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Resonant-tunneling theory of imaging close-packed metal surfaces by scanning tunneling microscopy

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We propose a resonant-tunneling theory of scanning tunneling microscopy (STM) by considering the general characteristics of a probe tip in which an electron trap, or impurity, causing the resonance is assumed to adsorb on an insulating contamination layer at the tip. The resulting constant-current STM image is the sum of two terms. The first term is due to the spatial variation of the conductance between surface and impurity, and the second term is due to the spatial variation of the force between surface and impurity. The relative contribution of the two terms to the image corrugation is determined by a constant K, which depends on the properties of insulating layer. Under the assumption of single atom adsorbed on a clean tip, our result reduces to the Tersoff-Hamann formalism, as expected. However, for a contaminated-tip approximation, we find that atomic corrugation of STM images can be dominated by the force corrugation between impurity and surface similar to that of atomic-force microscopy. The theory provides good agreement with experimental data on the corrugation as a function of z-axis piezoelectric element driving distance recently reported [J. Wintterlin *et al.*, Phys. Rev. Lett. **62**, 59 (1989)] for the Al(111)surface.

I. INTRODUCTION

The failure to interpret recent observations of atomic resolution on close-packed metal surfaces, Au(111) (Ref. 1) and Al(111) (Ref. 2), has raised a new challenge to existing theories of scanning tunneling microscopy (STM). For these surfaces, the corrugation of contour of constant local density of states (LDOS) at the Fermi energy is negligibly small at distances larger than 3 Å from the surface. Thus, a smooth STM image without any atomic corrugation, according to the Tersoff-Hamann (TH) theory,[3] is expected at a tunneling conductance of $10^{-7}\ \Omega^{-1}$ which corresponds to a gap distance of ~ 5 Å. In order to explain their results, Hallmark *et al.*[1] suggested that a localized surface state near the Fermi energy due to the presence of the bulk band gap of gold at the L point could possibly be the origin of the enhanced corrugation. However, this predominant electronic origin has been tentatively ruled out to be responsible for the atomic corrugation on Al(111) surface from the measurement of bias and gap-width dependence on the corrugation. From their observations, Wintterlin *et al.*[2] suggested that the elastic deformation of the adsorbed cluster on the tip, caused by adhesion forces between tip and sample, was the amplification mechanism behind both observations. Nevertheless, no real theoretical analysis was given. Wöll *et al.*[4] reported that the agreement between STM atomic corrugations on Au(111) and previous models of reconstruction suggests that STM measures spatially localized electronic states near the atomic cores. However, it is not clear how the localized electronic d states of the metal contribute more significantly to the tunnel current than the delocalized (sp) states.

The phenomenon of local-density corrugation enhancement was first observed on the basal plane of highly oriented pyrolytic graphite (HOPG).[5] During the past few years, several models have been proposed based on numerous experimental results obtained on this surface. The key point is the assumption of large elastic deformation of the surface due to the close approach to, or mechanical contact with, the surface by a contaminated tip.[6] The observed amplification effect and extremely low work function can thus be explained by the fact that a significant amount of the z-axis piezoelectric element driving distance contributes to the elastical deformation of the surface rather than to a change in the gap distance.

From the viewpoint of elasticity[7,8] and from computer simulation studies,[9] it appears that the close-packed metal surface, in contrast to the HOPG surface, is unlikely to be elastically deformed by forces in the 10^{-8}–10^{-7}-N range. The explanation proposed for HOPG is, therefore, not applicable. Moreover, the value of work function obtained on the aluminum surface by the measurement of tunneling current as a function of gap width was ~ 3.5 eV, which is close to the typical work function of clean metal surfaces. This observation strongly indicates that the change in gap width is approximately the same as the z-axis piezoelectric element driving distance,[10] and

therefore, the atomic corrugation observed is not simply caused by the anomalous amplification (as in the case of HOPG) of what is originally a small contour corrugation of constant LDOS of the surface. Batra and Ciraci[11] have proposed that the giant corrugations observed in STM images of HOPG is due to the chemical-bond formation between the surface and the tip atom. However, such a mechanism requires the tip to be at close proximity to the surface, i.e., ~1 to 2 Å, which does not agree with the high tunnel resistance ($10^8\Omega$) for a tunnel junction considered here.[3,12]

The role of a contaminated tip on the STM images of HOPG surfaces taken in air has been studied extensively,[13,14] and its various effects on the resolution are clearly demonstrated. The condition of the tip for imaging in ultrahigh vacuum (UHV), however, is not so clearly established. Kuk and Silverman[15] have conducted field-ion-microscopy (FIM) studies on a tunneling tip. They showed that a W tip prepared by field evaporation produced good resolution, but they also mentioned that the tip is often altered by adsorption of impurities during an experiment. Their FIM images also showed that the common practice of cleaning the tip *in situ* by applying a high field across the gap does not necessarily produce a sharp tip, despite the fact that STM workers could produce good images with such tips. Chiang and Wilson[16] also reported tip studies by scanning electron microscopy (SEM) and Auger-electron spectroscopy (AES). Their SEM images showed that heat and high-voltage treatments of a freshly etched W tip produced a blunting effect while AES studies showed varying degrees of contamination of carbon and oxygen on the tip with and without cleaning treatments. In view of the uncertainty surrounding the structure and cleanness of the tunneling tip, it is clear that much less is known about the condition of the tip than that of the surface under study in UHV. In the present paper, we propose a resonant tunneling theory for STM based on a contaminated-tip model to explain the atomic corrugations observed on close-packed metal surfaces.

Figure 1(a) shows schematically the structure of the model tip which we will use in the following discussions. The hatched area represents the conductive part of the tip. The region consisting of small open circles represents insulating contamination layers at the tip, while the solid circle at the end of this region represents an "impurity" atom which provides an isolated resonance near the Fermi energy. When a bias voltage is applied between the tip and surface, electrons tunnel first from the surface into the impurity and then out of the impurity into the tip. This special surface-vacuum-impurity-insulator-tip tunnel junction poses a resonant tunneling problem as shown in Fig. 1(b). The resonant tunneling aspect in scanning tunneling microscopy was noted previously by Lang[17] for a model tunnel junction consisting of two flat jellium surfaces with a single atom adsorbed on one of them. It was shown that the high lateral resolution is predominantly due to the localized nature of the wave function associated with the adatom, or impurity.

STM tips formed by electrochemical etching or mechanical grinding, unlike the field-ion-microscopy tip, usually has a contamination problem, such as an oxide layer. In most cases, especially in air STM experiments, these dirty tips are directly used to scan the surface without any further cleaning and very-high-resolution images can be obtained on various materials. For STM operated in UHV, a brief *in situ* cleaning of the tip using the field-desorption method is often performed. However, this can only temporarily remove the contamination. Recontamination can be caused by the diffusion of remaining contamination on the tip shank to the tip point. Therefore, a region of poor conductivity due to the contamination is likely to form at the end of a real STM tip. One possibility is that isolated scattering centers, or impurities, are introduced into this nonconducting inhomogeneous region during the initial preparation of the tip.[18] Another possibility is that during the STM operation, a surface atom is picked up and attached to the end of a contaminated tip. This conjecture is supported by the observations of both Hallmark *et al.*[1] and Wintterlin *et al.*,[2] who reported obtaining stable low-resolution images of pristine steps and terraces prior to

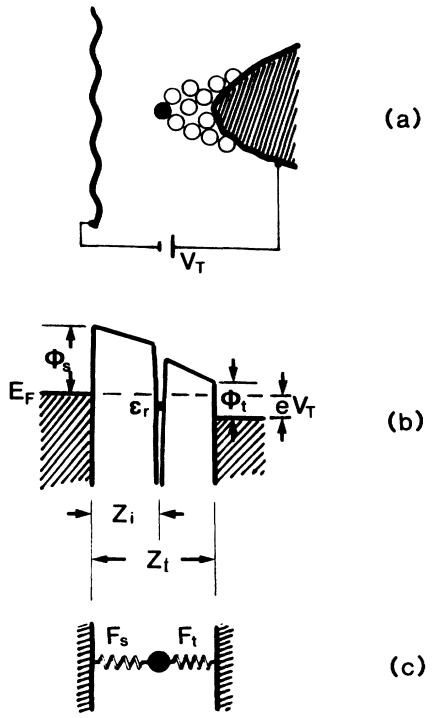

FIG. 1. (a) Schematic illustration of a contaminated tip near the surface. Hatched area is the conductive part of the tip, area consisting of open circles is the insulating layer, and the solid circle is the impurity causing the resonance. (b) The potential barriers of resonant tunneling corresponding to the tip model in (a). ϕ_s and ϕ_t are the effective barrier heights of surface-impurity and tip-impurity tunneling subsystems, respectively. ε_r is the resonant energy. (c) The simplified interaction of surface-impurity and tip-impurity subsystems. F_s represents the force between surface and impurity, and F_t represents the force between tip and impurity.

small tip changes which made the atomic corrugation visible. Regardless of how they are formed, the impurities act as minitips and provide very high spatial resolution. Obviously, for impurities buried deep inside the insulating layer, point contact between tip and surface is expected during the normal STM operation. If the repulsive force due to the mechanical contact does not reach a level to heavily damage the tip and the surface, the high lateral resolution is still expected due to the existence of resonances. Strong evidence of such an effect has been observed on a HOPG surface in the form of gigantic corrugation, extremely low work function, and large repulsive forces ranged from 10^{-6} to 10^{-8} N.

II. THEORY

We start with the transfer Hamiltonian method to evaluate the tunneling current[19] for the two subsystems: surface-impurity and tip-impurity. Considering a mathematically sharp resonance, the tunneling current for the surface-impurity subsystem is

$$I_{sr}=(2\pi e/\hbar)\sum_{\mu} f_s(E_\mu)(1-f_r)|M_{\mu r}|^2\delta(E_\mu-\varepsilon_r) \tag{1}$$

and the tunneling current for the tip-impurity subsystem is

$$I_{tr}=(2\pi e/\hbar)\sum_{\nu} f_r[1-f_t(E_\nu+eV_T)]|M_{\nu r}|^2\delta(E_\nu-\varepsilon_r)\ , \tag{2}$$

where f_s and f_t are the Fermi distribution functions of the surface and the tip, f_r is the occupancy of the resonant level, V_T is the tip bias, E_μ and E_ν, and ε_r are the energies of surface state Ψ_μ, tip state Ψ_ν, and resonant state Ψ_r. The transition matrix element $M_{\lambda r}$ ($\lambda=\mu,\nu$) is determined by Bardeen's formalism[20]

$$M_{\lambda r}=-(\hbar^2/2m)\int ds_\lambda(\Psi_\lambda\nabla\Psi_r-\Psi_r\nabla\Psi_\lambda)\ , \tag{3}$$

where the integral is over any surface lying entirely within the potential barrier of individual subsystem.

When the steady resonant tunneling state is reached, $I_{sr}=I_{tr}$. Combining Eqs. (1) and (2) to solve for f_r, we readily obtain the resonant tunneling conductance at small bias V_T and low temperature,

$$\sigma_T=\sigma_s\sigma_t(\sigma_s+\sigma_t)^{-1}\ , \tag{4}$$

with the subsystem conductance σ_α ($\alpha=s,t$) determined by

$$\sigma_\alpha=(2\pi e^2/\hbar)\sum_{\lambda}|M_{\lambda r}|^2\delta(E_\lambda-\epsilon_r) \tag{5}$$

Here we have assumed that the resonant level is near the Fermi energy and the resonant tunneling channel is open when the bias is applied.

A number of methods can be used for model calculations of the transition matrix element $M_{\lambda r}$ of each subsystem as defined in Eq. (3). The detailed discussion of them is beyond the scope of this paper. For a quick and reasonable estimation of the conductance σ_s of the surface-impurity subsystem, the TH formalism[3] can be used. In the following discussions, based on the localized nature of the wave function ψ_r, we need only to assume that the conductance of surface-impurity subsystem depends only on the impurity position (x_i,z_i) and the conductance of tip-impurity subsystem depends only on the distance z_t-z_i between the impurity and the end of the conductive part of the tip as shown in Fig. 1(b). Here x_i is the coordinate of the impurity on the x-y plane and z_i is that along the z axis. Mathematically, we write $\sigma_s=\sigma_s(x_i,z_i)$ and $\sigma_t=\sigma_t(z_t-z_i)$. Note that z_t-z_i is no longer a constant due to the existence and the flexibility of insulating layer.

The impurity position (x_i,z_i) depends on the forces on it from both surface and tip. For simplicity, we consider the surface and the conductive part of the tip as rigid. The insulating layer is regarded as a medium to transfer the force from tip to impurity by its own elastic deformation. An illustration of this simple interaction system is shown in Fig. 1(c). Similarly, we express the surface-impurity force as $F_s(x_i,z_i)$ and the tip-impurity force as $F_t(z_t-z_i)$. Because of its small mass, corresponding to a high resonant frequency of the system, the impurity during scanning follows a contour on which the total force is zero. In mathematical form, it is

$$F_s(x_i,z_i)-F_t(z_t-z_i)=0\ . \tag{6}$$

The small lateral component of the forces is neglected because the probing tip has to be stable, at least for a period of time to collect the entire image.

In principle, in the constant-current mode of STM, knowing the conductance and the force of each subsystem, we can solve z_i and z_t from Eqs. (4) and (6) as functions of x_i. Let us write

$$z_i(x_i)=z_e+\Delta_i(x_i) \tag{7a}$$

and

$$z_t(x_i)=z_s+\Delta_s(x_i)\ , \tag{7b}$$

where z_e and z_s are the average distances of the impurity and the tip measured from the surface; $\Delta_i(x_i)$ and $\Delta_s(x_i)$ are the corresponding corrugations. To the first order of Δ_i and Δ_s, Eq. (6) becomes

$$F_s(x_i,z_e)-c_s(x_i,z_e)\Delta_i(x_i)-F_t(z_s-z_e)+c_t(z_s-z_e)[\Delta_s(x_i)-\Delta_i(x_i)]=0\ , \tag{8}$$

where $c_s=-\partial F_s/\partial z$ and $c_t=-\partial F_t/\partial z$. Equation (8) can be rewritten as

$$\Delta_i(x_i)=(1+c_s/c_t)^{-1}\Delta_s(x_i)+(1+c_t/c_s)^{-1}[F_s(x_i)-F_t]/c_s\ , \tag{9}$$

where all the quantities are evaluated at the average positions, z_e and z_s. The dependence of c_s on x_i is not important.

Performing the similar expansion in Eq. (4) to the same order of Δ_i and Δ_s, we obtain

$$[\sigma_s-\sigma_s(x_i,z_e)]/\sigma_s'\simeq(1-\beta)\Delta_i(x_i)+\beta\Delta_s(x_i)\ , \tag{10}$$

where σ_s is the average value of $\sigma_s(x_i)$ and defined by $\sigma_s^{-1}=\sigma_T^{-1}-\sigma_t^{-1}(z_s-z_i)$, and

$$\beta=(\sigma_s^2\sigma_t')/(\sigma_t^2\sigma_s')\simeq(\kappa_t/\kappa_s)(\sigma_s/\sigma_t) .$$

Here $\sigma_\alpha'=\partial\sigma_\alpha/\partial z$ and κ_α is the decay length and is defined as $(2m\phi_\alpha/\hbar^2)^{1/2}$.

Solving for corrugation $\Delta_s(x_i)$ using Eqs. (9) and (10), we obtain

$$\Delta_s(x_i)\simeq K\Delta_e(x_i)+(1-K)\Delta_f(x_i) , \quad (11)$$

where $\Delta_e(x_i)$ and $\Delta_f(x_i)$ are the contours of the constant conductance σ_s and constant force F_s for the surface-impurity subsystem. K is approximately independent of x_i and determined by

$$K=(1+c_s/c_t)[1+(c_s/c_t)(\phi_t/(\phi_s)^{1/2}(\sigma_s/\sigma_t)]^{-1} . \quad (12)$$

Equation (11) indicates that contributions to the atomic corrugation in the constant-current image of STM generally arise from two terms. The first term represents the electronic contribution of surface, or the contour of constant LDOS of surface at Fermi energy under TH's spherical-tip approximation,[3] magnified by a constant K. The second term, similar to the atomic-force microscopy,[21] represents the surface-impurity interaction, or the contour of constant interatomic force, magnified by a constant $(1-K)$. The magnitude of K is determined through Eq. (12) by the ratios of conductance, σ_s/σ_t, of potential barrier heights, ϕ_s/ϕ_t, and of spring constant, c_s/c_t, which all strongly depend on the distance of impurity from surface.

III. DISCUSSION

The requirement that the resonance level is sharp and coincides exactly with the Fermi level is not necessary for the theory established in the last section. The impurity level can shift and broaden due to the interactions with the electronic states of the surface and the tip. In the case that the resonance peak is significantly away from the Fermi energy, we may still expect appreciable density of states of the impurity lying at the Fermi energy[17] for the impurity-assisted, or resonance, tunneling to occur, and the treatment can be represented by the integration of the transmission probability over energies surrounding the peak[22] without seriously affecting our presentation of the mechanism.

The possibility exists that more than one impurity center can occur in the contamination region of the tip, and more than one state can associate with each impurity. Exact treatment of such a complicated system is impossible without knowing the details of the impurity structure, but a result similar to Eq. (11) should be expected based on the following arguments. The first term in Eq. (11) is due to the spatial difference of electronic structure of the surface as it is established by other STM theories,[3,23] and the contribution to this term is dominated by the most protruding impurity center regardless of the location of other impurity centers. The second force term in Eq. (11) is due to the conjecture that the interaction between the tip and surface causes the elastic deformation of the tip which in turn changes the impurity structure and therefore the tunneling current. This again does not strongly depend on the impurity structure except for a minor change in constant K. In order to assure the appearance of the force term in Eq. (11), a significant change in tunnel current due to the slight deformation of the tip has to be assumed, which is, of course, unlikely if the tip is clean.

The constant K as introduced in our theory can be regarded as a fitting parameter because of the unknown structure of the tip. Nonetheless, a general discussion of its magnitude at two extreme cases is still in order. At one extreme, we consider a single atom adsorbed on a clean metal tip. The strong chemical bond between the adsorbate and the electrons in conduction band of the metal produces a high conductance of the impurity-tip subsystem, σ_t. Therefore, we have $\sigma_s/\sigma_t \ll 1$ at normal STM imaging conductance and $\phi_t/\phi_s \ll 1$ because the barrier height ϕ_t of the impurity-tip subsystem almost collapses.[11] Also the gap distance is in general about 5 Å (Refs. 3 and 12), and tip-surface interaction is mainly due to weak, delocalized van de Waals forces. c_s is small compared to c_t at this distance because the impurity is strongly bound to the tip. Therefore, $K\simeq 1$, and the first term dominates the corrugation of the image. Such a clean-tip configuration, usually called single-atom imaging, has been previously discussed in detail by Lang.[23] At the other extreme, we consider a single atom absorbed on a dirty tip where σ_t may be much smaller than σ_s. The tunneling barrier is mainly established in the contaminated tip. For such a case, the gap between the tip and the surface will be very small (comparable to the lattice spacing of the surface), the barrier height ϕ_s will collapse[11,24] (ϕ_t is in the order of 0.1 eV), and the interaction between the tip and the surface becomes strong. We therefore expect that $\phi_t > \phi_s$ and $c_s \sim c_t$. Incidentally, c_s cannot be too large compared to c_t; otherwise serious damage could happen to the tip. Therefore, $K\simeq 0$ in this case and the second term dominates the corrugation.

For a K value between the two extremes which could be due to the slight contamination of the tip, both terms contribute to the corrugations of the STM image. The consideration of the second term has important implications for the interpretation of STM images when the contour of constant force differs largely from that of constant LDOS. In that case, the position of bright spots in the image may not represent the exact position of the peaks of the contour line of constant LDOS. This effect is likely to be expected on those semiconductor surfaces on which various energy-dependent surface states localized at different positions exist.

IV. APPLICATION: Al(111)

As an application of Eq. (11), we choose the Al(111) surface because it is the only close-packed metal surface on which a systematic study[2] has been done. Considering the high lateral resolution of STM images,[1,2,4] we assume a single aluminum atom attached to the end of the tip. Although consideration of the tip shape is important in the interpretation of many asymmetric STM images,[25] a

good starting point would be considering only a single-atom interaction with the surface.[6] The next layer of atoms in the tip does not play a significant role except for a minor distortion of the image.[26] To calculate the force between the impurity and the surface, we use the effective medium immersion potential energy of a free aluminum atom in a jellium surface.[27] The force calculation below results in an inward relaxation of the adatom which provides a simple explanation of the oscillatory phenomenon,[27] but may not give a correct value for the unit-cell length.[28] Within the range of total charge density of our interest, the potential energy can be approximately expressed in the form

$$V(x_i,z_i)\simeq a_0[\rho(x_i,z_i)-\rho_0]^2+V_0 , \tag{13}$$

where $\rho(x_i,z_i)$ is the total charge density of the surface at the impurity position, $a_0\simeq 1.3\times 10^4$ eV a.u.^{6}, $\rho_0\simeq 7.8\times 10^{-3}$ a.u.$^{-3}$, and V_0 is a constant. The z component of the force, $F_s(x_i,z_i)$, is given by a $-\partial V(x_i,z_i)/\partial z_i$, where $F_s=-2a_0(\rho-\rho_0)\partial\rho/\partial z_i$. The van de Waals interaction is not considered here because it only dominates at large distances. For the computation of total charge density of the surface, we use the approach of superposition of atomic charge density[3] and choose the exponential form $\rho_a\exp(-2\kappa r)$ for the aluminum atomic charge density. The contour lines of constant total charge density thus calculated with $\rho_a\simeq 0.4$ a.u.$^{-3}$ and $\kappa\simeq 1.1$ Å^{-1} agree reasonably well with those obtained by more rigorous calculations.[29]

Figure 2(a) shows the contour lines of total charge density of Al(111) surface in the vacuum region on the $(1\bar{1}0)$ plane. z is the distance measured from surface. The space between the two neighboring (111) planes is 2.3 Å. Correspondingly, Fig. 2(b) shows the contour lines of constant force between a free aluminum atom and a jellium surface. The numbers marked on every other contour in Fig. 2(a) represent the value of total charge density of the contour in a unit of millielectrons per cubic bohr, and those in Fig. 2(b) represent the force value of the contour in units of eV/Å or 1.6×10^{-9} N. It is clearly seen that the measurable contour corrugation in both cases lies within a distance of less than 3 Å, as expected. The observed corrugation of STM images on this surface, therefore, implies a close approach of the impurity atom to the surface. The conductance σ_s of the surface-impurity subsystem within this region, according to the TH formalism,[3] is thus larger than 10^{-3} Ω^{-1}. However, such an estimation is not warranted because the transfer Hamiltonian method on which TH theory is based may fail when the transition probability between the two electrodes becomes large. Using a tight-binding method, Ferrer *et al.*[30] calculated the tunneling current at small gap distances and found that the contact resistance, corresponding to gap distances of 1.5–3 Å,[12] is on the order of 10^4 Ω, which is about 3 to 4 orders of magnitude less than the experimental value. Therefore, at a tunneling resistance of 10^7 Ω, we have $\sigma_s/\sigma_t\simeq 10^3$ ($\gg 1$), $\phi_s\simeq 0$,[24] and $c_s/c_t\simeq 1$. The estimation of c_s/c_t is based on the fact that the position of the impurity atom is around the valleys of both potential-energy curves for surface-impurity and tip-impurity subsystems. Therefore, $K\simeq 0$, and the second term in Eq. (11), i.e., the atomic-force contribution, dominates the corrugation.

Figure 3 shows the calculated contour corrugation Δ_f, or Δ_s, as a function of average impurity distance z_e from the surface as defined in Eq. 7(a). The force axis, $F_s(z_e)$, as shown below the z_e axis, indicates the force value of each contour line. The scale of contour corrugation is labeled on the right side, while the natural logarithmic scale of the corrugation is on the left. For the comparison of our results with experimental data, the change of the z-axis piezoelectric element driving distance z_s, as correlated with that of z_e through the first term of Eq. (9), is calculated with $c_s/c_t\simeq 1$ and marked on the top as the z_s axis.

A good agreement between the theoretical curve (solid line in Fig. 3) and the experimental results[2] (solid circles in Fig. 3) is obtained, especially the rapid fall of the corrugation on the part where the force becomes attractive. Although the impurity is very close to surface, less than 2

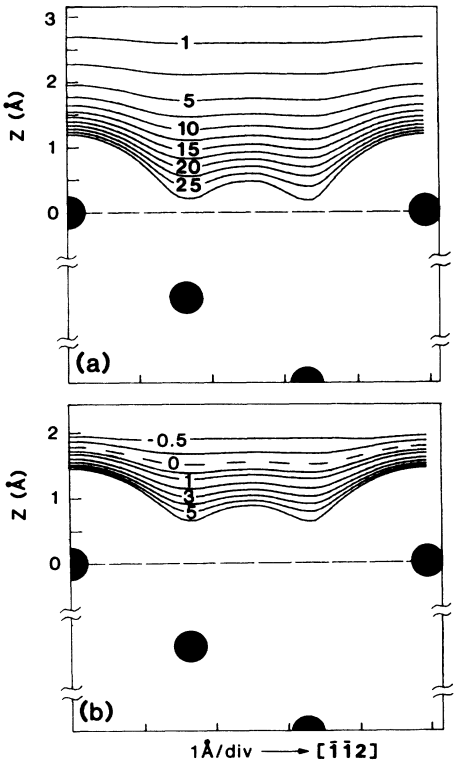

FIG. 2. (a) The contour lines of total charge density on the Al$(1\bar{1}0)$ plane. The numbers on every other contour are the values of total charge density of the contours in units of millielectrons per cubic bohr, or 10^{-3} a.u.$^{-3}$. (b) The contour lines of constant force between a free aluminum atom and aluminum surface. The numbers on the contours are the force values of the contours in units of eV/Å, or 1.6×10^{-9} N. The horizontal dashed lines in both (a) and (b) indicate the Al(111) surface, and z is the distance measured from the surface. Solid circles represent Al atom positions on the $(1\bar{1}0)$ plane.

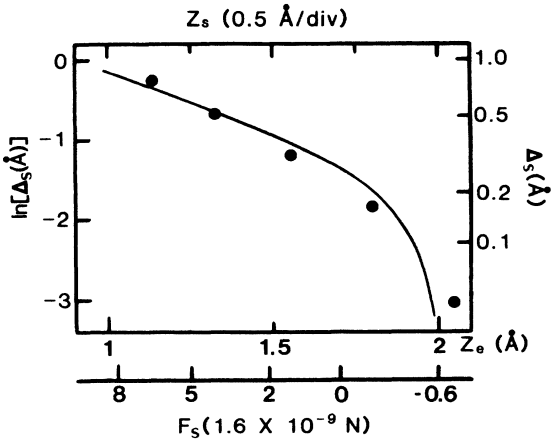

FIG. 3. Calculated curve (solid line) of contour corrugation of constant surface-impurity force as a function of the force F_s and average distance z_e of impurity from surface. F_s and z_e are related as shown in Fig. 2(b). Δ_s is the corrugation, i.e., the difference between the maximum and minimum in any given force contour in Fig. 2(b). z_s is the relative change of the z-axis piezoelectric element driving distance calculated with the ratio $c_s/c_t=1$ (see text). z_s corresponds to the $z-z_0$ axis given in Ref. 2. The solid circles are the experimental data points from Ref. 2.

Å, the force is very small, only on the order of 10^{-9} N. We found that the maximum corrugation of this surface is about 0.9 Å at ~ 1 Å away from the surface, and the force correspondingly is about 2×10^{-8} N. The attempt of further increasing the corrugation by decreasing the tunneling resistance may cause the impurity atom to be trapped on the surface or significant plastic deformation of the tip.[31] The image of STM when operated under these conditions will become extremely unstable, as reported.[1,2] Obviously, the most stable case is when the tip follows the contour of zero force which is shown in Fig. 2(b) as a dashed curve. The contour corrugation is correspondingly 0.28 Å, which incidentally is the same as the typical corrugation 0.3 Å reported for both gold and aluminum surfaces.

Finally, we wish to point out that the observed work function of Wintterlin *et al.*,[2] ~ 3.5 eV, is dominated by the barrier height ϕ_t between impurity and tip instead of vacuum barrier height ϕ_s when the impurity is at such a close approach to the surface. The apparent work function ϕ_A is defined through the equation $d(\ln I_T)/dz_s=-2(2m\phi_A/\hbar^2)^{1/2}$ (Ref. 24). We found that when $\phi_s\simeq 0$, $\phi_A\simeq\phi_t/(1+c_t/c_s)^2$ and ϕ_t has to be about 14 eV in order to generate 3.5 eV for ϕ_A with $c_s/c_t\simeq 1$. Such a large value of ϕ_t could be due to a variety of reasons, e.g., significant contribution to the resonant tunneling current from states with nonzero wave-vector components parallel to the surface[22] or the highly asymmetric nature of the insulating barrier where the most direct path of the tunneling current between the conductive part of the tip and the impurity is not necessarily along the z direction.

V. CONCLUSIONS

We have proposed a resonant tunneling theory of scanning tunneling microscopy by considering the general properties of a contaminated probing tip with an adsorbed impurity acting as a resonance. We find that the constant current STM image generally contains two contributions, i.e., spatial variations of both conductance and interatomic force of the surface-impurity subsystem. The relative contribution of the two terms to the observed corrugation strongly depends on the cleanness of the tip characterized by a constant K. We believe that the second term in Eq. (11) due to spatial variations of the interaction of the surface-impurity is important for a proper interpretation of STM observations. This applies not only to close-packed metal surfaces as discussed in the text, but also to other types of surfaces as long as contamination exists on the STM tip. While our proposed mechanism is certainly one possibility among several others (as reviewed in the Introduction), we have shown that for the Al(111) surface, a good agreement of our theory with the experimental results has been achieved with a proper choice of the ratio c_s/c_t. Our mechanism is also consistent with the suggestion of an adsorbed metal cluster on the probe tip by Wintterlin *et al.*[2] The instability of the "high-resolution" tip observed in Al(111) and Au(111) surfaces could conceivably be due to the attachment or detachment of the adsorbed resonance impurity according to our model.

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