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Simulation of tip–sample interaction in the atomic force microscope

Brian S Good† and Amitava Banerjea‡

† National Aeronautics and Space Administration, Lewis Research Center, Cleveland, OH 44135, USA

‡ S N Bose National Centre for Basic Sciences, DB17 Salt Lake City, Calcutta 700064, India

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Abstract. Recent simulations of the interaction between planar surfaces and model atomic force microscope (AFM) tips have suggested that there are conditions under which the tip may become unstable and 'avalanche' toward the sample surface. Here we investigate via computer simulation the stability of a variety of model AFM tip configurations with respect to the avalanche transition for a number of fcc metals. We perform Monte Carlo simulations at room temperature using the equivalent-crystal theory (ECT) of Smith and Banerjea. Results are compared with recent experimental results as well as with our earlier work on the avalanche of parallel planar surfaces. Our results on a model single-atom tip are in excellent agreement with recent experiments on tunnelling through mechanically controlled break junctions.

1. Introduction

Several recent studies have reported [1–5] an avalanche effect in adhesion. These reports indicate that there are conditions under which solid surfaces will collapse together even when the initial interfacial spacing is significantly larger than the bulk interplanar spacing. This, of course, is intimately tied to the question of the stability of the tip in the scanning tunnelling microscope (STM) or the atomic force microscope (AFM) when the probe tip is brought into near contact with the sample surface. In fact, the first suggestion that solid surfaces could jump together was made by Pethica and Sutton [1] who were primarily interested in the interaction of a metallic tip with a flat surface because of its relevance to the STM/AFM. Their analyses were based on a Lennard-Jones pair potential and on continuum elasticity theory. These approximations have serious limitations which the authors themselves have pointed out [1]. Subsequently others have investigated [2–5] the stability of adhering flat surfaces using more appropriate semi-empirical methods and have found quantitative evidence for an avalanche effect.

Some investigations of the interaction of a model STM/AFM tip with a sample surface have been carried out in the recent past [6–9]. These have either involved tight-binding [6] (TB) or self-consistent-field pseudopotential [7] studies with no relaxations of the atoms in the tip and sample or molecular dynamics (MD) studies using semi-empirical methods such as the Stillinger–Weber potential for Si [8]. The former have generally focused on small model tips with or without a 'support' and concentrated on the electronic effects such as the creation of tip-induced localized states. The latter group of investigations have tended to model larger and considerably blunter tips often concentrating on actually crashing the tip into the sample much as a nano-indenter does or on the friction involved in sliding a tip

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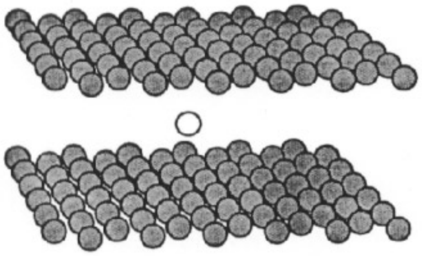
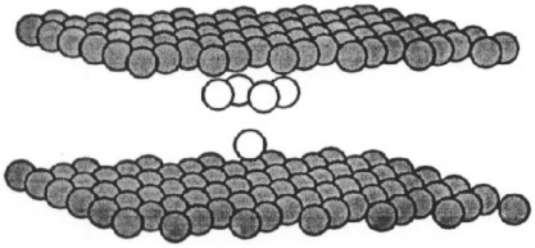
over a sample surface [9]. They have not, in general, worried about the stability of the tip when in proximity with the sample surface.

In this paper we present a study of tip stability in a model of the AFM using the equivalent-crystal theory (ECT) introduced by Smith and co-workers [10–12] and later modified by Smith *et al* [13]. We present results of simulations of the interactions between tips of two different geometries—a single atom or a pyramid of five atoms attached to the flat surface of a semi-infinite slab—and a flat sample surface. The simulations have been conducted using the Metropolis Monte Carlo algorithm [14] at a temperature of 300 K for a number of fcc metals and for fcc iron. Preliminary results of similar simulations for Ni at zero temperature have been presented elsewhere [15].



(a) Single-atom tip



(b) Five-atom tip

Figure 1. The geometry of (a) single-atom and (b) five-atom STM tips. Note that the vertical layer spacing has been expanded by a factor of 1.5 for clarity.

2. Simulation procedure

The results presented below are obtained from Monte Carlo simulations performed using the ECT [10–12] which is based on the universal binding energy relation (UBER) [16] and has been shown to provide accurate energetics in a wide variety of reduced-symmetry situations, including layerwise avalanche [2, 4, 5], surface relaxation [11, 12, 17], and surface reconstruction [18]. The ECT, which has now been modified [13] to better handle shear-type distortions, expresses the energy of a collection of atoms as a sum over individual atomic contributions. Each atomic contribution comprises four different terms. The first of these terms depends essentially on the local density in the immediate neighbourhood of the atom in question and is generally the largest single contribution to the surface or interface energy. The second term accounts for local deviations in symmetry away from that of the ground-state crystal and local variations in nearest-neighbour distances. The other two terms depend on changes in bond angles and account for shear-like distortions. It has been shown [18] that the last two, bond-angle-dependent terms contribute little to the relaxation energies of metal surfaces. Hence, in this study we have neglected the last two terms of the ECT energy expression [13] and essentially used the earlier version [10–12] of the ECT.

The model system used in this work consists of two parallel slabs of metal atoms separated by a gap normal to the fcc (001) interface. Each slab consists of seven atomic layers, each layer being 5 × 5 lattice constants. Projecting into the gap from one of the slabs is an atomically sharp tip in perfect registry with the underlying atomic plane. The two slabs are arranged so that the 'tip' comes down on the fourfold hollow in the centre of the surface of the other, 'sample' slab. In this work we have, for computational reasons, restricted our attention to tips containing either a single atom, or a five-atom pyramid consisting of a single-atom tip layer atop a four-atom base layer. This tip, either the single atom or the five-atom pyramid, is attached to one of the slabs as described above. The geometry of the two tips and adjacent layers is shown in figure 1.

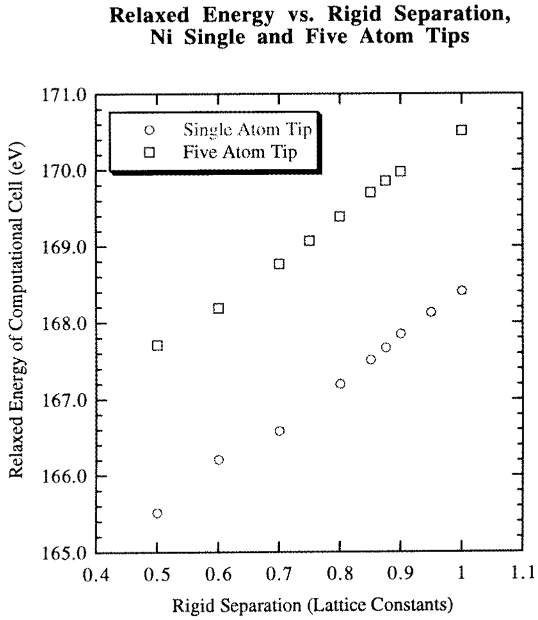


Figure 2. Plots of relaxed energy versus rigid separation for single- and five-atom Ni tips approaching a Ni(001) surface.

In our method, the initial configuration of the computational cell is set by adjusting the gap to a value between zero (where the single tip atom is in its ideal crystallographic position with respect to both slabs), and two lattice constants, a separation known to be larger than the critical separation at which avalanche occurs for planar surfaces approaching each other [2]. Subsequently, all atoms in the tip and in the three layers of each slab closest to the

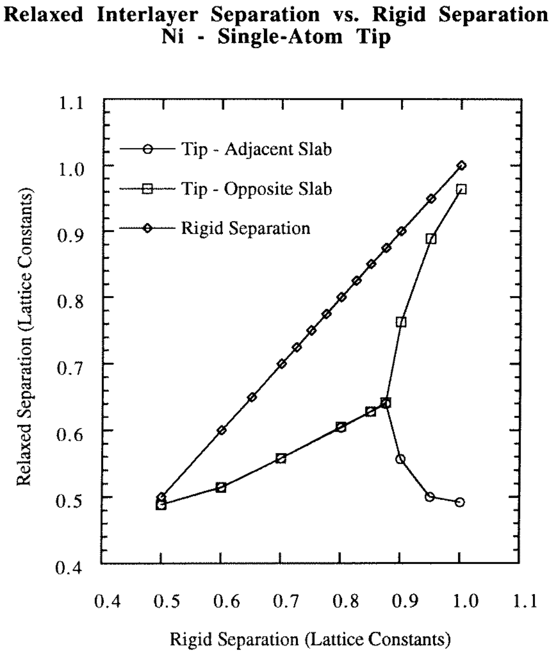


Figure 3. Plots of relaxed interplanar separations versus rigid separation for a single-atom Ni tip approaching a Ni(001) surface.

gap are allowed to relax so as to minimize the total energy of the computational cell. The relaxations are performed on a cubic lattice, but there are no additional constraints, e.g. the relaxations are atomwise, rather than layerwise as in previous work [4]. A sequence of four refinements are performed, using progressively smaller step sizes, with the smallest being 0.001 lattice constants. The standard Metropolis Monte Carlo algorithm [14] is used, with a temperature of 300 K.

3. Results

Simulations have been carried out for the fcc metals Cu, Ni, Ag, and Au, as well as for fcc-Fe. The results for all of these are qualitatively the same with the possible exception of those for Au. Hence, we present here only the results for Ni, as representative of four of the metals studied, and for Au, which appears to be somewhat different from the other metals.

Displayed in figures 2–4 are the results of the simulations of single- and five-atom Ni tips. While figure 2 displays plots of the relaxed energy of the appropriate systems as a function of the rigid separation, figures 3 and 4 show plots of a variety of interlayer separations as functions of rigid separation. The scale of the horizontal axis in all three figures is chosen so that a rigid separation of 0.5 lattice constants corresponds to the situation in which all atoms are in their bulk crystallographic positions. Figure 3 shows the separations between the tip atom and the adjacent slab (to which the tip atom remains attached at large separation), and between the tip atom and the opposite slab, for the single-atom tip. The rigid separation is also plotted for comparison. It can be seen that the tip atom exhibits clear avalanche behaviour—for separations larger than a material-dependent critical separation,

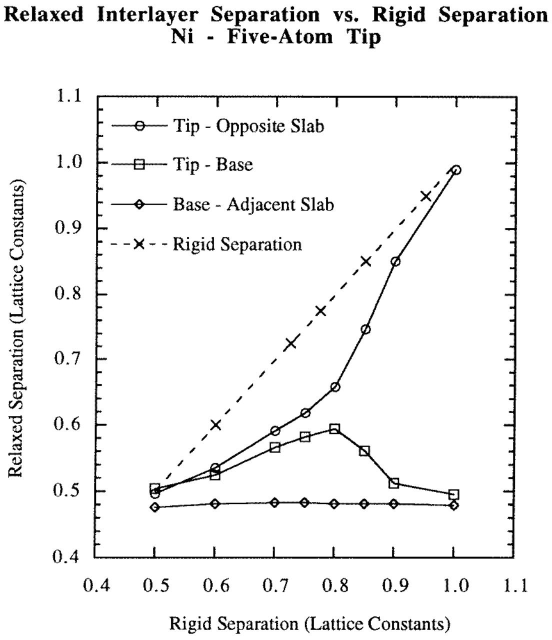


Figure 4. Plots of relaxed interplanar separations versus rigid separation for a five-atom Ni tip approaching a Ni(001) surface.

the tip atom remains in the vicinity of the slab to which it is initially attached. When the separation falls below the critical value, however, the tip atom finds it energetically favourable to occupy a position in the centre of the gap. It should be noted that the two tip–slab separations do not add up to the rigid separation because there is relaxation of the slab layers as well. It should also be noted that the behaviour of the slabs differs from that exhibited in the layerwise avalanche of metal surfaces [2–5] These studies found that when two slabs are brought closer together than a critical separation, not only will the surface layers avalanche together, but the adjacent layers in each slab will follow, giving rise to a rarefaction wave which propagates away from the gap. In the current work, in all cases the slab surface layers remain further apart than the critical separation, even when the rigid separation is 0.5. We therefore do not expect to see a layerwise avalanche. In addition, the atoms directly beneath the tip atom are more strongly bound to the slab than to the tip, and are unlikely to avalanche towards the tip as it migrates toward the centre of the gap. This is precisely the behaviour exhibited by our model system. While there is a distinct puckering of the slab surface directly under the tip atom on either side of the gap, the puckered atoms never complete the avalanche process and remain attached to their respective slabs.

The relaxed interfacial energies of the computational cell for both Ni tips are displayed in figure 2. The energy plots do not clearly exhibit the sharp drop characteristic of layerwise avalanche. This can be understood by recalling that, of over 1000 atoms in our computational cell, only the single tip atom avalanches, so the fractional difference in energy is small. This is unlike the case of layerwise avalanche [2] between approaching flat surfaces where the entire surface on either side moves out and the energy released in the process is comparable to the surface energy of the appropriate surface. A similar situation arises in the case where the approaching flat surfaces are out of registry [5]. There, too,

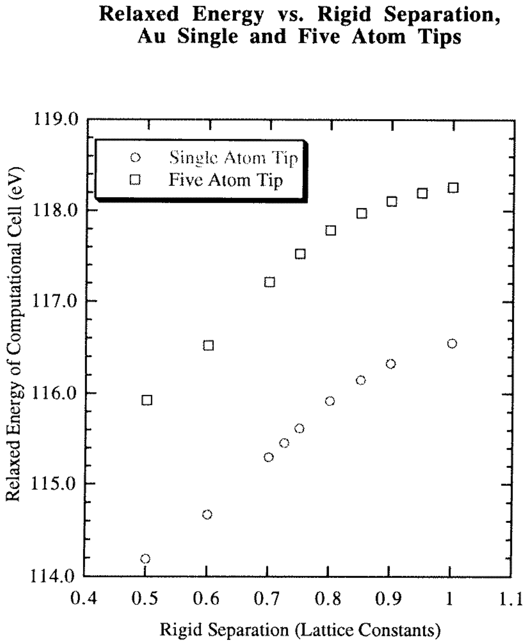


Figure 5. Plots of relaxed energy versus rigid separation for single- and five-atom Au tips approaching a Au(001) surface.

there is little or no evidence of avalanche in the energy plot but the phenomenon clearly shows up in plots of the appropriate interlayer distances.

Results for the five-atom Ni tip are displayed in figures 2 and 4. Again the tip atom avalanches, but the slab layers do not. Further, the four atoms which constitute the 'base' of the five-atom pyramid behave like surface atoms and do not avalanche although they do relax outward by a small amount. The main reason for this is that these atoms do not stand to gain much energy by moving outward as they have only one nearest neighbour in that direction—the tip atom. So this reduced coordination in the 'outward' direction suppresses the avalanche effect even in the base of the five-atom pyramidal tip. Once again the avalanche effect does not show up in the plot of the energy for the same reasons as in the case of the single-atom tip.

Figures 5–7 show results for a single- and five-atom Au tips approaching a Au(001) surface. One can see from figures 6 and 7 that in this case while the tip atom does move out into the gap between the 'support' and the 'sample', there is no sharply defined avalanche in the case of either the one-atom or the five-atom tip. The reason for this apparent absence of a sharp transition in the case of Au is not clear. However, Au surfaces are known to behave differently from those of other fcc metals [18]. It is not clear whether or not the different behaviour seen for Au here is related to the different behaviour of Au surfaces. We are currently investigating similar phenomena in the case of the related metals Pt, Pd, and Ir in order to help clarify this matter.

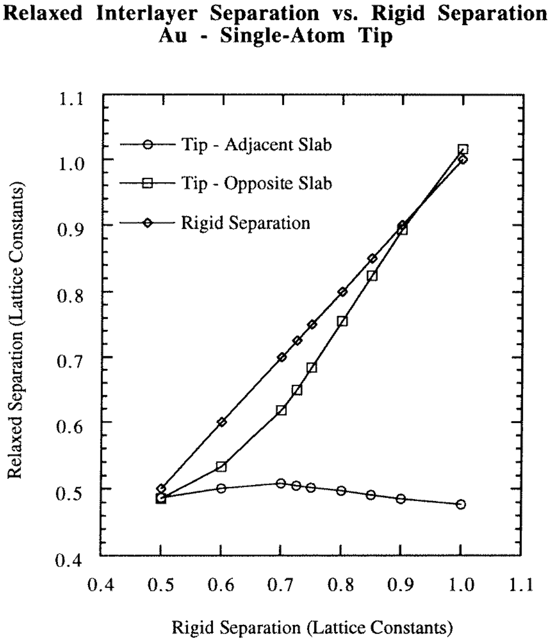


Figure 6. Plots of relaxed interplanar separations versus rigid separation for a single-atom Au tip approaching a Au(001) surface.

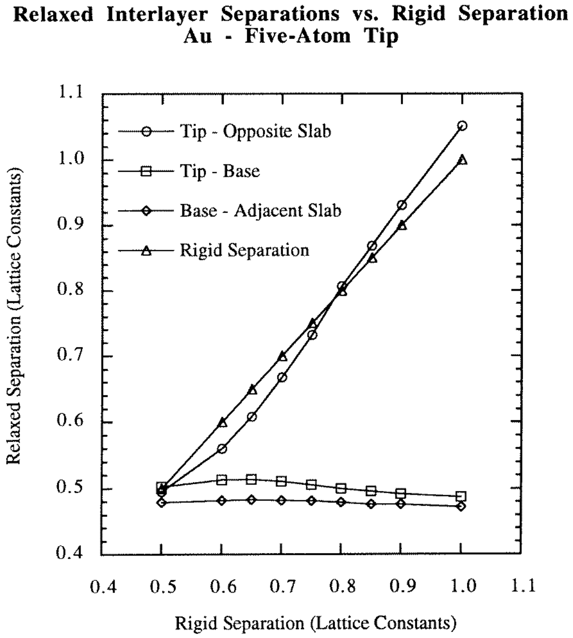


Figure 7. Plots of relaxed interplanar separations versus rigid separation for a five-atom Au tip approaching a Au(001) surface.

4. Discussion

We have carried out Monte Carlo simulations of the stability of AFM tips for a variety of fcc metals at room temperature. We find that an atomically sharp tip will undergo avalanche—that is, when the interfacial gap between the tip atom and an atomically flat slab falls below a critical value, the tip will move away from the slab to which it was initially attached, to a new equilibrium position within the gap. For the symmetric case of a single tip atom between two semi-infinite planes, the equilibrium position is exactly halfway between the two slabs. This is in excellent agreement with the results of recent experiments on tunnelling in mechanically controlled break junctions (MCBJ) [19] in which the authors see evidence of tunnelling through 'a single atom' in the much necked down junction and conclude that this solitary atom is situated midway between the two sides of the broken junction. In addition, we find that the atomic layers underneath the tip relax outward into the gap but do not go far enough to avalanche. Similar conclusions may be drawn for the five-atom pyramidal tip although in this case, for obvious reasons, the tip atom does not sit exactly midway between the two surfaces.

As we have already mentioned, the behaviour of the Au tip approaching a Au surface is quite different, qualitatively, from that of the other metals that we have studied. The reason for this is not clear yet. However, we hope that our ongoing investigations of similar systems involving Pt, Pd, Ir, etc will shed some light on whether or not this difference is related to the fact that Au surfaces, unlike those of the other metals studied here, undergo symmetry-reducing reconstructions.

In the case of adhesion between flat planar surfaces we have shown [5, 17] that the avalanche phenomenon is affected by the degree of registration between the two approaching surfaces. Avalanche is strongest and sharpest when the two surfaces are in perfect registry and is considerably weakened when the registry is lost and more so when only a few surface layers are permitted to relax. We are currently investigating the equivalent effect in the case of avalanche at an atomically sharp tip, i.e. when the tip is brought down onto the sample at sites other than the fourfold hollow of the fcc (001) surface.

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