ELSEVIER

Applied Surface Science 140 (1999) 352–357

applied surface science

Calculation of the optimal imaging parameters for frequency modulation atomic force microscopy

Franz J. Giessibl *, Hartmut Bielefeldt, Stefan Hembacher, Jochen Mannhart

Universität Augsburg, Institute of Physics, Electronic Correlations and Magnetism, Experimentalphysik VI, Universitätsstrasse 1, D-86135 Augsburg, Germany

Received 1 July 1998; accepted 11 August 1998

Abstract

True atomic resolution of conductors and insulators is now routinely obtained in vacuum by frequency modulation atomic force microscopy. So far, the imaging parameters (i.e., eigenfrequency, stiffness and oscillation amplitude of the cantilever, frequency shift) which result in optimal spatial resolution for a given cantilever and sample have been found empirically. Here, we calculate the optimal set of parameters from first principles as a function of the tip–sample system. The result shows that the either the acquisition rate or the signal-to-noise ratio could be increased by up to two orders of magnitude by using stiffer cantilevers and smaller amplitudes than are in use today. © 1999 Elsevier Science B.V. All rights reserved.

PACS: 07.79 Lh; 61.16 Ch; 87.64 Dz; 34.20 Cf

Keywords: Atomic force microscopy; Frequency modulation atomic force microscopy; Dynamic force microscopy; Atomic resolution; Tip–sample interaction; Dissipation; Thermal noise

1. Introduction

Although Binnig, Quate and Gerber anticipated that the atomic force microscope (AFM) they invented in 1985 [1] would ultimately achieve true atomic resolution in vacuum, it took almost 10 years before the Si (111)-(7 × 7) reconstruction [2–7] and other conducting [8] and insulating surfaces [9,10] were imaged with atomic resolution by AFM. Frequency modulation (FM) AFM, originally invented by Albrecht et al. in 1991 [11] for magnetic force microscopy, is the method which was used in the first demonstration of true atomic resolution in vacuum and is now common practice in vacuum AFM. In this technique, a cantilever (CL) with spring constant k and eigenfrequency f_0 is subject to positive feedback such that it oscillates with a constant amplitude A_0. When the oscillating CL is approached to a sample, its oscillation frequency changes from f_0 to $f = f_0 + \Delta f$ due to the forces between the tip of the CL and the sample. Scanning the CL across the sample (x–y plane) and adjusting z such that f is constant yields a map $z(x, y, \Delta f, k, f_0, A_0)$. This map provides an atomic picture of the surface if the vertical noise is smaller than the atomic corrugation. Up to now, combinations of Δf,

* Corresponding author. Tel.: +49-821-598-3675; Fax: +49-821-598-3652; E-mail: franz.giessibl@physik.uni-augsburg.de

PII: S0169-4332(98)00553-4

Table 1
Parameters used for imaging various surfaces by FM-AFM newline

k [N/m]	f_0 [kHz]	Δf [Hz]	A_0 [nm]	kA_0 [nN]	γ^a[fN$\sqrt{\text{m}}$]	Sample	Ref.	Lateral resolution
43.0	276.0	−60	40.0	1720	−74.7	Si(111)	[3]	atomic
17.0	114.0	−70	32.0	544	−65.4	Si(111)	[2]	atomic
23.5	153.0	−70	19.0	447	−28.2	Si(111)	[6]	atomic
33.0	264.0	−670	4.0	132	−21.2	Si(001)	[7]	atomic
30.0	168.0	−80	13.0	390	−21.2	NaCl(001)	[10]	atomic
36.0	160.0	−63	12.7	457	−20.3	InAs(110)	[12]	atomic
28.0	270.0	−80	15	420	−15.2	TiO_2(110)	[13]	atomic
37.0	276.0	−50	10.0	370	−6.7	Si(111)	[7]	atomic
41.0	172.0	−10	16.0	654	−4.8	Si(111)	[14]	atomic
34.0	151.0	−6	20.0	680	−3.8	InP(110)	[8]	atomic
10.0	290.0	−95	10.0	100	−3.3	Si(111)	[5]	atomic
37.0	276.0	−350	1.5	55.5	−2.7	Si(111)	[7]	atomic
2.5	60.0	−16	15.0	37.5	−1.2	KCl(001)	[15]	≈ 3 nm
2.5	60.0	−32	3.3	8.25	−0.3	Si(111)	[15]	≈ 0.6 nm (x), 2 nm (y)

[a] $\gamma = \Delta f k A_0^{3/2} / f_0$, see Ref. [16].

k, f_0, and A_0 which do provide true atomic resolution have been found empirically. With currently available CLs, the oscillation amplitude A_0 needs to be up to 100 times the interatomic distances for obtaining atomic resolution (see Table 1). However, the spring constant k and the eigenfrequency f_0 have to be selected from the discrete set of commercially available CLs. Since the spring constant of a CL cannot be freely chosen, it is important to clarify for which set of operating parameters (k, f_0, A_0) best performance is to be expected. Here, we present a calculation based on first principles for the optimal set of k, f_0 and A_0 as a function of the tip–sample potential $V_{ts}(x, y, z)$. The models for $V_{ts}(x, y, z)$ we use here include exponential and inverse-power laws.

2. Calculation of vertical noise

Since the imaging signal in FM-AFM is a frequency shift Δf, the best signal-to-noise ratio is expected for large Δf and little noise $\delta(\Delta f)$. However, for a given minimum distance d between the front atom of the CL and the sample both Δf and $\delta(\Delta f)$ decrease with amplitude. If Δf were independent of A_0, minimal noise would result for $A_0 \to \infty$. Since the magnitude of Δf decreases with amplitude, it is not straightforward to see whether there is an optimum (minimum in vertical noise) for a specific set of k, f_0 and A_0. These optimal parameters will depend on the characteristics of the tip–sample potential.

Three major contributors to the vertical noise in $z(x, y, \Delta f, k, f_0, A_0)$ can be identified (see Fig. 1).

(1) Frequency noise: a variation δd leads to a variation in the frequency shift according to $\delta(\Delta f)$

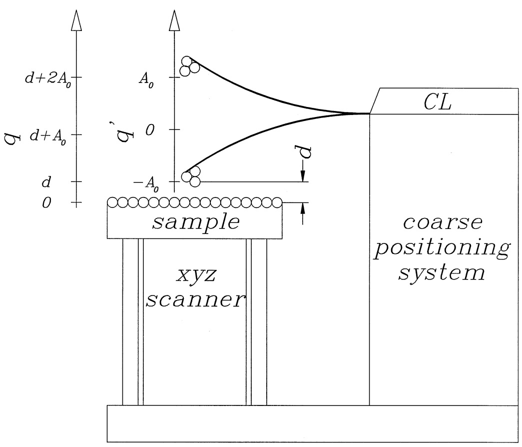

Fig. 1. Schematic of a frequency modulation atomic force microscope.

$=(\partial(\Delta f))/(\partial d)\delta d$. Thus, the vertical noise caused by frequency noise is:

$$\delta z_f = \frac{\delta(\Delta f)}{\frac{\partial(\Delta f)}{\partial d}}. \quad (1)$$

Albrecht et al. [11] have calculated the thermodynamic lower limit of the frequency noise

$$\delta f_{\text{thermal}} = \delta(\Delta f)_{\text{thermal}} = \sqrt{\frac{k_B T B f_0}{k A_0^2 \pi Q_0}} \quad (2)$$

where k_B is the Boltzmann constant, T the absolute temperature, B the detection bandwidth and Q_0 the quality factor of the CL [11]. The detection bandwidth B determines the imaging speed. If a section with a width of 100 atoms is to be imaged at an imaging speed of three lines per second, B needs to be at least $2 \times 100 \times 3/\text{s} = 600$ Hz.

There is also a contribution to frequency noise $\delta(\Delta f)_{\text{instrumental}}$ which depends on the quality of the frequency detector. Since these noise sources are uncorrelated, the total frequency noise is given by

$$\delta(\Delta f) = \sqrt{\delta(\Delta f)^2_{\text{thermal}} + \delta(\Delta f)^2_{\text{instrumental}}}. \quad (3)$$

The denominator in Eq. (1), $(\partial(\Delta f))/(\partial d)$, is calculated further below.

(2) Amplitude noise: the fluctuation of the total energy of the CL is approximately $k_B T$. Thus, $k(A_0 + \delta A_0)^2/2 \approx k A_0^2/2 + k_B T$ and the amplitude noise is given by:

$$\delta A_0 \approx \frac{k_B T}{k A_0}. \quad (4)$$

For typical values of kA_0 (Table 1), this contribution is negligible even at room temperature.

(3) Mechanical noise: the mechanical loop from CL to sample is closed by the xyz scanner and the coarse positioning system. Acoustic noise, building vibrations etc. cause a variation of the distance between CL and sample $\delta Z_{\text{instr.}}$. Proper design of the microscope and insulation from external vibrations help to bring $\delta Z_{\text{instr.}}$ down to a few picometers.

Since the noise contributions in z-direction are statistically independent, the total z-noise is:

$$(\delta z)^2 = \left(\frac{\delta(\Delta f)}{\frac{\partial(\Delta f)}{\partial d}}\right)^2 + (\delta A_0)^2 + (\delta Z_{\text{instr.}})^2. \quad (5)$$

Since amplitude- and mechanical noise are negligible, in the following, we only consider the noise contribution from frequency noise.

2.1. Calculation of the derivative of the frequency shift

2.1.1. Frequency shift for inverse-power forces

For tip–sample forces given by

$$F_{ts}(q) = \frac{C}{q^n} \quad (6)$$

where C is a constant and q is the distance between the center of the front atom of the tip and the plane defined by the centers of the surface atoms, the frequency shift $\Delta f = f - f_0$ is given by Ref. [16]:

$$\Delta f_{sA_0} = n \frac{f_0}{2k} \frac{C}{d^{n+1}} \quad (7)$$

if $A_0 \ll d$. For $A_0 \gg d$ the frequency shift is given by:

$$\Delta f_{lA_0} = Y_n \frac{f_0}{k A_0^{3/2}} \frac{C}{d^{n-1/2}} \quad (8)$$

with

$$Y_n := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{(1+y^2)^n} \mathrm{d}y. \quad (9)$$

Pertinent values of Y_n are $Y_1 = 1/\sqrt{2}$, $Y_2 \approx 0.36$, $Y_3 \approx 0.27$, $Y_4 \approx 0.22$, $Y_7 \approx 0.16$ and $Y_{13} \approx 0.11$ [16].

For functions $g_s(d) = cd^{-3/2}$ and $g_l(A_0) = A_0^{-3/2}$ a function

$$g(d, A_0) = \frac{1}{\left[c^{-m} d^{3m/2} + A_0^{3m/2}\right]^{1/m}} \quad (10)$$

fulfills $\lim_{A_0/d \to 0} g(d, A_0) = g_s(d)$ and $\lim_{A_0/d \to \infty} g(d, A_0) = g_l(A_0)$. The simplest case $m = 1$ yields an approximation for Δf which is sufficiently precise for intermediate amplitudes [1]

$$\Delta f = \frac{Y_n f_0}{k\left(A_0^{3/2} + \frac{2Y_n}{n} d^{3/2}\right)} \frac{C}{d^{n-1/2}} = \frac{Y_n f_0 C}{k} \frac{1}{A_0^{3/2} d^{n-1/2} + \frac{2Y_n}{n} d^{n+1}}. \quad (11)$$

The variation of the frequency shift with distance is given by the derivative:

$$\frac{\partial(\Delta f)}{\partial d} = -\frac{Y_n f_0 C}{k} \times \frac{(n-1/2) A_0^{3/2} d^{n-3/2} + 2Y_n(1+1/n) d^n}{\left(A_0^{3/2} d^{n-1/2} + \frac{2Y_n}{n} d^{n+1}\right)^2}. \quad (12)$$

2.1.2. Frequency shift for exponential forces

For exponential forces

$$F_{ts}(q) = F_0 e^{-q/\lambda} \quad (13)$$

the frequency shift for small amplitudes $A_0 \ll \lambda$ is:

$$\Delta f_{sA_0} = \frac{f_0}{2k\lambda} F_0 e^{-d/\lambda} \quad (14)$$

and the frequency shift for large amplitudes $A_0 \gg \lambda$ [16]:

$$\Delta f_{lA_0} = \frac{f_0\sqrt{\lambda}}{kA_0^{3/2}} \frac{F_0 e^{-d/\lambda}}{\sqrt{2\pi}}. \quad (15)$$

Again, we can create an approximation for all amplitudes

$$\Delta f = \frac{f_0}{2k\lambda\left(1 + \sqrt{\frac{\pi}{2}}\left(\frac{A_0}{\lambda}\right)^{3/2}\right)} F_0 e^{-d/\lambda} \quad (16)$$

with the derivative

$$\frac{\partial(\Delta f)}{\partial d} = -\frac{1}{\lambda}\Delta f. \quad (17)$$

With this calculation $(\partial(\Delta f))/(\partial d)$ all the elements of the z-noise are complete. Finally, we have to take into account that we cannot choose the stiffness of the CL k independently from the amplitude A_0. Forces between tip and sample in vacuum are in general attractive before the CL makes contact. Therefore, there is a distance region where the CL is unstable and snaps uncontrolled to the surface ('jump-to-contact'), unless either $k > \max(-(\partial^2 V_{ts})/(\partial d^2)) = k_{ts}^{max}$ [17] or $kA_0 > \max(-F_{ts}) = F_{ts}^{max}$ [16].

These two conditions can be merged to

$$k = s\frac{F_{ts}^{max}}{A_0 + F_{ts}^{max}/k_{ts}^{max}} \quad (18)$$

with a 'safety factor' $s > 1$.

2.2. Effect of nonconservative V_{ts}

The tip–sample potential has so far been treated as nondissipative. However, Erlandsson et al. [4], Bammerlin et al. [10], Sugawara et al. [14], Guethner [5] and others have found significant damping of the CL when it oscillates close to the surface. A general model in analogy to friction is that the dissipative force component is given by

$$F_{diss}(q) = -\mu F_{ts}(q)\frac{\frac{dq}{dt}}{\left|\frac{dq}{dt}\right|}\left|\frac{dq}{dt}\right|^r. \quad (19)$$

The parameter r determines the type of 'friction': $r = 0$ corresponds to velocity-independent friction, $r = 1$ is commonly used for treating damped oscillators and $r = 2$ describes friction in fluids. Unfortunately, little is known about the nature of the dissipation process in FM-AFM. For the simplest case $r = 0$, the energy loss per oscillation cycle ΔE_{ts} is given by:

$$\Delta E_{ts} = -\int_{d+2A_0}^{d} \mu F_{ts}(q)\,dq + \int_{d}^{d+2A_0} \mu F_{ts}(q)\,dq. \quad (20)$$

[1] For amplitudes in the order of the decay length ($A_0 = d, \lambda$), the error of the all-amplitude approximation is 7%, 2%, 4% and 90% for exponential forces and inverse-power forces $n = 13$, 7 and 1, respectively. A precise formula for $n = 1$ is given in H. Hölscher et al. [18].

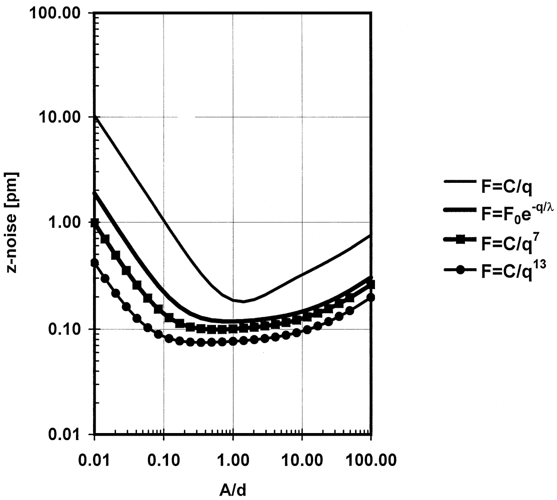

Fig. 2. Calculated noise in sample topography (perpendicular to surface) as a function of amplitude for exponential and inverse-power force models.

Since $\int F_{ts} \mathrm{d}q = V_{ts}$,

$$\Delta E_{ts} = 2\mu[V_{ts}(d + 2A_0) - V_{ts}(d)]. \tag{21}$$

This energy loss diminishes the quality factor Q_0 of the CL. Since $Q_0 = E/\Delta E_{CL}$, where $E = kA_0^2/2$ is the total energy in the CL and ΔE_{CL} is the energy loss due to internal friction in the CL, the effective Q-value is given by:

$$Q = \frac{E}{\Delta E_{CL} + \Delta E_{ts}} = \frac{Q_0}{1 + 2Q_0 \Delta E_{ts}/kA_0^2}. \tag{22}$$

The negative effect of dissipation on the Q factor is partially compensated with using large amplitudes. Bammerlin et al. [10] have measured the dissipation for a silicon tip interacting with potassium chloride. Analysis of their data yields $\mu \approx 0.05$.

3. Results and conclusion

The z-noise is thus given by

$$\delta z_f = \frac{k}{Y_n F_{ts}^{max}} \frac{d^2\left(\left(\frac{A_0}{d}\right)^{3/2} + \frac{2Y_n}{n}\right)^2}{\left(n - \frac{1}{2}\right)\left(\frac{A_0}{d}\right)^{3/2} + 2Y_n(1 + 1/n)} \times \sqrt{\frac{k_B T B}{\pi Q k A_0^2 f_0}} \tag{23}$$

for inverse-power forces and

$$\delta z_f = \frac{2k\lambda^2}{F_{ts}^{max}}\left(1 + \sqrt{\frac{\pi}{2}}\left(\frac{A_0}{\lambda}\right)^{3/2}\right)\sqrt{\frac{k_B T B}{\pi Q k A_0^2 f_0}} \tag{24}$$

for exponential forces. In both cases, the noise is proportional to $1/F_{ts}^{max}$, i.e., the greater the maximum attractive force, the easier it is to obtain true atomic resolution. Also, the noise is proportional to $1/\sqrt{f_0}$, i.e., the higher the frequency, the lower the noise. The most interesting implications of Eqs. (23) and (24) are the dependence of noise with amplitude. The stiffness of the CL is calculated with Eq. (18). The safety factor s is set to 100 (most authors use $s \gg 1$ see column 'kA_0' in Table 1).

Fig. 2 shows a plot of δz_f for inverse-power forces with $n = 1$, 7 and 13 and exponential forces with $F_{ts}^{max} = 3$ nN, $d = 250$ pm and $\lambda = a_{Bohr} = 52.9$ pm as a function of A_0/d. The corresponding force models are listed in Table 2. The properties of the CL in use are $Q_0 = 10\,000$, $f_0 = 100$ kHz, $T = 300$ K, the frequency detector is set to $B = 1$ kHz and its electronic noise is $\delta(\Delta f)_{instrumental} = 0.1$ Hz. For F_{ts}

Table 2
Models used for tip–sample potential

Force model	$V_{ts}(q)$	$F_{ts}(q)$	F_{ts}^{max}	k_{ts}^{max}	ΔE_{ts}
Inverse-power, $n > 1$	$\frac{C}{n-1}\frac{1}{q^n - 1}$	C/q^n	C/d^n	nF_{ts}^{max}/d	$\mu \frac{F_{ts}^{max} d}{n-1}\left[1 - \frac{1}{(1+2A_0/d)^{n-1}}\right]$
Inverse-power, $n = 1$	$C \ln(q)$	C/q	C/d	F_{ts}^{max}/d	$\mu F_{ts}^{max} d \ln(1 + 2A_0/d)$
Exponential	$F_0 \lambda e^{-q/\lambda}$	$F_0 e^{-q/\lambda}$	$F_0 e^{-d/\lambda}$	F_{ts}^{max}/λ	$\mu F_{ts}^{max} \lambda(1 - \exp^{-2A_0/\lambda})$

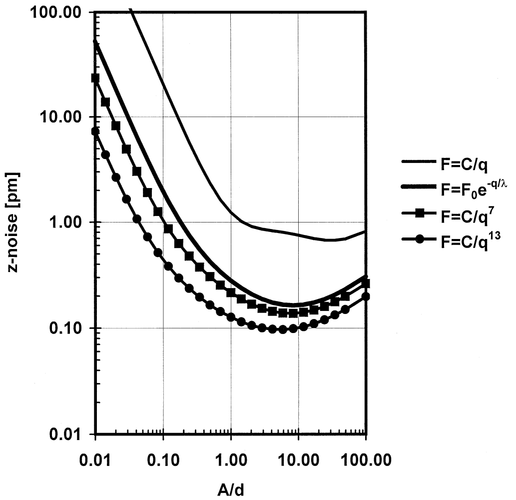

Fig. 3. Calculated noise in sample topography as a function of amplitude for exponential and inverse-power force models with dissipation.

$= C/q$, the optimum is reached for $A_0/d \approx 1$. The corresponding spring constant is $k = 500$ N/m. For forces with shorter ranges ($n = 7$, 13 and exponential), the lowest noise is obtained for even smaller amplitudes. The corresponding optimal spring constants range up to 3000 N/m.

Fig. 3 shows the noise for nonconservative potentials. For each cycle, an energy ΔE_{ts} is dissipated with $\delta E_{ts} = 2\ \mu(V_{ts}(d + 2A_0) - V_{ts}(d))$ with $\mu = 0.05$. As expected, larger amplitudes are required for minimum noise. The minimal noise is less pronounced than in the case without damping. The corresponding optimal stiffness is between 30 and 200 N/m.

In summary, we have shown why CLs with $k \approx 10$ N/m require amplitudes in the order of 10 nm. If CLs with $k \approx 300$ N/m were available, B could be increased by 100 or the vertical noise would drop by a factor of 10. Since the z-noise level is already comparable to the other noise sources δA_0 and δZ_{instr}, the major practical advantage is an increase in bandwidth which would allow faster scanning.

By comparing Figs. 2 and 3 it is clear that dissipation is crucial for determining the optimal operating amplitude—zero dissipation would favor stiff cantilevers and strong dissipation requires large amplitudes and softer cantilevers. More work on the investigation of the dissipation process between tip and sample needs to be done for improving the performance of FM-atomic force microscopy. Also, Eqs. (23) and (24) suggest that using CLs with higher f_0 results in less noise. However, if the dissipative part of the tip–sample force depends on the relative velocity between tip and sample ($r \geq 1$ in Eq. (19)), using CLs with higher frequencies might result in poorer resolution, since the dissipated energy will be proportional to f_0.

Acknowledgements

We thank Lukas Howald for discussions. This work was supported by BMBF Grant 13N6918/1.

References

[1] G. Binnig, C.F. Quate, Ch. Gerber, Phys. Rev. Lett. 56 (1986) 930.
[2] F.J. Giessibl, Science 267 (1995) 68.
[3] S. Kitamura, M. Iwatsuki, Jpn. J. Appl. Phys. 34 (1995) L145.
[4] R. Erlandsson, L. Olsson, P. Martensson, Phys. Rev. B 54 (1996) R8309.
[5] P. Güthner, J. Vac. Sci. Technol. B 14 (1996) 2428.
[6] R. Lüthi, E. Meyer, M. Bammerlin, A. Baratoff, T. Lehmann, L. Howald, Ch. Gerber, H.J. Guntherodt, Z. Phys. B 100 (1996) 165.
[7] S. Kitamura, M. Iwatsuki, Jpn. J. Appl. Phys. 35 (1996) L668.
[8] Y. Sugawara, M. Ohta, H. Ueyama, S. Morita, Science 270 (1995) 1648.
[9] J. Patrin, presentation at STM 95, Aspen, CO, 1995.
[10] M. Bammerlin, R. Lüthi, E. Meyer, A. Baratoff, J. Lü, M. Guggisberg, Ch. Gerber, L. Howald, H.J. Güntherodt, Probe Microsc. 1 (1997) 3.
[11] T.R. Albrecht, P. Grütter, D. Horne, D. Rugar, J. Appl. Phys. 69 (1991) 668.
[12] W. Allers, A. Schwarz, U.D. Schwarz, R. Wiesendanger, Rev. Sci. Instr. 69 (1998) 221.
[13] K. Fukui, H. Onishi, Y. Iwasawa, Phys. Rev. Lett. 79 (1997) 4202.
[14] Y. Sugawara, H. Ueyama, T. Uchihashi, M. Ohta, Y. Yanase, T. Shigematsu, M. Suzuki, S. Morita, Materials Research Society 1996 Fall Meeting, in: J. Michel, T. Kennedy, K. Wada, K. Thonke (Eds.), Proceedings E: Defects in Electric Materials II, Boston, December 1996, p. 16.
[15] F.J. Giessibl, Jpn. J. Appl. Phys. 33 (1994) 3726.
[16] F.J. Giessibl, Phys. Rev. B 56 (1997) 16010.
[17] N. Burnham, R.J. Colton, J. Vac. Sci. Technol. A 7 (1989) 2906.
[18] H. Hölscher, U.D. Schwarz, R. Wiesendanger, Appl. Surf. Sci. 140 (1999) 344.