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Calculation Method for the Geometric Dimensions of a Scanning Near-Field Optical Microscope Optical Fiber Probe and Experimental Verification

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Keywords: SNOM, optical fiber probe, simulative measurement, geometric dimension

ABSTRACT

This study proposes an innovative calculation method for the geometric dimensions of a scanning near-field optical microscope (SNOM) optical fiber probe. We employ molecular mechanics and vibration theory to construct a simulative measuring model of a SNOM. We use a complex Boolean operation to arrange the probe and the sample atom-by-atom and then establish an atomic model for the simulative measuring model of SNOM. We conduct a scanning electron microscopy (SEM) photographing experiment to measure the geometric dimensions of the probe and then draw a relational diagram of the geometric dimensions and deduce their relational equations. We also find the potential energy parameter values of the Morse potential energy model among different atoms in order to solve the problem of the unknown potential energy parameter value by using the Lorenz—Berthelot mixing rule. We combine the optimal search of the Levenberg—Marquardt method with a reasonable convergence criterion to acquire the optimal geometric dimensions. In addition, a SNOM optical fiber probe is used to compare the results of the experimental and simulative measurements.

INTRODUCTION

In a measurement conducted using a scanning near-field optical microscope (SNOM), the geometric dimensions of the optical fiber probe, including the aperture and end protrusion sizes, the thickness of aluminum coating, and the bevel angle of the probe, have a significant effect. Currently, the analysis of SNOM measurement is extremely difficult, and the geometric dimensions of the optical fiber probe cannot be easily obtained. To confirm these geometric dimensions, researchers currently use a scanning electron microscope (SEM); however, this method results in the destruction of the fiber probe, rendering it unusable. To solve this problem, this study combines a theoretical model and an SEM experiment to develop a nondestructive method for calculating the geometric dimensions of the optical fiber probe.

Binning et al. (1982) conducted micro displacement scanning using an extremely small probe to sense the changing physical field of the sample and then drew the profile and 3D map of the sample surface. Pohl et al.(1984) completed the development of the first SNOM. A metal film-coated optical fiber probe with a sharp and fine aperture at its end was used as the probe, and the transverse amplitude of the quartz tuning fork of a simple harmonic vibration was used as the feedback signal. In an analytical study of the optical fiber probe, Novotny et al. (1994) used the multiple multipole method to calculate the near-field light intensity distribution and found that the aperture and shape of the metal film-coated probe affected the luminous flux efficiency and light decay rate. Therefore, it was concluded that aperture and shape are important characteristics of an optical fiber probe and affect SNOM measurement. Karrai and Grober (1995) analyzed the oscillation phenomenon when an optical fiber probe was fixed on the tuning fork, and then proposed a theoretical analysis model for the probe’s vibration. Cortes et al. (2014) designed and constructed a collection-mode scanning near-field microwave microscope using electronics and software, and demonstrated its operability. In their study, a collection-mode near-field microscope was demonstrated using a 10.56 GHz (X-band) frequency illumination. Imaging of a standing evanescent microwave was experimentally used to evaluate the

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capabilities of the microscope.

While solving an inverse problem in the engineering field, an unknown situation is first assumed in the analysis process, and the finite element method or finite difference method is then used to solve the problem by obtaining a set of numerical solutions. Huang et al. (1992) used the conjugate gradient method to inversely calculate the unknown contact conductive value during metal casting. Schnur and Zabaras (1992) applied the concept of the Levenberg—Marquardt method to inversely calculate the material characteristics of an elastic material and its material interface. Balan et al. (1998) used the quasi-Newton method to inversely determine the optimal shape of the cast pre-formed forging die. Chang and Weng (1999) applied an inverse solution to predict the moisture content distribution in a material, which cannot be easily measured. Lin et al. (2000) applied the inverse problem of engineering to solve the heat conduction problem. As for the application to the manufacturing problem, Romanov (2003) explored an inverse problem of laminated elastic plates. Lin and Chen (2004) took the load of the experimental measurement as the criterion and inversely solved the change in the friction coefficient in a rough forging process. Lin and Chen (2005) considered the experimental processing load as the foundation and combined the analytical Levenberg—Marquardt method with the finite element model of a thermo-elastic-plastic large deformation of metal forming, inversely acquiring the changing process of the friction coefficient of the contact surface between the rough forging sample and the mold.

Unlike the abovementioned studies, this study provided an innovative nondestructive method for finding solutions for the aperture and end protrusion sizes, thickness of the Al coating, and bevel angle of the optical fiber probe.

As mentioned, in an SEM measurement, the electrical conductivity of the optical fiber probe is poor. Thus, it is always required to be sputtered with a silver or gold conductive layer and separated from the tuning fork. Consequently, the SNOM optical fiber probe is destructed, and is rendered unusable. To address this problem, this study combines the measuring experiment of SNOM with its simulative measuring model, and proposes a nondestructive calculation method by innovatively applying the measurement of a ladder standard sample. Thus, the solutions for significant geometric dimensions, including the aperture size, end protrusion size, thickness of the Al coating, and bevel angle of the probe, can be obtained. This study first follows the results of the SEM experiment conducted to derive the relational diagram and equations of the geometric dimensions of a real Al-coated SNOM optical fiber probe with a silicon (Si)-made optical fiber. It then proposes the use of a complex Boolean operation and the concept of cutting-off radius to employ an accurate and workable simplification for decreasing the number of atoms substantially. The Al-coated SiO_2 SNOM optical fiber probe arranged by atoms and the ladder standard sample are used, establishing an atomic model for the simulative measuring model of SNOM.

The Lorenz—Berthelot mixing rule is also used to solve the problem of Morse potential energy parameters among different atoms. Morse force is used to calculate the interaction between atoms of the probe and the sample. We correct the vibration equation of the SNOM optical fiber probe developed by Novotny et al. (1994) which does not consider Morse force, and further develops a . simulative measuring model of SNOM for analyzing the effects of the geometric dimensions of the optical fiber probe on SNOM measurement. Focusing on the ladder standard sample, we first find the error between the sample plane’s shape acquired in the SNOM experiment by using two optical fiber probes and that acquired in the SNOM simulative measurement. This error is squared, multiplied by 1/2, and then added the inverse Barrier function to it to obtain the inverse solutions for the target function values of the geometric dimensions of the optical fiber probe. We combine the optimal search of the Levenberg—Marquardt method with a reasonable convergence criterion, and then conduct an SEM experiment to derive the relational diagram and equations of the geometric dimensions of the SNOM optical fiber probe, establishing a nondestructive calculation method and procedures for determining these dimensions; the optical fiber probe is used to confirm the feasibility of the calculation method and procedures. This study can also address the existing disadvantage that the optical fiber probe is destructed before acquiring its geometric dimensions from the SEM experiment. Thus, we provide an innovative nondestructive method for finding the solutions for the geometric dimensions of the optical fiber probe.

CONSTRUCTION of A SINULATIVE MEASURING MODEL OF AL-SiO_2/Si-SNOM

This study uses an optical fiber probe with Al coated externally and a SiO_2 optical fiber material used in the middle layer. It is a tuning-fork SNOM optical fiber probe of 1640-00 model manufactured by Veeco Instruments Inc. (2002), as shown in Fig. 1. In addition, we use a Si-made TGZO1 ladder standard sample manufactured by NT-MDT Company (2003), as shown in Fig. 2. The optical fiber probe and the ladder standard sample are used to establish a simulative measuring model of Al-SiO_2/Si-SNOM and conduct SNOM experiment. According to the selected SNOM optical fiber probe, a measuring experiment of the SNOM ladder standard sample is carried out. Through the shape of the optical fiber probe acquired in the

SEM experiment, a relational equation of the geometric dimensions of the SNOM optical fiber probe is deduced. We propose the use of a complex Boolean operation and the concept of cutting-off radius r_c to establish an atomic model for the simulative measuring model of SNOM, and use the Lorenz—Berthelot mixing rule to find the Morse potential energy parameter values among different atoms, after completing the development of the simulative measuring model of Al-SiO_2/Si-SNOM. The dimensions of the optical fiber probe acquired in the SEM measuring experiment are substituted in the simulative measuring model of Al-SiO_2/Si-SNOM. From the difference between the results of the experiment and the simulation, the simulative measuring model of Al-SiO_2/Si-SNOM is considered reasonable. Using the geometric dimensions of different optical fiber probes and through the established simulative measuring model of Al-SiO_2/Si-SNOM, simulative measurement is performed to analyze the effects of these geometric dimensions on the surface profile.

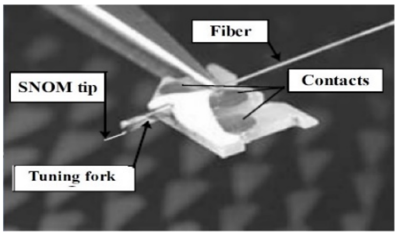
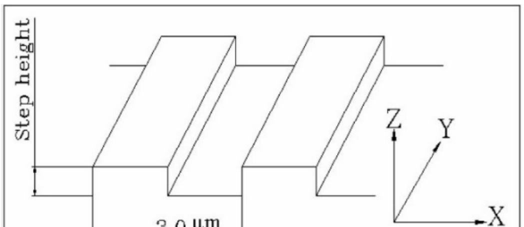


Fig. 1. Veeco's tuning-fork SNOM optical fiber probe of 1640-00 model



Part number	Step height	Accuracy	Pitch*
TGZ01	20..25nm	±1nm	3.0μm
TGZ02	90..104nm	±1.5nm	3.0μm
TGZ03	496..503nm	±1%	3.0μm
TGZ04	1000nm	±1%	3.0μm
TGZ11	1500nm	±1%	10.0μm

Active area........3×3mm(all models)
Chip dimensions.......5×5×0.45mm(all models)

Fig. 2. TGZ01 ladder standard sample

THEORETICAL MODEL FOR THE SIMULATIVE MEASURING MODEL of Al-SiO_2/Si-SNOM

Through the SEM experiment, we acquire the shape of the optical fiber probe, derive the relational equations of the geometric dimensions of the probe, and propose the use of subtraction (SUB) operation and the concept of cutting-off radius. SiO_2 atoms are arranged to form the central spindle of the optical fiber probe, Al atoms are arranged to form the Al coating of the probe, and Si atoms are used to arrange the TGZ01 ladder standard sample, thus establishing the atomic model for the simulative measuring model of Al-SiO_2/Si-SNOM. Then, the Lorenz—Berthelot mixing rule is applied to determine the Morse potential energy parameters among different atoms. In addition, Morse force is used to calculate the interaction between the probe and sample atoms. We correct the vibration theory of the optical fiber probe proposed by Novotny et al. (1994) in order to analyze the relationship between the tip-sample interaction and amplitude of the probe, deduce the amplitude equation of the simulative measuring model of Al-SiO_2/Si-SNOM constructed by Al-SiO_2/Si, and then establish the simulative measuring model of Al-SiO_2/Si-SNOM. The related theoretical model is explained herein.

Relational Equations of the Geometric Dimensions of the Optical Fiber Probe

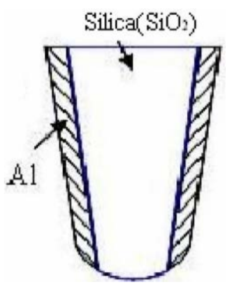
According to the SNOM tuning-fork optical fiber probe of 1640-00 model manufactured by Veeco Instruments Inc. (2002) and the TGZO1 ladder standard sample manufactured by NT-MDT Company (2003), this study establishes a simulative measuring model of Al-$Si0_2$/Si-SNOM. Through the SEM experiment, we first find out the geometric dimensions of the SNOM optical fiber probe, which include (a) the aperture of the probe (S), (b) the end protrusion size of the probe tip (h), (c) the thickness of the Al coating (t), and (d) the bevel angle (θ). Then, we draw a relational diagram of the geometric dimensions of the real Al-coated and Si-made SNOM optical fiber probes, as shown in Fig. 3(a) and (b), and derive their relational equations [Eqs. (1)-(3)].

$$S=f_1(R,h)=2\sqrt{2Rh-h^2} \tag{1}$$

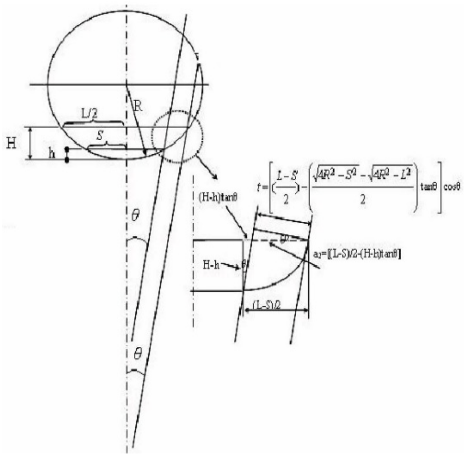
$$h=f_2(R,S)=\frac{2R-\sqrt{4R^2-S^2}}{2} \tag{2}$$

$$t=f_3(L,S,R,\theta)=\left[\left(\frac{L-S}{2}\right)-\left(\frac{\sqrt{4R^2-S^2}-\sqrt{4R^2-L^2}}{2}\right)\tan\theta\right]\cos\theta \tag{3}$$

where R denotes the arc radius of the probe shape, S denotes the aperture of the probe, L denotes the chord length measured from the probe shape, h denotes the Si protruding height at the probe tip, t denotes the thickness of the Al coating, and θ denotes the gradient.



(a). Cross-sectional view of the optical fiber probe



(b). Magnified view and interrelationship among the geometric dimensions of the SNOM probe

Fig. 3. Schematic of the geometric dimensions of the SNOM optical fiber probe

Atomic Model

According to the dimensions obtained by SEM, we propose the use of a complex Boolean operation and the concept of cutting-off radius r_c, to employ an accurate and workable simplification method for decreasing the number of atoms substantially, and then establish an atomic model for the simulative measuring model of SNOM. AI atoms are used to arrange and form the atomic model of the optical fiber probe cone, $FCC_{tip}(a_{AI})$, and SiO_2 atoms form the central spindle cone of the optical fiber probe, $SiO_{2\_tip}(a_{si}/ox.)$. According to the bevel angle and cutting-off radius of the optical fiber probe, the SUB operation and union (UNI) operation are conducted, cutting and forming the atomic model AM, with the required correct dimensions of the optical fiber probe, as shown in Eq. (4). On the other hand, Si atoms are used to arrange and form an atomic model of a large hexahedral sample, $DC_{sample}(a_{si})$. Based on the set cutting-off radius, the SUB operation is conducted, cutting the atomic model AM_{sample} with the required correct dimensions of the standard sample, as shown in Eq. (5).

$$AM_{tip} = UNION(SUBTRACTION(FCC_{tip}(a_{AI}) - R_{C\_AI}(a_{AI})) + SIO_{2\_tip}(a_{si/ox})) \qquad (4)$$

where a_{AI} is the lattice constant of Al atom, $a_{si/ox.}$ is the lattice constant of Si or O atom, $FCC_{tip}(a_{AI}))$ is the atomic model for the conic Al-coating part of the optical fiber probe, $R_{c_AI}(a_{AI})$shows that the atomic model for the conical Al-coating part of the optical fiber probe is greater than the atomic model encircled by the cutting-off radius, and SiO_{2_tip}, $(a_{si/ox})$ is the atomic model for the conic central spindle part of the optical fiber probe.

$$AM_{sample}= SUBTRACTION(SUBTRACTION(Si_{sample}(a_{si})- R_{c\_si}(a_{si})) \qquad (5)$$

where a_{si} is the lattice constant of a Si atom, $Si_{sample}(a_{si})$ is the atomic model of the large hexahedral sample, and $R_{c\_si}(a_{si})$ is the atomic model of the sample greater than that encircled by the cutting-off radius, which is shown as a solid in Fig. 4.

Per the aforementioned relational equations of the geometric dimensions, we draw the geometric shape of the Al-coated SNOM optical fiber probe with the SiO_2-made optical fiber, as shown in Fig. 3(a). Fig. 4(a) shows the atomic model of the real Al-coated and the Si-made SNOM optical fiber probes. Fig. 4(b) shows the atomic model of the TGZO1 ladder standard sample arranged by Si atoms. Furthermore, the atomic models of the optical fiber probe and the ladder standard sample are adjusted to the corresponding positions for simulation, completing the development of the atomic model required for the established simulative measuring model of Al-SiO_2/Si SNOM, as shown in Fig. 4(c) and exploring the SNOM simulative measurement. During the simulation in this study, the dimensional profiles of the SNOM optical fiber probe and the standard sample are arranged by atoms. To save the simulation time, we take 29 nm as the length of the SNOM optical fiber probe and 25.5 nm + r_c, as the height of the sample. The atoms exceeding the cutting-off radius r_c, are removed to carry out the arrangement of the atoms in the SNOM optical fiber probe.

Potential Energy Function and Morse Parameter Value

We employ the Morse potential energy function of two-body potential energy to describe the interatomic interaction. The Morse potential energy function is mostly applied to the simulation of solids and metals (Rieth,2003). Since its calculation results are identical to many experimental results and are suitable for describing the interatomic interaction of solids, we use this function to analyze the tip-sample interaction and the relation between them. The Morse potential energy function is defined as follows (Rieth, 2003):

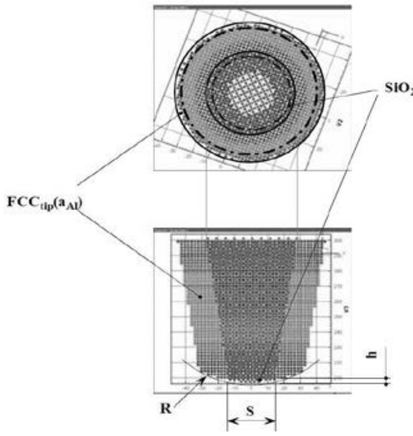
$$\emptyset(r) = D \cdot \left\{e^{-2\alpha(r-r_0)} - 2 \cdot e^{-\alpha(r-r_0)}\right\} \qquad (6)$$

where D is the cohesion energy, α is the material parameter, r is the interatomic distance, and r_0 is the equilibrium distance.

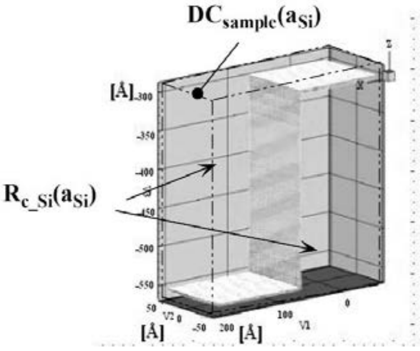
The interatomic interaction is defined as follows:

$$F(r) = \frac{\partial\emptyset(r)}{\partial r} = -D(-2\alpha e^{-2\alpha(r-r_0)} + 2\alpha e^{-\alpha(r-r_0)}) \qquad (7)$$

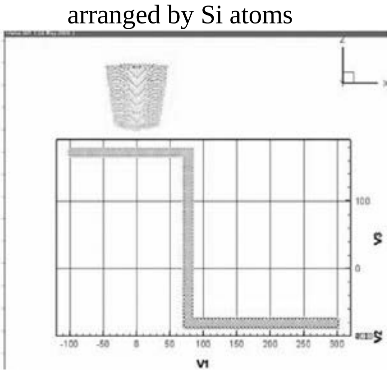
The different parameter values of the Morse potential energy function used in this study are shown in Table 1 (Girifalco and Weizer, 1959; Martin et al, 1986; Peng and McCABE, 2007; Graves and Brault, 2008). The molecular interaction rapidly decreases with an increase in distance γ between molecules. When this distance r exceeds 2.5 times the equilibrium interatomic distance(r_0), the force approaches zero.



(a). Atomic model of optical fiber probe



(b). Atomic model of TGZ01 ladder standard sample arranged by Si atoms



(c) Atomic model of Al-SiO_2/Si SNOM

Fig. 4. Atomic model for simulative measurement model of Al-SiO_2/Si SNOM

Therefore, in defining the distance of a cutting-off radius r_c, when the distance exceedscthe molecule's action force beyond r_c is very small, and hence, need not be calculated. Therefore, the calculation time can be effectively shortened. The relation between the cutting-off radius and the cutting-off potential energy $\emptyset_c(r)$ is given as follows:

$$\emptyset_c(r) = \begin{cases} \emptyset(r), r \leq r_c \\ 0, r > r_c \end{cases} \tag{8}$$

where $\emptyset(r)$ is the potential energy function, $\emptyset_c(r)$ is the cutting-off potential energy, r is interatomic distance, and r_c, is the cutting-off radius. To obtain a near-real situation, three times the value of r_0 is selected as the cutting-off radius to carry out the simulative analysis.

Table 1 Parameter values of the Morse potential energy function of the SNOM simulative measuring model (Girifalco and Weizer, 1959; Martin et al., 1986; Peng and McCABE, 2007; Graves and Brault, 2008)

Parameter	D(J)	$\alpha(10^{10}m^{-1})$	$r_0(10^{-10}m)$
Al- Al	4.330×10^{-20}	1.1646	3.253
Si-Si	4.8573×10^{-19}	0.7891	4.208
O–O	8.202×10^{-19}	0.268	1.208
Al -Si	1.45028×10^{-19}	0.97685	3.69981
Si–O	6.311×10^{-19}	0.52855	2.758

The central spindle body of a real SNOM optical fiber probe is made of SiO_2 , around which Al is coated. The TGZO1 ladder standard sample is made of Si. Therefore, during the SNOM simulative measurement, the interrelationship between the SiO_2 material at the protruding end of the optical fiber probe and the Si material of the ladder standard sample, as well as that between the Al material of the Al coating and Si material of the ladder standard sample, must be considered. We use a real optical fiber probe to simulate the measurement of the ladder standard sample made of Si, as shown in Fig. 5. Moreover, from Table 1, the Al-Al (Girifalco and Weizer, 1959), Si-Si (Martin et al., 1986), and O-O (Peng and McCABE, 2007; Graves and Brault, 2008) potential energy parameter values of Al in the Al coating, SiO_2 in the central spindle, and Si in the TGZ01 ladder standard sample can be determined, respectively.

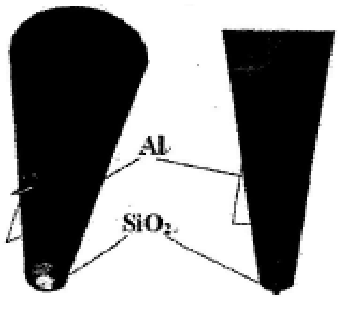


Fig. 5. Schematic of the real Al-coated and Si-made SNOM optical fiber probes

We use the Lorenz—Berthelot mixing rule to determine the Morse potential energy parameters between Si-O and Si- Al, which are taken as the parameter values of the simulative measuring model of the study. It is known that the aperture and protruding end of the optical fiber probe are made of SiO_2, the conical surface of the probe is coated with Al, and the nanoscale ladder standard sample is made of Si. Therefore, for the atomic Morse potential energy function between the Al atoms in the Al coating of the optical fiber probe and the Si atoms in the Si-made nanoscale ladder standard sample, the Morse potential energy functions of Eq. (6) are expressed as Eqs. (9) to (11).

$$\emptyset_{SiAl}(r_{SiAl}) = D_{SiAl}(e^{-2\alpha_{siAl}(r_{SiAl}-r_{0(SiAl)})} - 2e^{-\alpha_{SiAl}(r_{SiAl}-r_{0SiAl})}) \quad (9)$$

$$\emptyset_{Si}(r_{Si}) = D_{Si}(e^{-2\alpha_{Si}(r_{Si}-r_{0Si})} - 2e^{-\alpha_{si}(r_{si}-r_{0Si})}) \quad (10)$$

$$\emptyset_{SiO}(r_{SiO}) = D_{siO}(e^{-2\alpha_{SiO}(r_{SiO}-r_{0SiO})} - 2e^{-\alpha_{SiO}(r_{SiO}-r_{0SiO})}) \quad (11)$$

We use the Lorenz—Berthelot mixing rule to acquire the related parameter values of the Morse potential energy function between the Al coating of the Si-made optical fiber probe and the Si-made nanoscale ladder standard sample, as shown in Eqs. (12)-(17). The parameter values of the Morse potential energy function between Si-Al and Si-O are shown in Table 1

$$D_{SiAl} = \sqrt{D_{Si}D_{Al}} \quad (12)$$

$$D_{SiO} = \sqrt{D_{si}D_{OX}} \quad (13)$$

where D_{Al}, is the size of the Al-Al Morse cohesion energy, D_{Si} is the size of the Si-Si Morse cohesion energy, D_{OX}, is the size of the O-O Morse cohesion energy, D_{SiO} is the size of the Si-O Morse cohesion energy, and D_{siAl} is the size of the Al-Si Morse cohesion energy.

$$\alpha_{SiAl} = \frac{1}{2}(\alpha_{Si} + \alpha_{Al}) \quad (14)$$

$$\alpha_{SiO} = \frac{1}{2}(\alpha_{Si} + \alpha_{Ox}) \quad (15)$$

where $\propto_{AI}$ the size of the Al-Al Morse material parameter value, $\propto_{SI}$ is the size of the Si-Si Morse material parameter value, $\propto_{OX}$ is the size of the O-O Morse material parameter value, $\propto_{sio}$ is the size of the Si-O Morse material parameter value, and $\propto_{SiAl}$ us the size of the Al-Si Morse material parameter value.

$$r_{SiAl} = \frac{1}{2}(r_{Si} + r_{Al}) \quad (16)$$

$$r_{SiO} = \frac{1}{2}(r_{Si} + r_{Ox}) \quad (17)$$

where r_{AI} is the AI-AI Morse equilibrium radius, r_{OX} is the O-O Morse equilibrium radius, r_{SI} is the Si-Si Morse equilibrium radius, r_{SiAI} is the Al-Si Morse equilibrium radius, and r_{SiO} is the Si-O Morse equilibrium radius.

RESULTS AND DISCUSSIONS

Atomic Force Borne by the Optical Fiber Probe

The sample and probe of the study are both composed of atoms. Under the dimensions of the atom, the two-body potential energy function is used to analyze the tip-sample interaction, correct the vibration theory of optical fiber probe proposed by Karrai et al., and construct an equation for the simulative measuring model of SNOM. First, the Morse potential energy functions of two-body potential energy are expressed as Eq. (6) and Eq. (7). The interaction between the single Al, Si, or O atom of the optical fiber probe made of Al or SiO_2, and the single Si atom of the ladder standard sample made of Si is expressed as $F_{Fact}(r_{((AI,SiorOx.)Si)l})$ as shown in Eq. (18). Therefore, we acquire the total action force, $F_{\emptyset\_Fact}$ on each atom of the probe functioned by other atoms, as shown in Eq. (19).

$$F_{FACT}(r_{pqi}) = 2\alpha_{pqi}D_{pqi}(e^{-2\alpha_{pqi}(r_{pqi}-r_{0pq})} - e^{-\alpha_{pqi}(r_{pqi}-r_{0pq})}) \quad (18)$$

$$F_{\emptyset\_FACT} = \sum_{i=1}^{n} 2\alpha_{pqi}D_{pqi}(e^{-2\alpha_{pqi}(r_{pqi}-r_{0pq})} - e^{-\alpha_{pqi}(r_{pqi}-r_{0pq})}) \quad (19)$$

where p is the Al, Si, or O atom on the optical fiber probe; q is the Si atom on the TGZ01 ladder standard sample; $F_{Fact}(r_{AISii})$ is the atomic force between the Al and Si atoms; $F_{Fact}(r_{SiSii})$ is the atomic force between the Si atoms; and $F_{Fact}(r_{SiO.i})$ is the atomic force between the Si and O atoms.

Mathematical Equation of Probe Vibration for the Simulative Measuring Model of Al-SiO2/Si-SNOM

According to the vibration of the optical fiber probe, we correct the vibration equation of the optical fiber probe borne with driving force used by Karrai et al., which is expressed as Eq. (20). In addition, the measurement of the optical fiber probe is affected by the interatomic Morse force on the ladder standard sample. The vibration equation for the optical fiber probe of the Morse force produced from the atoms is expressed as Eq, (21).

$$M_{eff}\frac{\partial^2 x_1}{\partial t^2} + C\frac{\partial_{x1}}{\partial_t} + \mathrm{k}x_1 = F_d e^{iw_a t} \quad (20)$$

$$M_{eff}\frac{\partial^2 x_2}{\partial t^2} + C\frac{\partial_{x2}}{\partial_t} + \mathrm{k}x_2 = F_{\emptyset\_FACT} \quad (21)$$

where $F_d e^{i\omega_a t}$ is the driving force produced from the vibration of the optical fiber probe driven by a piezoelectric material; $F_{\emptyset\_FACT}$ is the total action force borne by atoms; ω_a is the driving angular frequency of the vibration of the optical fiber probe, being $\omega_a = 2\pi f_a$, with f_a being the driving vibration frequency; x_1 is the amplitude of the optical fiber probe produced from the driving force; x_2 is the amplitude of the optical fiber probe produced from the atoms; *k* is the spring constant of the optical fiber probe; and C is the damping coefficient of the probe. The effective mass M_{eff} is expressed as follows (1994):

$$M_{eff} = 0.2427\rho BHL \quad (22)$$

where ρ is the density of the optical fiber probe, *B* is the width of the tuning fork of the probe, *H* is the thickness of the tuning fork of the probe, and *L* is the length of the tuning fork of the probe.

The amplitude change explored in the study is extremely small, just several nanometers. Compared with the driving force borne by the SNOM optical fiber probe, the Morse force is extremely small. Moreover, the interaction distance between the SNOM optical fiber probe and sample is extremely short, and the Morse force change produced is also not significant. To simplify the calculation and complexity of the system, we assume that the tip—sample interatomic interaction is approximately linear. Hence, through Laplace transforms, the change in the probe amplitude caused by the change in the tip-sample interatomic force can be acquired, Therefore, we propose applying the concept of linear combination to combine the vibration size $x_1(t)$ produced from the force driving the tuning fork, as shown in Eq. (23), with the size of the vibration amplitude $x_2(t)$ produced from the effects of atomic force, as shown in Eq. (24). The thus-established vibration equations are used to conduct the simulative measurement, When the SNOM optical fiber probe is operated by a driving force, a driving amplitude is produced. During simulative measurement, to keep the optical fiber probe at a fixed amplitude value, the probe must be moved to bring it close to the standard sample surface. The corresponding Morse force is made to produce in order to reduce the vibration amplitude of the optical fiber probe and make it reach the set amplitude of the SNOM simulative measurement. We also record the position of the optical fiber probe and draw the surface profile acquired from the simulative measurement of the standard sample.

$$x_1(t) = \frac{F_d}{M_{eff}\sqrt{({\omega_n}^2-{\omega_a}^2)^2+(2\xi\omega_n\omega_a)^2}}(({\omega_n}^2 - {\omega_a}^2)Cos\omega_a t + 2\xi\omega_n\omega_a Sin\omega_a t) \quad (23)$$

$$x_2(t) = \frac{F_{\emptyset\_Fact}}{M_{eff}{\omega_n}^2} + \frac{F_{\emptyset\_Fact}}{M_{eff}{\omega_n}^2}e^{-\xi\omega_n t}\left[\frac{\xi\omega_n}{\omega_d}Sin\omega_d t + Cos\omega_d t\right] \quad (24)$$

According to the geometric dimensions of the optical fiber probe acquired from the SEM experiment, and from the related dimensions of the tuning fork, we obtain the required effective mass M_{eff} and spring constant K. As to the driving force F_d produced from the vibration of the tuning fork driven by piezoelectric material, referring to the study of Karrai and Grober (1995) and the related information of SNOM machines in models AURORA-2 and AURORA-3 manufactured by Veeco Instruments Inc. (2002), F_d and the driving vibration angular frequency ω_a are set, During the simulation, the resonance angular frequency ω_n damping factor ξ , and damping vibration frequency ω_d are set according to the values acquired from the SNOM scanning measurement of the TGZO1 ladder standard sample on AURORA-3. When the SNOM machine conducts scanning measurement of the profile, the maximum resonance amplitude of the optical fiber probe is generally 1 nm (2002). Therefore, during simulative measurement of the standard sample, we take x = 0.98 nm as the resonance amplitude. The aforementioned related parameters are substituted in the derived equation. Through adjustment of the position of the SNOM optical fiber probe, the size of the atomic force $F_{\emptyset\_Fact}$ is changed to achieve the size of the preset fixed amplitude. We record the corresponding positions of the optical fiber probe and the sample in order to draw the surface profile acquired from the simulation.

PROCEDURES FOR CONSTRUCTING THE SIMULATIVE MEASURING MODEL OF Al-SiO2/Si-SNOM

The optical fiber probe used in the study for the SNOM scanning measuring experiment is developed by melt-pulling of SiO_2, material and coating of Al; the standard sample is made of Si. As mentioned, we use Al-SiO_2/Si to construct a simulative measuring model of SNOM in the following steps:

Step 1: Use an SNOM optical fiber probe of 1640-00 model to carry out measurement of TGZ01 ladder standard sample by an SNOM machine of AURORA-3 model, acquiring the surface profile diagram of the sample.

Step 2: Confirm the dimensions and shape of the SNOM optical fiber probe. Conduct an SEM experiment of the SNOM optical fiber probe of 1640-00 model, to confirm the dimensions and shape of the SNOM optical fiber probe.

Step 3: According to the SEM experimental results, deduce the relational equations of the geometric dimensions of the SNOM optical fiber probe.

Step 4: Establish an atomic model for the simulative measuring model of SNOM. The SNOM optical fiber probe and the measured sample surface are considered as an ideal atom-arranged model. Using the SUB operation, UNI operation, and the concept of cutting-off radius r_c arrange the central spindle of the SNOM optical fiber probe by SiO_2 atoms. Use the Al atoms of the face-centered cubic structure to arrange the Al coating of the SNOM optical fiber probe to complete the development of the atomic model of the real Al-coated and Si-made SNOM optical fiber probes rapidly. Use the Si atoms of diamond cubic (DC) structure to arrange the atomic model of the sample in order to construct the simulative measuring model of SNOM. Use the ideal atoms to arrange the atomic models for the Al-coated and Si-made optical fiber probes as well as the surface of the Si-made nanoscale ladder standard sample.

Step 5: Set the related Morse potential energy parameters including cohesion energy D_{AI} , material parameter $\propto_{AI}$, equilibrium distance r_{0AI} , and cutting-off radius r_{cAI}. The Lorenz—Berthelot mixing rule is used to determine the Si-Al Morse potential energy parameter value, the size of the Si-O Morse cohesion energy D_{SiOx}, the size of the Al-Si Morse cohesion energy D_{AISI}, the size of Al-Si Morse material parameter value $\propto_{AISI}$, the size of the Si-O Morse material parameter value $\propto_{SIOx}$, the Ai-Si Morse equilibrium radius r_{SIAI}, and the Si-O Morse equilibrium radius r_{SiOx}.

Step 6: Set the related parameter values of the SNOM vibration mechanism, including the force required for driving the vibration of the tuning fork, quality factor, dimensions of the tuning fork, effective mass M_{eff}, damping coefficient C, and the spring constant value K of the tuning fork of the simulative model, as shown in Table 2.

Table 2 Related parameters of SNOM simulative measurement (Veeco Metrology Group, 2000)

Quality factor	Elastic modulus	Dimensions of tuning fork	Spring constant	Effective mass
1000	78.7 [Gpa]	4[mm]×0.6[mm] ×0.4[mm]	26600 [N/m]	6.174288 ×10^{-7}[kg]

Step 7: Construct a theoretical model for the simulative measurement of Al-SiO_2/Si-SNOM, indicating the correction of the theory of the simulative measurement of Al/Al-SNOM. Derive an amplitude equation $x(t)$ of the optical fiber probe during the simulative measurement of Al-SiO2/Si -SNOM.

Step 8: Set the fixed amplitude value x=0.98nm for the SNOM simulative measurement.

Step 9: Adjust the corresponding positions of the probe and the sample. Use Morse force to calculate the tip-sample interatomic interaction $F_{\emptyset\_Fact}$.

Step 10: Calculate the amplitude of the optical fiber probe during the simulative measurement by SNOM. By adjusting the position of the optical fiber probe, the optical fiber probe is made to reach the fixed amplitude value. Record the corresponding height positions of the probe and the sample.

Step 11: Draw the surface profile of the standard sample. Calculate the coordinates of the absolute position of the SNOM optical fiber tip and record the values. Draw the surface profile of the standard sample during simulative measurement.

Step 12: Substitute the parameters of the optical fiber probe acquired by SEM photographing, including the aperture and end protrusion sizes, thickness of Al coating, and the bevel angle of the probe, in the simulative measuring model of Al-SiO_2/Si-SNOM. Compare the results of the measuring experiment of SNOM and the simulative measuring model of Al-SiO_2/Si-SNOM, and find the error between them, to prove the rationality of the simulative measuring model of Al-SiO_2 /Si-SNOM.

Step 13: According to the simulative measuring model of Al-Si O_2 /Si-SNOM, perform simulative measurement of the aperture and end protrusion sizes, thickness of Al coating, and bevel angle of the optical fiber probe.

Step 14: Explore the simulation measurement results of the simulative measuring model of Al-SiO_2 /Si-SNOM and the edge effects produced from the aperture, end protrusion size, thickness of Al coating, and bevel angle of the probe.

METHOD AND PROCEDURES FOR CALCULATING THE GEOMETRIC DIMENSIONS OF THE OPTICAL FIBER PROBE

This study applies the simulative measuring model of Al-SiO_2/Si-SNOM to establish an innovative model and determine the calculation method for the geometric dimensions of the SNOM optical fiber probe. To find solutions for the geometric dimensions, the optical fiber probe must be measured by SEM. In case of an SEM measurement, the optical fiber probe, because of its poor conduction, must be sputtered with a silver or gold conductive layer and separated from the tuning fork, thus destructing the SNOM optical fiber probe and rendering it unusable. According to the established simulative measuring model of SNOM and through the SEM experiment, we deduce the relational equations of the geometric dimensions of the Al-SiO_2/Si-SNOM optical fiber probe. An SNOM optical fiber probe is used to carry out the measurement. After one of the SNOM optical fiber probes is used to measure the ladder standard sample and SEM experiment is conducted, its shape is obtained. Then, the aperture and end protrusion sizes of the optical fiber probe and thickness of the probe's Al coating are measured. These results are compared with those acquired using the nondestructive calculation method proposed in this study, thus proving that our nondestructive calculation method is reasonable and acceptable. The SEM photographing experiment carried out by the SNOM optical fiber probe belongs to an experimental measurement destructing the functions of the SNOM optical fiber probe.

Calculation Method for the Geometric Dimensions of the Optical Fiber Probe by Applying Measurement of the Ladder Standard Sample

This study carries out an SNOM measurement experiment of the ladder standard sample using an optical fiber probe, and proposes the force bearing the relation between the SNOM optical fiber probe and the ladder standard sample. The error between the surface profile of the plane measured through the experiment and that measured through SNOM simulation is squared, multiplied by 1/2, and then added the Barrier function to it, achieving solutions for the target function values of the geometric dimensions of the SNOM optical fiber probe. Next, using the

Levenberg—Marquardt method, according to the results simulated by the simulative measuring model of SNOM and the suitable convergence criterion, we find solutions for the aperture S of the optical fiber probe, the end protrusion size h of the optical fiber probe, and the thickness t of the Al coating. Regarding the bevel angle of the probe, based on the bevel shape of the vertical edge profile of the ladder standard sample measured in the SNOM experiment, we analyze that the bevel angle of the bevel edge obtained in the measurement is just the bevel angle of the SNOM optical fiber probe. As mentioned, the target function E^* of the study is acquired by squaring the error between the surface profile of the plane measured through experiment and that measured through SNOM simulation, multiplying the squared error by 1/2, and then adding the Barrier function to it. The target function values of the geometric dimensions of the optical fiber probe can be solved as shown in Eq. (25).

$$E^* = \frac{1}{2}\sum_{i=1}^{n}((H_M)_i - (H_N)_i)^2 + \varphi_i(S) \tag{25}$$

where H_M is the measured data, being the height of the surface profile measured on the cross-sectional plane of the ladder standard sample acquired in SNOM measurement; H_N is the result of numerical calculation, being the height of surface profile on the plane of the ladder standard sample simulated by the simulative measuring model of SNOM; and n is the number of measuring points on the ladder standard sample. In the study, n=9; S is the unknown parameter value of the system, which is the aperture of the optical fiber probe here; and ψ_j is the Barrier function, with Eq.(26) as follows:

$$\psi_j = 0.0001 \times E(S) \tag{26}$$

where ψ_j is a weight value, which serves as an adjustable factor in the process of searching optimal parameter values, and is beneficial to the optimal searching process.

The optimal steps in the general numerical optimization method are shown in Eqs. (27) and (28). If the Gauss—Newton Method is added with a regularization parameter (Λ), ite., Marquardt parameter, the optimal step of the Levenberg-Marquardt method can be obtained (2005) as shown in Eg. (29):

$$\text{Steepest Descent Method}: \delta = -J^T r \tag{27}$$

$$\text{Gauss-Newton Method}: \delta = -(J^T J)^{-1}\ J^T r \tag{28}$$

$$\text{Levenberg-Marquardt Method}: \delta = -(J^T J + \Lambda I)^{-1}\ J^T r \tag{29}$$

Where I is the unit matrix, J is the Jacobian matrix, J=$\begin{bmatrix} \frac{\partial r_1(S)}{\partial S} \\ \vdots \\ \frac{\partial r_n(S)}{\partial S} \end{bmatrix}_{ax1}$, and r is the residual matrix of the system, $r_i(S) = (H_M)_i - (H_N)_i$, r=$\begin{bmatrix} r_1(S) \\ \vdots \\ r_n(S) \end{bmatrix}_{ax1}$

Here, we take the Levenberg—Marquardt method as the searching rule to find solutions for the geometric dimensions of the optical fiber probe. The error between the surface profile acquired from SNOM experiment and that acquired from SNOM simulation is squared, multiplied by 1/2, and then added the Barrier function to it, achieving solutions for the target function values of the geometric dimensions of the optical fiber probe. To make the search smoother, we further correct the concept of Tikhonov's method (Huang et al. 1992) and make it a target function, as shown in Eq. (25).

Procedures of Calculating the Geometric Dimensions of the Optical Fiber Probe

Combining the SNOM measurement experiment and SNOM simulative measuring model, we propose a nondestructive method to find solutions for the geometric dimensions, including the aperture and end protrusion sizes, thickness of Al coating, and bevel angle of the probe. First, the established simulative measuring model of Al-SiO_2/Si-SNOM is used. Then, we square the error between the surface profile measured through experiment and that measured through simulation, multiply the squared error by 1/2, and then add the Barrier function to it, in order to obtain solutions for the target function values of the geometric dimensions of the optical fiber probe. We combine the optimal search of the numerically optimized Levenberg-Marquardt method with a reasonable convergence criterion to establish the study's nondestructive calculation method for geometric dimensions of the SNOM optical fiber probe. This method solves the problem of destruction of the optical fiber probe before the measurement of its geometric dimensions. The detailed steps of such an innovative nondestructive calculation method are explained as follows:

Step 1: Carry out SNOM measurement. Obtain the experimental surface profile of the ladder standard sample.

Step 2: Set the height H_M of the surface profile of the plane acquired in the experimental measurement of the ladder standard sample. It refers to the use of the optical fiber probe to carry out SNOM measurement to obtain the surface profile measured in the experiment of the TGZ01 ladder standard sample, and calculate the height values $(H_M)_{i\ \ i=1\sim9}$. of the surface profile at the nine points within the considered area. Through SNOM experiment,, the bevel angle of the bevel edge of the vertical edge profile of the ladder standard sample is obtained, and the bevel angle of the θ SNOM optical fiber probe is acquired.

Step 3: Conduct an SEM experiment of the SNOM optical fiber probe to obtain the related geometric dimensions, including S_{1_LAB}, h_{1_LAB}, R_{1_LAB}, θ_{1_LAB}, L_{1_LAB}, and t_{1_LAB}, ,and derive their relational diagram and equations. The geometric dimensions.

Step 4: As the initial values, let the aperture size of the probe be S_0, the thickness of the Al coating be t_0, the bevel angle of the probe be θ_1, and the protruding height at the probe tip be h_0. First, set S_0, and t_0 according to the aperture and Al-coating thickness of the probe stated in the catalog. Then, let the protruding height h_0 at the probe tip be a layer arranged with atoms.

Step 5: Calculate the initial large round-angle radius R_0 of the shape of the optical fiber probe and the geometric arc length L_0 of the probe. Through the use of complex Boolean operation, establish the atomic model, as shown in Fig. 4(a). Apply the relational diagram of the probe to measure the arc length L_0 of the atomic model in the geometric relational equations. According to Eq. (1) or Eq. (2), the large round-angle radius R_0 of the probe is obtained.

Step 6: Use the various initial values to carry out SNOM simulative measurement, obtaining the simulative surface profile of the standard sample.

Step 7: Obtain the height H_N of the surface profile of the simulated plane of the ladder standard sample. The initial value of the first optical fiber probe alone is required to carry out SNOM simulative measurement and obtain the surface profile of the simulated plane of the standard sample. Calculate the height $(H_N)_{i \quad i=1\sim9}$ of the surface profile of the simulated plane at the nine points within the considered area.

Step 8: Calculate the geometric dimensions of the optical fiber probe as follows.

(1) Take S_0, θ_1, R_0, L_0, and t_0 obtained from the foregoing steps as the initial parameter values.

(2) Carry out SNOM simulative measurement to acquire the simulated surface profile of the ladder standards sample. The $(H_M)_i$ and $(H_N)_i$ obtained in Step *7* are substituted in Eq. *(*25) in order to calculate the target function value $E^{*(0)}$ of the initial algorithm, where

$$E^{*(0)} = \frac{1}{2}\sum_{i=1}^{9}((H_M)_i - (H_N)_i)^2 + \psi(S) \text{and} \ \ \psi_0 = 0.0001 \times E^{*(0)}(S).$$

(3) Calculate the J, g, and H values of iteration (2003),

$$\text{Where } \mathrm{J} = \begin{bmatrix} \frac{\partial r_1(S)}{\partial p} \\ \vdots \\ \frac{\partial r_n(S)}{\partial (S)} \end{bmatrix}_{n\times1}, \quad \mathrm{g} = -\frac{d\psi}{dS}, \ H = \frac{d^2\psi}{dS^2}.$$

(4) Calculate the amount of change in the iteration as ΔS(Romanov et al.,2003),

Where $\Delta S = (-\mathrm{J}^T\mathrm{r} + \mathrm{g})/(\mathrm{J}^T\mathrm{J} + \mathrm{H} + \Lambda)$.

(5) Calculate the next iteration parameter, acquiring the aperture Value S_{k+1} of the optical Fiber probe:$S_{k+1}=S_k+\Delta S_k$,where k starts from 0.

(6) Calculate the large round-angle radius R_{k+1} of the probe shape. As seen from this atomic model, the protruding height at the probe tip is equivalent to the height of a single row of atoms. Therefore, h_{k+1} is known. Thus, from Eq. (1) or Eq. (2), the large round-angle radius, $R_{k+1,}$ can be acquired.

(7) According to the relational diagram of the geometric dimensions of the probe shape, find the arc length L_{k+1}

(8) Correct the thickness of the Al coating, t_{k+1}. From the relational equations of the geometric dimensions of the optical fiber tip, shown in Eq. (3), calculate the t_{k+1}, where

$$t_{k+1} = \left[\left(\frac{L_{k+1} - S_{k+1}}{2}\right) - \left(\frac{\sqrt{4R_{k+1}{}^2 - S_{k+1}{}^2} - \sqrt{4R_{k+1}{}^2 - L_{k+1}{}^2}}{2}\right) \tan\theta_1\right]\cos\theta_1$$

(9) According to the solution for the aperture value, S_{k+1}, large round-angle radius R_{k+1}, bevel angle θ_1, arc length L_{k+1}, and Al-coating thickness t_{k+1} of the first optical fiber probe, perform simulative measurement by SNOM, acquiring the simulated surface profile of the plane of the TGZ01 standard sample and the newly simulated height value $(H_N)_{i \quad i=1\sim9}$.

(10) Calculate the new target function value

$$E^{*(k+1)} = \frac{1}{2}\sum_{i=1}^{9}((H_M)_i - (H_N)_i)^2 + \psi(S_{k+1}),$$

and then check whether the new target function value is smaller than the old target function value $E^{*(k)}$. If it is, proceed with item (11) of Step 8. If it is not, magnify the Levenberg-Marquardt parameter, which indicates the magnification of the increment of the parameter, i.e., $\Lambda = 10 \times \Lambda$. Return to Item (5) of Step 8.

(11) Here, let$\{|\Delta S_k|/(10^{-5} + |S_k|)\} < 10^{-4}$ be the convergence criterion used for solving and analyzing the aperture of the optical fiber probe. If the convergence criterion is met, finish this step, and start with Step 9. If it is not met, reduce Λ, which indicates the reduction of the increment of the parameter, i.e., $\Lambda = 0.1 \times \Lambda$. Return to Item (4) of Step 8. Through the Levenberg-Marquardt method, obtain the solution for the aperture of the optical fiber probe. Proceed until the defined convergence criterion is met. During this time, the geometric dimensions of the optical fiber probe, including

$S_{1\_method} = S_{k+1}$, $h_{1\_method} = h_{k+1}$,
$R_{1\_method} = R_{k+1}$, $\theta_{1\_method} = \theta_{k+1}$,
$L_{1\_method} = L_{k+1}$, and $t_{1\_method} = t_{k+1}$,
can be solved.

Step 9: Compare these acquired geometric dimensions of the optical fiber probe with the related geometric dimensions of the optical fiber probe acquired from SEM experiment. Thus, the feasibility of the nondestructive calculation method of applying the ladder standard sample to obtain the geometric dimensions of the optical fiber probe is proved.

RESULTS AND DISCUSSION

To solve the edge effect caused by the geometric dimensions of the optical fiber probe and the surface profile of the sample during SNOM measurement, as well as to overcome the disadvantage of destructive measurement and analysis of the geometric dimensions by SEM, this study uses a tuning-fork SNOM optical fiber probe of 1640-00 model manufactured by Veeco Instruments Inc. and a ladder standard sample of TGZ01 model manufactured by NT-MDT Company to carry out SNOM measurement on the SNOM machine in AURORA-3 model.

This study combines the experimental measurement of SNOM with the simulative measuring model of SNOM, and proposes a nondestructive method for determining the important geometric dimensions of the optical fiber probe, including the aperture and end protrusion sizes, Al-coating thickness, and bevel angle of the probe. Using a complex Boolean operation and the concept of cutting-off radius r_c, we employ an accurate and workable simplification method to decrease the number of atoms substantially. The Al coating arranged by Al atoms and the central spindle of probe arranged by SiO2 atoms form the SNOM optical fiber probe. The atomic model of the ladder standard sample is formed by arranging the Si atoms, establishing the atomic model for the simulative measuring model of SNOM. After combining the optimal search of the numerically optimized Levenberg-Marquardt method with the reasonable convergence criterion, we establish a nondestructive calculation method for the geometric dimensions of the SNOM probe.

This study acquires the surface profile of the plane of the TGZ01 ladder standard sample using the experimental measurement of SNOW, as shown in Fig. 6. In Fig 6, Zone 1 and Zone 3 are the plane surface parts of the ladder standard sample. The main reasons for the surface profile error of the plane of the ladder standard sample are the effects of both the aperture of the optical fiber probe and the protruding height at the probe tip. When Zone 2 in Fig. 6 is partially magnified, the bevel angle of the optical fiber probe is almost equivalent to the gradient of the surface profile, which is approximately 8.5°. Therefore, we can calculate the aperture of the optical fiber probe (Si_method = 78.4 nm) and the protruding height at the probe tip (h_1_method = 0.639nm). The value of h_1_method is almost equal to that of a layer of atoms in the **at**omic model of the probe arranged by SiO_2 atoms. Therefore, from Eq. (1) or Eq. (2), the round angle of the optical fiber probe shape can be acquired (R_1_method =1202.698 nm). Furthermore, on the basis of the various dimensions solved earlier, and from Fig. 3(b) and Eq. (3), we can calculate the thickness of Al coating (t_1_ method = 100.6 nm) and the geometric arc length of the optical fiber probe (L_1_method = 299.257 nm).

We establish an atomic model for the calculated geometric dimensions of the optical fiber probe, as shown in Fig. *7*, with the cutting-off radius being 1.2624 nm and the total number of atoms being 110080.

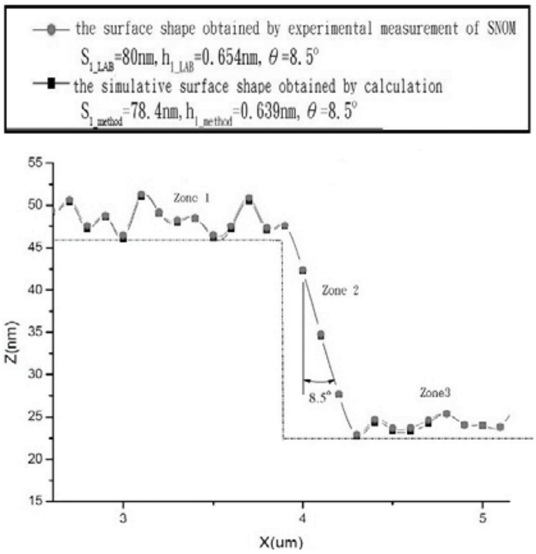


Fig. 6. SNOM simulation and experimental results acquired after calculation of the ladder standard sample by the optical fiber probe

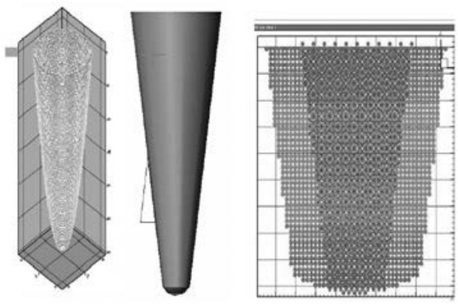


Fig. *7*. Atomic model of the optical fiber probe acquired after calculation

Then, we also carry out the simulative measuring of the surface profile of the plane of the TGZ01 ladder standard sample by using the simulative measuring model of SNOW. The acquired surface profile of the plane of the TGZ01 ladder stander sample is shown in Fig. 6. Then, we calculate the related geometric dimensions of the optical fiber probe for actual measurement of the TGZ01 ladder standard sample, as shown in Table 3. After that, according to the nondestructive calculation method of the geometric dimensions of the optical fiber probe, the geometric dimensions of the optical fiber probe are obtained, as shown in Table 3. Through SEM experiment, the geometric profile of the optical fiber probe is obtained, as shown in Fig. 8 and Table 3.

Table 3 Geometric dimensions of the optical fiber probe acquired from SEM experiment and calculation

The SNOM Optical Fiber probe	Geometric dimensions of optical fiber probe					
	Optical fiber aperture of central spindle of optical fiber probe	Large Round-angle Radius of probe shape	Protruding height at the probe tip	Thickness of Al coating of probe	Bevel angle of probe	Arc length at the probe tip
Result of SEM experiment	S_{1_LAB} = 80.0nm	R_{1_LAB} = 1223.568nm	h_{1_LAB} = 0.654nm	t_{1_LAB} = 100nm	$\theta_{1\_LAB} = 8.5^{\circ}$	L_{1_LAB} = 299.298nm
Calculation result	S_{1_method} = 78.4nm	R_{1_LAB} = 1202.698nm	h_{1_LAB} = 0.639nm	t_{1_LAB} = 100.6nm	$\theta_{1\_method} = 8.5^{\circ}$	L_{1_method} = 299.257nm
Average height difference between the plane part of TGZ01 Ladder stand sample measured by SNOM and the simulated Surface profile					0.28nm	

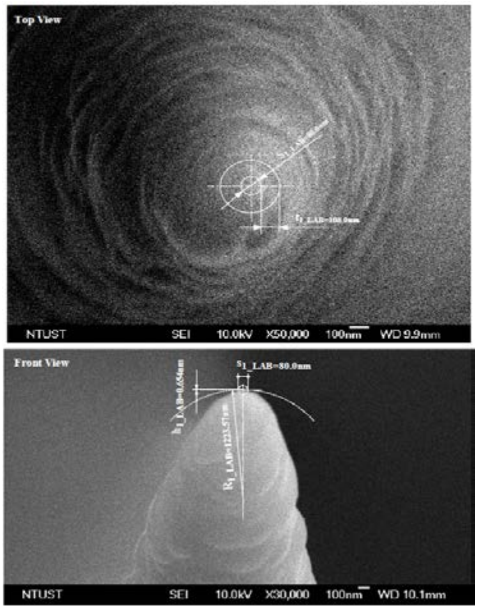


Fig. 8. Geometric profile of the optical fiber probe obtained in SEM experiment

Comparing the simulated surface profile results of the plane by using the geometric dimensions of the optical fiber probe acquired from SNOM measurement and those by calculation, it is found that the simulated average height error of the plane between the measured result of the plane of the ladder standard sample and the calculated geometric dimension of the optical fiber probe is 0.28 nm is an extremely small value, as shown in Fig. 6 and Table 3. From Table 3, it can be found that the difference between the geometric dimensions of the optical fiber probe acquired from the SEM experiment and that from the calculation is also small. Therefore, it can be confirmed that the nondestructive calculation method proposed by the study for solving the geometric dimensions of the optical fiber probe is feasible.

CONCUSION

We combine experiments with theories to complete the development of a simulative measuring model of SNOM and establishes an innovative and nondestructive calculation method for the geometric dimensions of the SNOM optical fiber probe to overcome the technical disadvantage of the destructive measurement of the geometric dimensions by SEM measurement. We apply the plane of a ladder standard sample to establish a nondestructive calculation method for the geometric dimensions, and use atoms to establish the required simulative measuring atomic model. According to the vibration mechanism of the SNOM probe, we apply Morse force to analyze the tip-sample interaction in order to construct a fixed-amplitude simulative measuring model of SNOM. To complete the development of the required atomic model rapidly, we propose the use of a complex Boolean operation and the concept of cutting-off radius to decrease the number of atoms. substantially, achieving the effect of simplified arrangement work of the atomic model. On the other hand, in the simulative study of the measuring model of SNOM, we conduct a photographing experiment of the geometric dimensions of the optical fiber probe by SEM, and establishes the relational equations of the geometric dimensions of the real Al-coated and SiO_2-made SNOM optical fiber probes. In the selection of the potential energy parameter, the Lorenz-Berthelot mixing rule is employed to find the Morse potential energy parameters among different atoms in order to solve the problem of the unknown potential energy parameter value, which serves as the potential energy parameter value of the simulative measuring model. When using the calculation method of the geometric dimensions of the SNOM optical fiber probe, we square the error of the plane shape of the ladder standard sample, multiply the squared error by 1/2, and then add it to the Barrier function to solve the target function values of the geometric dimensions. We combine the optimal search of the Levenberg-Marquardt method with a reasonable convergence criterion, and then derive the relational diagram and equations of the geometric dimensions, establishing an innovative and nondestructive calculation method and procedures for these dimensions. We compare the results of the nanoscale ladder standard sample measured by the SNOM optical fiber probe with those of the sample simulated by the probe. Through SEM experimental photographing, the geometric dimensions of the optical fiber probe are confirmed, proving the feasibility of the proposed nondestructive calculation method.

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掃描近場光學光纖探針之幾何尺寸計算方法和實驗驗證

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摘要

本文建立一個掃描近場光學(SNOW)光纖探針之幾何尺寸計算方法。我們應用分子力學和振動理論去建立一個 SNOW 的模擬量測模式。在建立 SNOW 的模擬量測模式中的原子模式，我們使用布林運算去安排探針和量測試片的原子模式。我們先做掃描電子顯微鏡(SEM)實驗，量測出探針的幾何尺寸並繪出光纖探針幾何尺寸的關係圖，進而推導出光纖探針的幾何尺寸的相關公式。我們並使 Lorenz-Berthelot mixing rule 去得到不同種類原子間的 Morse potential energy 的參數值。我們再用 Levenberg-Marquardt 方法進行最佳化的搜尋，配合合理的收斂準則，進而獲得最佳的光纖探針的幾何尺寸。此外，我們也使用 SNOW 的光纖探針進行幾何尺寸量測實驗，並比較實驗所得的光纖探針幾何尺寸和模擬所得的光纖探針幾何尺寸，驗證本文所建立的非破壞性光纖探針幾何尺寸計算方法為可行的。