Jpn. J. Appl. Phys. Vol. 34 (1995) pp. L 789–L 792
Part 2, No. 6B, 15 June 1995

Simulation of Atomic Force Microscopy Image Variations along the Surface Normal: Presence of Possible Resolution Limit in the Attractive Force Range

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(Received April 17, 1995; accepted for publication May 16, 1995)

Variations of atomic force microscopy (AFM) images as tip-sample distance is varied were examined using a newly developed AFM simulation code ACCESS (AFM simulation Code for Calculating and Evaluating Surface structures) with a Morse-type pairwise potential. A model system consisting of a single atom tip (an "ideal" AFM tip) and a face-centered cubic (fcc) (100) surface with or without point defect showed perfect atomic resolution when scanning was performed in the repulsive force range. In the attractive force range, image contrast inversion was observed twice with the increase of tip-sample distance. Simulation on the point defect surface indicated that this inversion is due to a collective force from more than one atom being imaged as one bright spot. Exact correspondence between the sample surface registry and the simulated image in this force range appears to be coincidental.

KEYWORDS: atomic force microscopy, attractive force, noncontact mode, simulation, point defects, resolution limit, Morse potential

1. Introduction

The use of atomic force microscopy (AFM) is rapidly expanding in diverse fields such as material sciences, electrochemistry and biology.[1)] Recent efforts being made in AFM involves its operation in the attractive force range,[2)] in order to avoid sample damage by the contact of the tip and to enable the imaging of soft samples such as polymers and biological samples. The imaging in the attractive force range is also claimed to have better resolution compared to the contact-mode scanning in the repulsive force range.[2)]

Despite these potential merits associated with the attractive force (noncontact mode) operation, reports on successful imaging are scarce, mainly due to experimental difficulties associated with AFM operation in the weaker force fields, and the characteristics of the AFM images taken at the attractive force range are not well known. This calls for the use of computational simulation techniques. While several attempts have already been made, most of them are concerned with tip-sample interactions,[3-12)] and examinations through the simulations of AFM images themselves[13-17)] are scarce. Furthermore, all the latter studies deal with imaging in the repulsive force range that corresponds to the contact-mode AFM operation, and imaging in the attractive force range has not been adequately addressed. We started examining this problem with a simulation using a newly developed AFM simulation code ACCESS (AFM simulation Code for Calculating and Evaluating Surface Structures)[18)] and preliminary results obtained using a Morse-type pairwise potential are described here.

2. Methods

The present AFM simulation using ACCESS was performed by calculating the pairwise forces acting between the AFM tip atom and the atoms that constitute the sample, in order to determine the total surface forces acting on the AFM tip. For this purpose a Morse-type potential (1) was used.

$$U_{ij}(r_{ij}) = D_{ij}\left[\exp\{-2\beta_{ij}(r_{ij}-r^*_{ij})\} - 2\exp\{-\beta_{ij}(r_{ij}-r^*_{ij})\}\right] \quad (1)$$

Here D_{ij} denotes bond energy, β_{ij} shape of potential curve, r_{ij} distance and r^*_{ij} average distance between atoms i and j. The parameters used in the present study, listed in Table I, were obtained by first determining their pure-component values through a fit with experimental bulk crystallographic parameters, then choosing appropriate values for the Cu-Fe pair. $\beta_{\mathrm{Cu-Fe}}$ was set equal to its bulk metal value, which happened to be the same for both Cu and Fe. $r^*_{\mathrm{Cu-Fe}}$ was set as the sum of Cu and Fe metal atom radii. It should be noted that these parameter values, including the potential shape, are not critical in the present simulation results and their interpretations. Forces involved in actual AFM systems are diverse,[2,19)] including Coulomb, dipole and van der Waals forces, and the present potential is only a representative and is not meant to cover all the possible potentials existing in the actual AFM systems.

In the present calculations, the tip was represented by an Fe atom, although any materials may be used for the present purpose. The use of a single-atom tip simulates the most ideal situation for AFM measurements. Copper (100) was chosen as the sample surface. The purpose behind the use of the metal tip and the metal surface as a model AFM system is to simplify forces acting between the tip and the sample compared to systems which are covalent and/or partially ionic. A Cu(100) metal slab with 4 layers of 11×11 atom arrays was constructed. Scanning was performed only on the center

Table I. Morse potential parameters used in the present study.

	D_{ij} [kJ/mol]	β_{ij} [1/Å]	r^*_{ij} [Å]
Fe-Cu	3.0	1.98	2.52

5×5 region (cf. Fig. 1(a)), in order to eliminate the edge effect.

The force representation in this paper is such that the attractive force is taken in positive direction and the repulsive in negative. Thus in the force images presented in this paper the gray scale indicates attractive force as bright, and as the attractive force weakens, or the force becomes repulsive, the gray scale becomes dark. This is the reverse of a common representation of actual AFM images obtained by the contact imaging-mode operation.

3. Results and Discussion

3.1 *Perfect surface*

Figure 1 shows the scanned area of a Cu(100) model sample surface (a) and the force distribution on the surface as is felt by the single-atom tip (b-d) at different tip-sample distances. The tip-sample distances, which are defined as the nucleus-nucleus distances between the topmost atomic layer of the sample and the tip atom, are 1.44, 2.89, and 3.52 Å in Figs. 1(b), 1(c) and 1(d), respectively. Again these values should not be taken as critical: they were chosen arbitrarily as representative distances for different force ranges. Thus force felt by the tip is repulsive at the tip-sample distance of 1.44 Å, while it is attractive at 2.89 and 3.52 Å. Comparison of the images presented in Fig. 1 leads to a few interesting observations. Firstly, in the repulsive force range (Fig. 1(b)), the dark spots in the image (stronger repulsive force) correspond exactly to the sample atomic position. Apparently, the tip feels the force from the sample atom nearest to it most strongly, and thus each dark spot in the force image represents the corresponding atom on the surface. This image simulates contact-mode imaging in actual AFM operations, thus confirming the common notion that under ideal conditions (viz., single-atom tip), AFM captures "true" atomic images.

When the scanning is performed in the attractive force range, the situation changes. Stronger attractive force regions (lighter tone) in Fig. 1(c) are not found directly above each atom position, but are located at the center of the squares made by four Cu atoms. This is not a tip effect of any sort, because the tip employed here is an "ideal" single-atom tip. This phenomenon is interpreted as indicating that, at this tip-sample distance with the present potential, composite force from a collection of atoms becomes stronger than the force from a

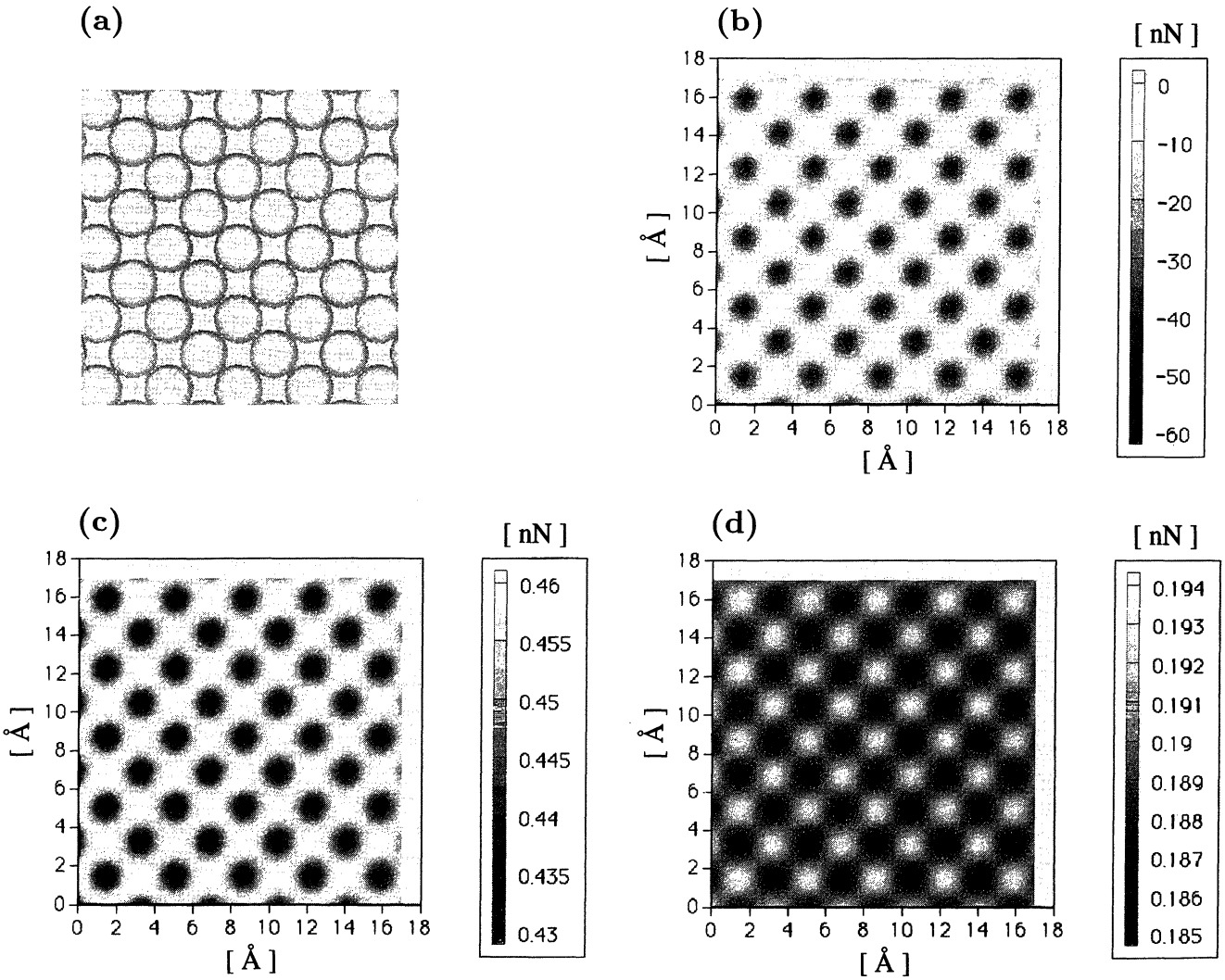

Fig. 1. Model sample surface of perfect lattice (a) and its simulated AFM images at the tip-sample distances of 1.44 Å (b), 2.89 Å (c) and 3.52 Å (d) using a single-atom tip.

single atom. Obviously, in the present case the composite force originates from at least four atoms that form a surface unit cell, rendering an image at the center of each unit cell. It should be noted that the image shown in Fig. 1(c) gives the appearance of an atomically resolved image although in reality it is not.

At the tip-sample distance of 3.52 Å, a simulated image shown in Fig. 1(d) is obtained. Here the bright spots (stronger attractive force) returns to the surface atomic positions again. This, however, is not a "true" atom-resolved image any more, considering the fact that at the tip-sample distance of 2.89 Å, atomic resolution has already been lost. Then the correspondence between the surface atom positions and the bright spots must be purely coincidental. This occured in the present case because the examined surface has fourfold symmetry and the used potential is spherical, producing a composite force field with exactly the same periodicity as that of the sample surface all the time with or without a phase shift. It is noted again that such conditions also produce an apparently "atomically resolved" image even though it does not reflect true atomic positions.

As mentioned earlier the present simulation results are not critically dependent on the potential shapes and their parameters. However, they should be strongly affected if the force field around a sample atom is anisotropic in any way. In that case the image variation as a function of tip-sample distance may take a very different appearance from what is observed here. With this reservation, however, we would like to question the claim made by Ohnesorge and Binnig[2] that AFM operation in the attractive force range provides the most reliable resolution.

3.2 *Point defect surface*

Observation of surface point defects is often taken as evidence of true atomic resolution.[2] Thus it may be interesting to simulate the tip-sample distance variation of a point defect surface with the present simulation model. Figure 2 shows a Cu(100) model sample surface with a point defect at the center of the surface (a) and the force distribution on this surface as it is felt by the single-atom tip at the three different tip-sample distances (b-d). In the repulsive force range (Fig. 2(b)), the single-atom tip precisely reproduces the defect position as well as other atom positions, as may be expected and in agreement with the results of Ohnesorge and Binnig.[2]

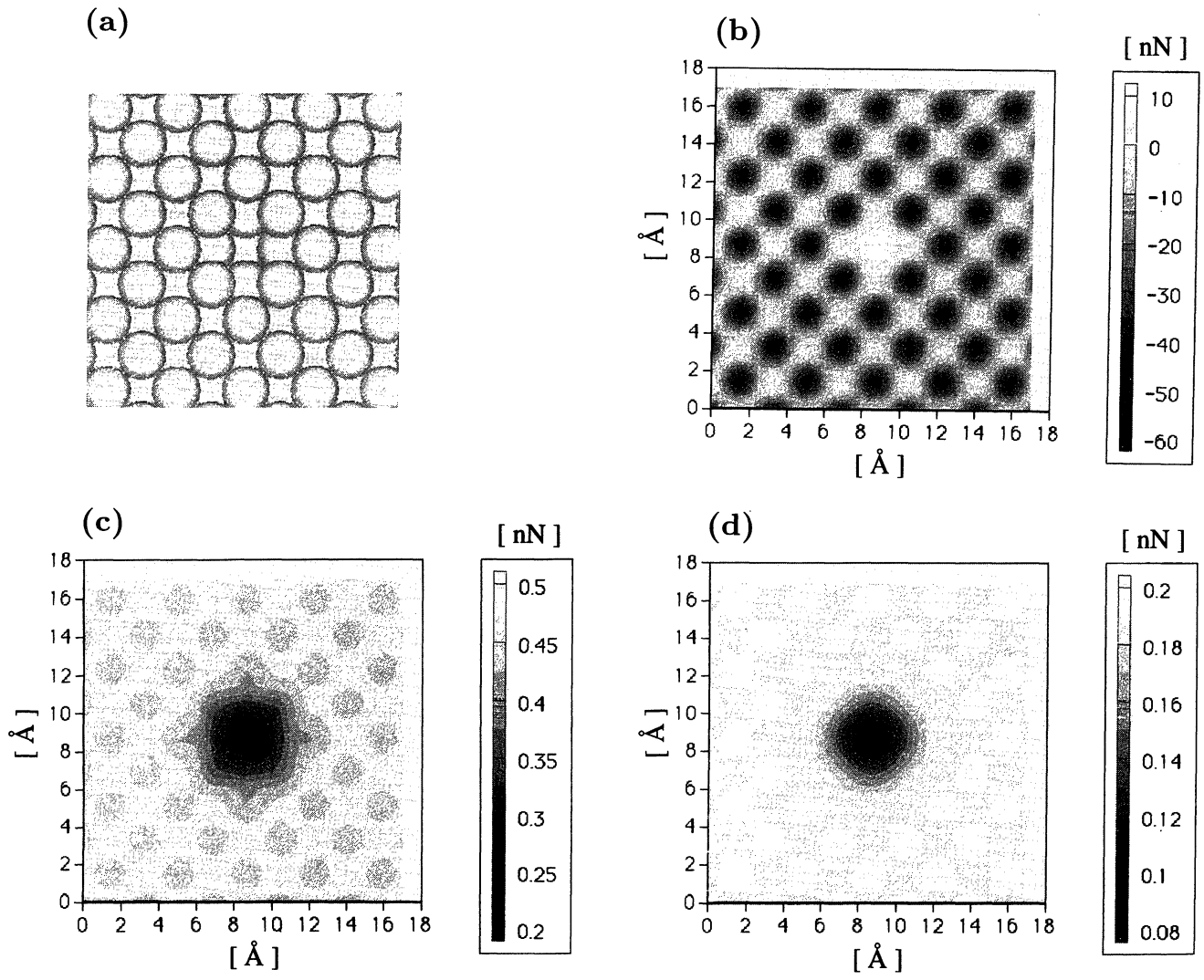

Fig. 2. Model sample surface with a point defect (a) and its simulated AFM images at tip-sample distances of 1.44 Å (b), 2.89 Å (c) and 3.52 Å (d) using a single-atom tip.

In the attractive force range (Figs. 2(c) and 2(d)), the defect image is found centered at the defect position but its size is much larger than the one found in Fig. 2(b). In Fig. 2(c) which is scanned at the tip-sample distance of 2.89 Å, the eight atoms surrounding the point defect are barely visible and they are not clearly resolved. This fact, along with the observation made in the previous section that at this tip-sample distance the strongest attractive force is found at the center of each four-atom unit cell, indicates that the collective force which produces the bright spots in Fig. 1(c) and Fig. 2(c) comes from two neighboring atoms, not a single one. In the present sample with a square surface symmetry, this results in the formation of an image at the center of each 2×2 surface unit cell.

At the tip-sample distance of 3.52 Å, the eight atoms surrounding the point defect almost completely lost their resolution (Fig. 2(d)). From this it is deduced that at this distance, the tip is always under the effect of forces from the nearest 9 (viz., 3×3) atoms. At the center of this 3×3 unit, there exists an atom in the case of the present square lattice, thus the registry formed with this force field coincides with that of the original surface (cf. Fig. 1(d)).

It is noted in Fig. 2(d) that a weaker effect of the point defect is also detected in the entire image of this 5×5 scanned region, as the observed shapes of the bright spots show apparent radial variation, becoming more smeared with increasing distance from the defect. This is not an edge effect, because such phenomenon is not observed in Fig. 1(d) which is scanned at the same distance in exactly the same manner.

4. Conclusions

A simple simulation of AFM images using a Morse-type pairwise potential indicated that the AFM image contrast may vary as a function of tip-sample distance. This is due to the fact that the force exerted on the tip comes from different numbers of surface atoms at different tip-sample distances: it comes from one atom when the tip-sample distance is very short, and from an increasing number of atoms with increasing tip-sample distance. It is found that a particular surface symmetry may produce coincidental "atomic" images at the distance where the tip is affected by more than one surface atom. It is confirmed that a point defect can be used as a test structure to examine true atomic resolution.

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