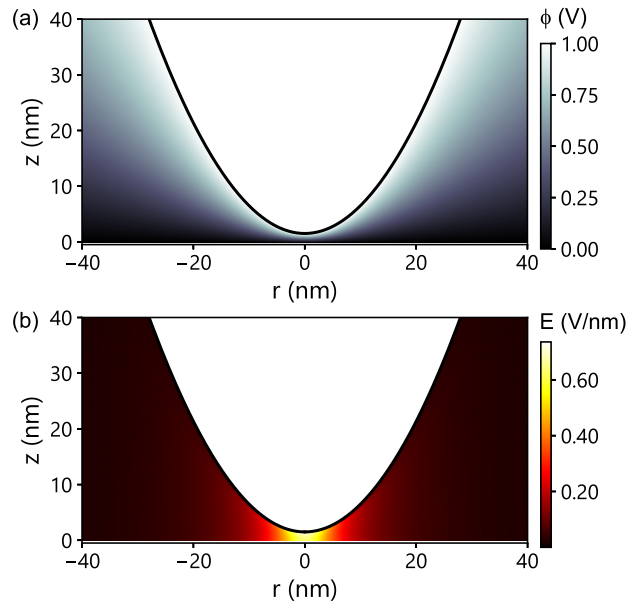


FIG. 1. Calculated maps of (a) the electrostatic potential ϕ and (b) the electric-field magnitude $|\mathbf{E}|$ in the vacuum region near the tip apex for a representative tip-sample geometry ($R = 10$ nm, $\alpha = 10^\circ$, and $s = 1.5$ nm). The tip is held at $U = 1$ V and the sample surface is grounded (0 V).

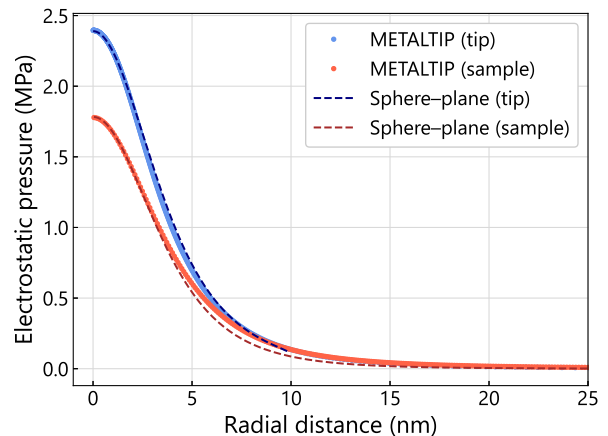


FIG. 2. Radial profiles of the electrostatic pressure on the tip and sample surfaces, calculated for the same geometry and bias conditions as in Fig. 1. Solid circles show the METALTIP results, evaluated on the tip surface (blue) and the sample surface (red). Dashed lines indicate the analytical sphere-plane solution.

required for the tip-side and sample-side force evaluations to achieve quantitative agreement (typically within $\sim 5\%$). This agreement serves as an action-reaction consistency check.

The convergence behavior of the cumulative vertical electrostatic force also provides a basis for estimating the influence of probe parts not explicitly included in

the present model, such as the macroscopic sensor body and the transition region between the modeled hyperbolic tip and the sensor body. In the present calculations, the hyperbolic metallic tip is included within a computational domain extending in the z direction to approximately $18\text{ }\mu\text{m}$ from the apex, where the cumulative vertical electrostatic force is already close to saturation, as shown in Supplementary Fig. S3. In typical self-sensing force sensor configurations, the metallic parts outside this modeled region are located much farther from the tip-sample junction, typically several hundred micrometers from the apex. Their additional contribution beyond the included computational domain is therefore expected to be small. Moreover, for the FM-KPFM response primarily considered here, such distant contributions are further suppressed because the frequency shift is governed by the force gradient rather than by the absolute force, and can therefore be regarded as negligible.

When the tip-sample separation is sufficiently small compared to the tip radius ($s \ll R$), the near-apex electrostatic response is expected to be governed primarily by local curvature and narrow-gap geometry. Accordingly, in the immediate vicinity of the apex, the pressure profile should approach that of the canonical sphere-plane model [12], for which an analytical solution is available via the method of images [44].

To test this expectation, we compared the pressure distributions calculated by METALTIP with the corresponding analytical sphere-plane solution. For this comparison, the sphere radius and sphere-plane gap were chosen to match the apex curvature and tip-sample separation of the hyperbolic tip geometry. As shown in Fig. 2, the METALTIP results closely follow the sphere-plane profiles on both the tip and sample sides for $r \lesssim 3\text{ nm}$, with deviations below 1.0%. This excellent agreement in the near-apex region supports the validity of the electric-field evaluation and the subsequent Maxwell-stress-based force calculation. In contrast, the logarithmic-scale plot in Supplementary Fig. S4 shows that, at larger r , the sample-side pressure increasingly deviates from the sphere-plane prediction. This discrepancy is naturally attributed to contributions from the tip shank.

C. Bias dependence of electrostatic force

Figure 3 shows the bias dependence of the electrostatic force (F - U curve) calculated with the same geometric parameters as in Fig. 1. The calculated $F(U)$ characteristic is well described by a parabola,

$$F(U) = a(U - U_0)^2 + F_0, \quad (3)$$

where U_0 and F_0 denote the bias and force offsets, respectively. In the present calculation, the tip-sample CPD is set to zero, and only the electrostatic force above a laterally homogeneous surface is considered; accordingly,

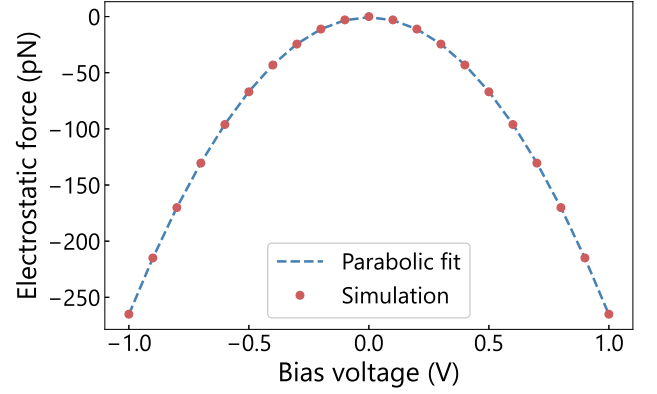


FIG. 3. Bias dependence of the electrostatic force (F - U curve) calculated for the same tip-sample geometry as in Fig. 1. Solid circles denote the calculated values, and the dashed line shows a parabolic fit using Eq. (3).

$U_0 = 0$ and $F_0 = 0$. This parabolic behavior confirms the expected dominant U^2 scaling of the electrostatic force.

As the tip radius R increases, the parabolic curvature parameter a increases monotonically and follows an approximately linear dependence on R over the range examined here (2–100 nm), as quantified in Supplementary Fig. S5. This scaling is consistent with the near-field limit ($s \ll R$) of the semi-analytical sphere-plus-cone model of Hudlet *et al.* [12], which predicts that $a \simeq \pi\epsilon_0(R/s)$. The observed $a(R)$ dependence therefore further supports the validity of the force calculation.

D. Conversion from force to frequency shift

In FM-AFM and KPFM, the experimentally accessible observable is the resonance-frequency shift of the oscillating force sensor rather than the force itself. The z component of the tip-sample force, F_z , can be converted into the resonance-frequency shift Δf using the standard expression [45, 46],

$$\Delta f(z_0) = -\frac{f_0}{kA^2} \langle F_z(z_0 + q(t)) q(t) \rangle, \quad (4)$$

where A , f_0 , and k are the oscillation amplitude, resonance frequency, and spring constant of the force sensor, respectively, and z_0 denotes the mean tip position. The tip deflection during one oscillation cycle is given by $q(t) = A \cos(2\pi f_0 t)$, and $\langle \dots \rangle$ denotes the average over one oscillation period. In the implementation, this cycle average is evaluated by sampling $F_z(z)$ at discrete tip positions along the oscillation trajectory and calculating the corresponding weighted average.

One motivation for developing METALTIP is to quantitatively simulate KPFM under experimental conditions aimed at high spatial resolution. In this regime,

KPFM is often performed in UHV using sharp metallic tips mounted on self-sensing force sensors [37, 38]. In such measurements, the tip-sample separation is frequently regulated in STM mode using the averaged tunneling current (I) as the feedback signal. Accordingly, in simulations of FM-mode experiments, the tip-sample separation s determined by STM feedback under static conditions (i.e., with the tip oscillation switched off) was used as an input parameter. For electrostatic calculations under oscillating conditions, s was converted into the mean tip-sample distance $\langle s \rangle$ by taking into account the oscillation amplitude and the tunneling-current decay constant κ . Assuming $I \propto \exp(-2\kappa s)$, the conversion is given by $\langle s \rangle = s + (2\kappa)^{-1} \ln[I_0(2\kappa A)]$, where I_0 is the modified Bessel function of the first kind (see Supplementary Note I for the detailed derivation). In the present analysis, we used $\kappa = 11.2 \text{ nm}^{-1}$, as experimentally determined from the distance dependence of the tunneling current. Hereafter, s refers to the nominal input separation defined by the static STM setpoint and should be distinguished from $\langle s \rangle$.

Supplementary Fig. S6 shows the Δf - U curve calculated using the same geometric parameters as those in Fig. 3. The parameters $f_0 = 30 \text{ kHz}$ and $A = 500 \text{ pm}$ were chosen to represent typical experimental conditions, while k was set to the nominal design value of the qPlus sensor (1852 N/m for our sensors). As for the F - U curves, the calculated Δf - U curve is well described by a parabola. The resulting frequency-shift values also fall within the range typically observed experimentally.

E. 3D simulation of CPD profiles for a laterally inhomogeneous surface

The 3D implementation of METALTIP allows arbitrary surface-potential distributions to be prescribed and can therefore be applied to laterally inhomogeneous samples. As the simplest demonstration, we considered a surface consisting of two regions with different surface potentials, separated by a straight boundary passing through the origin. The potential difference between the two regions was set to 0.5 V. To avoid an unphysical discontinuity on the numerical grid, the potential contrast was introduced not as an ideal step function, but as a smooth interpolation described by a hyperbolic tangent function with the interfacial width parameter $w_{\text{interface}} = 1.0 \text{ nm}$ (see Supplementary Fig. S7). The tip-sample geometry parameters were set to $R = 5.0 \text{ nm}$, $s = 1.0 \text{ nm}$, and $\alpha = 10^\circ$.

The interfacial width parameter $w_{\text{interface}}$ was introduced as a numerical regularization parameter, rather than as a physical length representing the intrinsic transition width of the surface potential at a particular boundary. A mathematically discontinuous surface-potential step produces an artificial singularity on the numerical grid, whereas the actual electrostatic potential near an interface is expected to vary over a finite atomic-scale

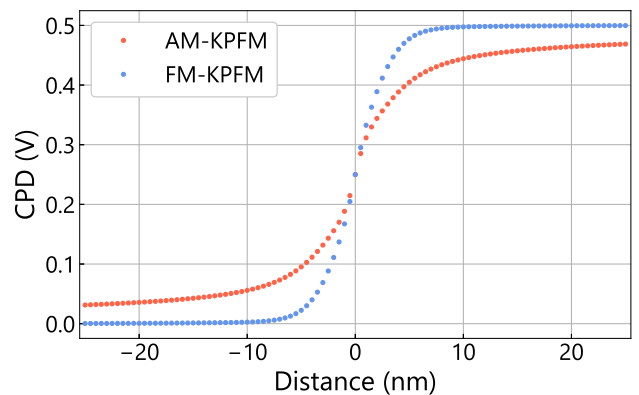


FIG. 4. Simulated CPD profiles across a lateral surface-potential boundary for a two-region model surface with a potential difference of 0.5 V. The calculations were performed with $R = 5.0 \text{ nm}$, $s = 1.0 \text{ nm}$, and $\alpha = 10^\circ$. The CPD profiles were extracted by parabolic fitting of simulated F - U and Δf - U spectra at each lateral tip position, corresponding to AM- and FM-KPFM, respectively. Here, $x = 0$ corresponds to the interface.

length because of charge redistribution and screening. We therefore used $w_{\text{interface}} = 1.0 \text{ nm}$ as a practical smoothing width: it is larger than the expected atomic-scale screening length and the local grid spacing near the interface, but still small compared with the several-nanometer CPD broadening caused by the finite tip size.

Using this prescribed surface-potential distribution, the tip was scanned laterally across the interface, and at each position the corresponding F - U and Δf - U curves were calculated. CPD profiles were then obtained by parabolic fitting of the simulated spectra at each lateral position. The profiles extracted from the F - U and Δf - U curves correspond to the responses measured in AM- and FM-KPFM, respectively. Figure 4 presents the resulting CPD profiles. The calculated profiles clearly show that the FM-mode signal yields a sharper transition across the interface. This reflects the stronger weighting of the tip-apex contribution in the frequency-shift signal [23] and is consistent with the higher spatial resolution generally achieved in FM-KPFM [21].

F. Fitting to experimental data and parameter extraction

Fitting the experimental data serves three purposes: (i) externally validating the numerical framework under realistic operating conditions, (ii) enabling quantitative interpretation of the experimental data, and (iii) extracting key parameters that are otherwise difficult to access, such as the electrically effective tip radius and tip-sample separation. In this context, the electrically effective tip radius denotes the radius parameter of the ideal hyperbolic metallic tip that reproduces the mea-

sured electrostatic response, including the CPD-profile broadening and the Δf - U curvature. This value may differ from the geometric tip radius estimated from SEM images, because the actual tip shape can deviate from the ideal hyperbolic geometry and the electrostatic interaction reflects the conducting surface contour over a finite region around the apex rather than only the local apex curvature.

The third objective, parameter extraction, is not generally straightforward because electrostatic observables often depend on multiple geometric parameters in a strongly correlated manner. Fitting a single dataset alone therefore does not necessarily yield a unique parameter set. Here, we address this identifiability issue by combining two complementary measurements acquired with the same tip: a CPD line profile across a heterogeneous interface and a Δf - U spectrum measured on a laterally homogeneous metallic surface.

1. SEM-based evaluation of tip geometry

In this study, we used commercially available electrochemically etched W tips (Unisoku). To characterize the statistical variation in tip geometry, we extracted the geometric parameters (R and α) from SEM images. The tip radius spanned approximately 5–30 nm, and more than half of the tips exhibited $R < 10$ nm. The full shank opening angle ranged from 5° to 20° , with most tips showing values below 10° .

For many tips, the outer profile could be fitted well by a single hyperbolic curve over an axial range of several hundred nanometers from the apex, as exemplified in Supplementary Fig. S8(a). In contrast, some SEM profiles could not be reproduced over the entire fitting window (from the near-apex region to the shank) by a single hyperbolic curve (Supplementary Fig. S8(b)). In the hyperbolic parametrization, R and α are not independent: for a fixed R , decreasing α substantially increases the axial length scale over which the profile approaches its asymptotic shank taper. Consequently, for tips whose shank narrows more rapidly (i.e., becomes nearly conical close to the apex), the full SEM profile cannot be captured within the fitting window by a single hyperbolic curve, even when α is reduced to the smallest practical value.

We expect this residual mismatch to have only a limited impact on the electrostatic response, because the near-apex region (which dominates the electrostatic interaction for sharp metallic tips) is still reproduced reasonably well, whereas the contribution from the more distant shank region is comparatively weak. In addition, over the tip-radius range considered here (2–20 nm), the frequency shift signals changed only marginally when α was reduced below 10° , as shown in Supplementary Fig. S9. Based on these findings, we fixed the opening angle at $\alpha = 10^\circ$ in all simulations used for fitting throughout this work.

Another reason for fixing α at 10° is the computational cost associated with smaller opening angles. For smaller opening angles, the hyperbolic coordinate grid becomes increasingly elongated near the tip surface, and a substantially finer grid is required to maintain good consistency between the tip-side and sample-side force evaluations. This requirement becomes particularly demanding in the 3D implementation, where the computational cost increases rapidly with grid density. Therefore, using $\alpha = 10^\circ$ provides a practical compromise: it is consistent with the SEM-based estimate and the weak α dependence of the frequency-shift response, while avoiding the excessive computational cost associated with smaller opening angles in the 3D calculations.

2. Fitting to CPD profile

To compare the 3D simulation with experiment, we considered the sharp surface-potential-step model introduced in Section IV E. As an experimental test sample, we employed a Cu(111) surface partially covered with an ultrathin NaCl overlayer [35], for which the CPD changes abruptly at the NaCl/Cu(111) interface [36]. The measurements were performed across the interface between a two-monolayer-thick NaCl film and the Cu(111) substrate [47]. The blue curve in Fig. 5 shows an experimental CPD profile, in which the CPD changes by approximately 0.85 V across the interface. The sensor resonance frequency and oscillation amplitude were 30.0 kHz and 510 pm, respectively. An STM topographic image of the measured region is provided in Supplementary Fig. S10.

In the simulation, the potential difference between the two regions was fixed to the experimentally determined value. For simplicity, the topographic height difference between the Cu and NaCl regions was neglected, and the sample surface was treated as geometrically flat. The influence of this approximation is discussed at the end of this section. The solid circles in Fig. 5 show the simulated profile fitted to the experimental data. In the fitting, the shank opening angle was fixed at $\alpha = 10^\circ$, while R and s were varied. The dashed vertical line marks the interface position in the simulation, which coincides with the onset of the NaCl-island topographic rise (green curve). Reasonable agreement was obtained for $R = 3.0$ nm and $s = 0.9$ nm. A small deviation is visible near the onset of the Cu-to-NaCl transition, which may reflect the neglect of the topographic height difference between the Cu and NaCl regions in the present flat-surface model, a slight deviation of the actual tip shape from the ideal hyperbolic shape assumed in the model, or both.

The width of the Cu-to-NaCl transition region depended strongly on R , becoming narrower for sharper tips (Supplementary Fig. S11). In contrast, varying s within the physically reasonable range for STM-mode regulation (0.7–1.0 nm) produced no appreciable change in the CPD-profile shape (Supplementary Fig. S12). Similarly, varying the shank opening angle over the range

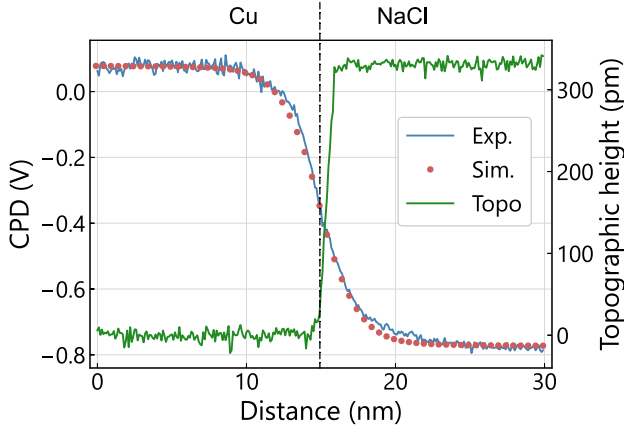


FIG. 5. Experimental CPD profile across a NaCl/Cu(111) interface (blue curve), together with the fitted simulated profile (red circles) and the corresponding topographic line profile (green curve). The dashed vertical line indicates the interface position used in the simulation. Reasonable agreement was obtained for $R = 3.0$ nm and $s = 0.9$ nm.

$\alpha = 5^\circ\text{--}20^\circ$ produced only a minor change in the CPD-profile width (Supplementary Fig. S13). These results indicate that, within the small-separation regime considered here, R is the primary parameter governing the interfacial broadening.

To estimate the robustness of the extracted tip radius, we performed a residual-based sensitivity analysis based on the root-mean-square error (RMSE) between the experimental and simulated CPD profiles. The RMSE showed a shallow minimum around $R = 2.5\text{--}3.0$ nm, as shown in Supplementary Fig. S14. When parameter sets with RMSE values within 20% of the minimum were regarded as acceptable, the CPD profile was consistent with $R \approx 2.0\text{--}4.0$ nm.

These results demonstrate that the transition width of a CPD profile across a potential-step interface can be used to constrain the electrically effective tip radius *in situ*. The representative value of $R = 3.0$ nm extracted from this CPD-profile fitting was then used as a fixed input parameter in an independent validation of the model by fitting the $\Delta f\text{--}U$ response measured on the Cu region.

We also assessed the possible influence of the approximately 320 pm apparent topographic height difference between the Cu(111) terrace and the 2 ML NaCl island, which was neglected in the flat-surface model. Because the present 3D implementation assumes a geometrically flat sample surface, explicitly treating the non-flat boundary geometry would require a substantial extension of the code. As a practical sensitivity test, we therefore performed an additional flat-surface simulation in which the tip-sample separation was increased by 320 pm (Supplementary Fig. S15). This calculation does not explicitly model the topographic step itself, but evaluates the separation-related effect associated with the measured height difference. The resulting CPD profile differed only

slightly from the original calculation, indicating that this effect is unlikely to substantially affect the CPD-profile broadening or the extracted effective tip-radius range.

3. Fitting to $\Delta f\text{--}U$ curve

Figure 6 shows the experimental $\Delta f\text{--}U$ curve analyzed here, together with a representative METALTIP fit. The spectrum was extracted from the same dataset used for the CPD-profile analysis, specifically from a Cu region where the CPD profile was flat and the influence of the NaCl/Cu(111) interface was negligible. Accordingly, this analysis was carried out using the 2D implementation of METALTIP. In the simulation, the tip radius was fixed at $R = 3.0$ nm, as determined from the CPD-profile fitting, and only the tip-sample separation was varied. Good agreement was obtained for a representative value of $s = 0.91$ nm, which lies within the physically reasonable range expected for STM-mode operation (0.7–1.0 nm) [48].

To quantify the sensitivity of the $\Delta f\text{--}U$ fitting to the tip-sample separation s , we evaluated the RMSE between the experimental and simulated curves as a function of s (Supplementary Fig. S16). The RMSE showed a clear minimum around $s = 0.91\text{--}0.92$ nm, with nearly identical values at these two separations. When parameter sets with RMSE values within 20% of the minimum were regarded as acceptable, the experimental $\Delta f\text{--}U$ curve was consistent with $s \approx 0.90\text{--}0.93$ nm. This range should be regarded as the sensitivity of the fit under the assumed model parameters, rather than as an absolute uncertainty bound on s . The absolute uncertainty range is likely larger than this estimate, because it is affected by systematic factors that are not fully captured in the present sensitivity analysis. These include the uncertainty in the electrically effective tip radius, possible deviations of the actual tip shape from the ideal hyperbolic model, and calibration uncertainties in the sensor parameters such as k and A .

Importantly, the representative fitted separation lies within the physically reasonable range expected for STM-mode regulation, and the experimental magnitude of the $\Delta f\text{--}U$ curve was reproduced without any arbitrary proportionality factor or unphysical mechanical parameters. The spring constant k was set to the nominal design value of the sensor, while the resonance frequency f_0 and oscillation amplitude A were taken directly from the experimental settings. The conversion from force to Δf was performed consistently using the established FM-AFM expression. This scale-free agreement supports not only the validity but also the high quantitative accuracy of the overall framework, including the electric-field evaluation, electrostatic-force calculation, and force-to- Δf conversion.

We performed the same combined analysis for several different tips. In many cases, the CPD profiles were well reproduced with effective tip radii in the range

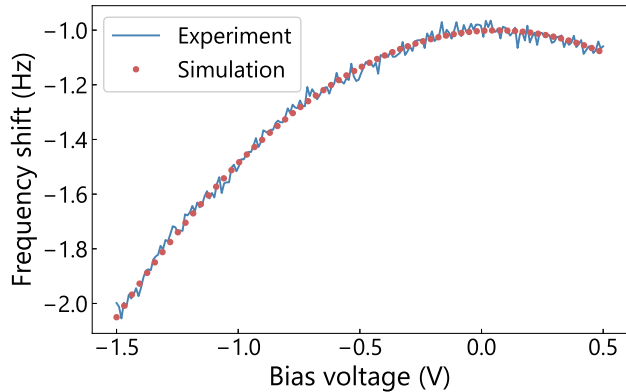


FIG. 6. Experimental Δf - U curve measured on a Cu(111) terrace (blue line) and a representative METALTIP fit (red circles). In the simulation, $\alpha = 10^\circ$ and $R = 3.0$ nm (from the CPD-profile fitting) were fixed, and the agreement shown was obtained at $s = 0.91$ nm.

of $R = 2$ –14 nm, and the corresponding Δf - U fitting yielded tip-sample separations of $s = 0.8$ –0.9 nm. In some cases, however, keeping s within a physically reasonable range ($s = 0.7$ –1.0 nm) required the tip radius used in the Δf - U fitting to differ by a few nanometers from the value obtained from the CPD-profile fitting. This tendency may indicate that the actual tip geometry deviates from the ideal hyperbolic geometry assumed in the model. We also found tips for which the CPD profile showed a sharp transition at the interface but did not become fully flat even in regions sufficiently far from the boundary (Supplementary Fig. S17). Such behavior may reflect an actual tip geometry that remains relatively sharp near the apex but becomes broader away from the apex than assumed in the ideal hyperbolic model.

Finally, we discuss a simple strategy for tip-parameter extraction using METALTIP. Under STM-mode distance regulation, the variation in s is expected to be limited as long as the same setpoint is used. Moreover, for tips fabricated by the same procedure, the variation in the shank opening angle is also expected to be relatively small. These considerations suggest that, by acquiring a Δf - U curve on a clean metallic surface at a fixed STM setpoint and fitting it with the 2D METALTIP model while treating R as the primary fitting parameter, the electrically effective tip radius can be evaluated *in situ* under experimental conditions.

V. SUMMARY

We developed a numerical software package for computing electrostatic interactions between a hyperbolic metallic tip and a conducting surface under AFM/KPFM-relevant conditions. This code enables direct simulation of the bias-dependent force and frequency-shift responses, $F(U)$ and $\Delta f(U)$. In addition, the full 3D implementation treats spatially varying surface potentials and reproduces CPD profiles across inhomogeneous interfaces. We validated the numerical framework by benchmarking against established theoretical models, confirming the expected scaling behavior and correct near-field limiting behavior. Using representative experimental datasets, we further demonstrated quantitative fitting without arbitrary scale factors, reproducing both CPD profiles across a potential-step interface and Δf - U spectra on a homogeneous metal surface. Combining these complementary observables provides stronger constraints on key experimental parameters—including the tip-sample separation and electrically effective tip radius—than fitting either dataset alone, and thereby enables *in situ* parameter identification with high quantitative accuracy. These results establish METALTIP as a practical platform for extracting key experimental parameters, enabling quantitative interpretation of KPFM data, analyzing contrast formation and measurement characteristics, and testing emerging KPFM measurement schemes under realistic tip-sample geometries.

SUPPLEMENTARY MATERIAL

See the supplementary material for additional numerical details, sample preparation, supplementary figures, and supporting analyses, including the numerical implementation of METALTIP, simulated surface-potential profiles, parameter-dependence plots, representative scanning electron microscopy images of the tips, and additional CPD profiles.

DATA AVAILABILITY STATEMENT

The METALTIP source code is publicly available on GitHub at <https://github.com/nobuyuki-ishidanim/metalip>. The data that support the findings of this study are available from the corresponding author upon reasonable request.

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