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LETTER TO THE EDITOR

Universal aspects of adhesion and atomic force microscopy

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Abstract. Adhesive energies are computed for flat and atomically sharp tips as a function of the normal distance to the substrate. The dependence of binding energies on tip shape is investigated. The *magnitudes* of the binding energies for the atomic force microscope are found to depend sensitively on tip material, tip shape and the sample site being probed. The *form* of the energy–distance curve, however, is universal and independent of these variables, *including tip shape*.

The scanning tunnelling microscope [1] (STM) and atomic force microscope [2] (AFM) have been demonstrated to be powerful new probes of solid surfaces at the atomic level. The STM and AFM have yielded topographic images of surfaces on the atomic scale. The topographic images obtained are not always easy to interpret and some theoretical modelling of the tip–sample interactions has been done [3, 4]. With the AFM there is the additional exciting possibility of mapping three-dimensional adhesive force contours for a tip and sample in intimate contact. Several authors have measured such force contours [2, 5, 6].

Typically, in the STM or the AFM, the tips are very sharp, containing a few atoms. It is difficult to determine the shape of the tip *in situ*. One might expect that the measured forces and energies and their variation with tip–sample separation will be sensitive to the shape of the tip. We will report results here, however, which suggest that while the magnitudes of adhesive energies and forces are sensitive to tip geometry, material, and sample site being probed, the variation of the energy, or of the force, with tip–sample separation has a universal form independent of these variables, *including tip shape*. Thus, atomic force microscopy can be expected to be a sensitive probe of material properties through relative magnitudes but not through the form of the force–distance relation. The universal binding energy relation (UBER) between total energy and interfacial separation was first discovered [7] for adhesion at flat interfaces between different pairs of simple metals. It was later found to extend to other cases of energy–distance variation [8, 9]. We will show here that this UBER also holds [10] for AFM tip interactions with a sample surface for a variety of sample materials, surface sites probed, and tip shapes.

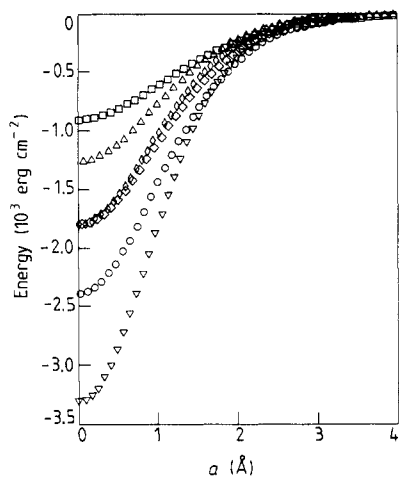


Figure 1. Variation of binding energy with separation for adhesion at the lowest-index interface between two slabs of Al (squares), Ni (circles), Cu (diamonds), Ag (triangles), Fe (narrow diamonds), and W (inverted triangles).

Recently, Smith and Banerjee [11, 12] have proposed a new theory that provides a simple and fast method for computing the total energy of solids. This theory provides accurate predictions of surface energies [11, 13] and surface relaxations in transition metals [12, 13] and in silicon [13]. Here we have used this equivalent crystal theory (ECT) to compute the binding energies in the cases of rigid adhesion (rigid fracture) and the binding of a STM/AFM tip to the surfaces of different metals, including transition metals. The accuracy and efficiency of this theory is particularly appropriate for the low symmetry problem of an atomically sharp tip probing a surface.

We have computed the binding energy for adhesion of two semi-infinite slabs of the same metal (in perfect registry across the lowest-index crystallographic plane) as a function of the separation between the slabs. This has been done for each of four face-centred-cubic (FCC) metals—Al, Ni, Cu and Ag—and two body-centred-cubic (BCC) metals—Fe and W. In each case the two semi-infinite slabs are separated rigidly with no surface relaxation or reconstruction being permitted [14]. Hence, we might describe this model process as rigid adhesion or rigid fracture.

Results for the variation of the binding energy with separation are shown in figure 1. These results should be of relevance to questions related to fracture, particularly transgranular fracture, in materials. In real materials, however, several other phenomena, such as elastic deformation, the presence and segregation of defects, plastic deformation, interaction with phonons, and relaxation, come into play before the fracture process is completed. Nevertheless, it is necessary to know the rigid-fracture contribution to the energy before one can begin to unravel the details of the other phenomena.

The rigid-adhesion curves shown in figure 1 can be scaled [7–9] as follows:

$$E^* = E/\Delta E \quad (1a)$$

$$a^* = (a - a_m)/l \quad (1b)$$

with a being the inter-slab separation (which is defined to be zero when the surface layers are at the equilibrium interplanar distance), ΔE the magnitude of the minimum adhesive energy, and a_m the separation at which this minimum occurs. It was discovered [7] that

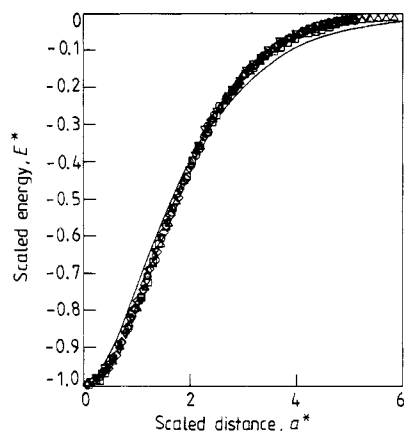


Figure 2. Scaled binding energies and separation for adhesion at the lowest-index interface for some metals. Symbols mean the same as in figure 1. Also plotted (full curve) is the Rydberg function given in equation (2).

such a scaling of adhesive energy curves for simple metals reduces them all to the UBER which is well described by the Rydberg function:

$$E^*(a^*) = -(1 + a^*) \exp(-a^*). \quad (2)$$

It is not at all obvious, *a priori*, that the UBER should also apply to adhesion in transition metals because the latter contain d orbitals which can be more directional and localized than the s-p orbitals of simple metals. As the UBER is known to apply to cohesion in transition metals [8, 9], however, there is reason to believe that it might apply to adhesion in transition metals as well. Since ECT provides very accurate predictions of surface relaxations in transition metals [12] and even semiconductors [13], we have reason to believe that it treats the directional-bonding effects in these materials adequately.

Results of the scaling are shown in figure 2. The *shape* of the rigid-adhesion curve is clearly universal—all the scaled curves fall on top of one another. As the Rydberg function of equation (2) described the simple-metal scaled results rather well [7], we have also plotted it on figure 2 for comparison. The fit between the scaled results in figure 2 and the Rydberg function is reasonably good.

Above we have computed adhesive energies of flat surfaces. Now we would like to determine the energetics of a tip on a flat surface. Ideally, in the STM or the AFM, the tip is atomically sharp and tunnelling occurs between the sample and a single atom at the end of the tip. However, the real STM/AFM tip is far from ideal and the tunnelling current has been known to jump from one asperity on the tip to another, creating complications in the interpretation and reproducibility of images. The effect of tip shape on the tunnelling current and the generated images has been the object of a number of studies [4, 15]. The effects of the interaction between the tip and the sample have also been investigated theoretically [3, 4]. The problem of rigid adhesion which we have just discussed may be viewed as the case of one extreme tip shape—an extremely dull STM ‘tip’. We now consider the other extreme situation where the tip is essentially a single atom but is connected to, and hence affected by the presence of, a solid support—the needle behind the tip. Our model of the tip, then, is a single atom on a flat semi-infinite slab. We have studied these two limiting cases with the tacit assumption that the behaviour of the other, intermediate, tip shapes will lie between these two extreme cases.

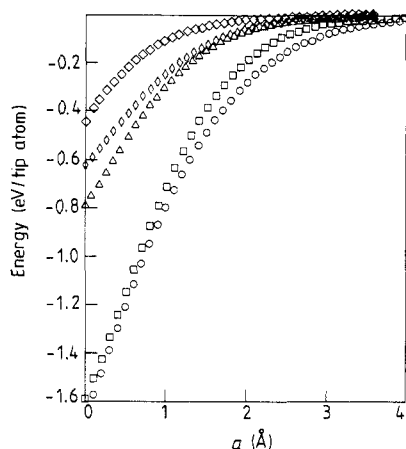


Figure 3. Variation of binding energy with separation for a STM/AFM tip moving normal to the (111) surface at the 'FCC'-hollow site for Ag (squares), the 'HCP'-hollow site for Al (circles), the bridge site for Cu (diamonds), the 'on-top' site for Ni (triangles), and a site of 1-fold symmetry (half-way between the bridge and on-top sites) for Cu (narrow diamonds).

Since in the real STM or AFM the tip may have a radius of curvature of 5–20 Å this single-atom-on-flat model is admittedly rather idealized. However, it is one extreme variant of the tip shape. Also, changing the pedestal to which the tip is attached from a flat surface to a pyramidal structure, for instance, will have a negligible effect on the adhesive energies and forces. Atoms in the pedestal are, at best, second neighbours to those on the sample surface. Their interactions, being at the second-neighbour distance and screened by the tip atom too, make only a negligible contribution to the overall adhesive energies and forces.

We consider a rigid tip, of the same material as the sample, moving normal to the rigid sample surface above different sites on the lowest-index plane. The results are shown in figure 3. The tip-sample separation, a , is zero when nearest-neighbour bonds between the tip atom and atoms in the top layer of the substrate are at the equilibrium nearest-neighbour bond length. Clearly the results are sensitive to both tip material and tip position on the surface. This suggests that the AFM has the potential to be a sensitive probe of surface energetics. As mentioned earlier, the sharpness of the tip is typically unknown and so one might be concerned about how much the results depend on tip sharpness. We are now in a position to investigate that question. Figures 1 and 2 give the results for a perfectly dull, i.e. flat, tip, while figure 3 gives the results for a perfectly, i.e. atomically, sharp tip. One can see, upon comparison of figures 1 and 3, that the sharpness of the tip does have a profound effect. In general, interaction energies of the ideally sharp tip are larger (per tip atom) than those of the perfectly dull tip. Perhaps one can understand this by realizing that the single tip atom is missing all in-plane neighbours (as opposed to an atom on the perfectly dull tip which is not) and, hence, is more 'reactive' than an atom on a flat surface.

One might wonder if the *shape* of the energy–distance curves is sensitive to the shape of the tip. In order to investigate this, as before, the data in figure 3 were scaled according to equations (1) and fitted to the Rydberg function of equation (2). In this case the minimum in the energy occurs at $a < 0$. Scaled results are plotted in figure 4. Also shown as a full curve in figure 4 is the Rydberg function (which was also plotted as a full curve in figure 2). Once again the data scale very well together on to a universal energy–distance curve and fit the Rydberg function very well too. We see that the shape of the energy–distance curves is approximately the same for a perfectly dull tip as it is for an

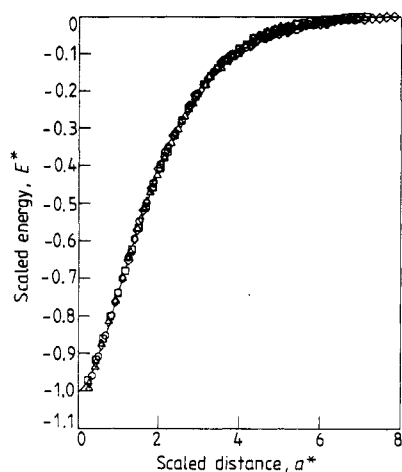


Figure 4. Scaled binding energies and separations for a STM/AFM tip at different sites on the (111) surfaces of different FCC metals. Symbols mean the same as in figure 3. Also plotted (full curve) is the Rydberg function given in equation (2).

ideally sharp one. This suggests that such curves are not sensitive to tip sharpness. We find, in addition, that the shape of these curves is not sensitive to tip material or to the position of the tip on the sample surface. This suggests that one cannot use the form of the force curves in the AFM to differentiate surface materials or sites. For that information one needs to determine the magnitude of the energy or force. As we have seen, the latter are sensitive to tip sharpness; hence, in order to obtain meaningful information from the AFM one needs to ensure that the tip does not change shape during the measurement.

In summary, we have computed binding energies for rigid adhesion (a very dull STM tip) as a function of normal interfacial separation [16] and for an atomically sharp STM tip moving normal to a flat sample surface. We have found that the magnitude of the AFM (or STM) tip-sample energetics is sensitive to tip sharpness, tip material, and the site on the sample surface that the tip is probing. This suggests that the AFM should be a sensitive probe of sample properties. However, none of these variables significantly influences the *form* of the dependence of the energy or the normal force on tip-sample separation. In other words, the form is universal even when all the aforementioned parameters, *including the shape of the tip*, are varied. Thus, it is the magnitude, and not the form of the energy or force curve, which is sensitive to information about the sample surface and the shape of the tip.

These results are generally supported by both experiment [6] and *ab initio* theory [4]. Dürig *et al* [6] have found that the force, and hence the energy, vary exponentially, and not according to a power law, with the normal tip-sample distance in the range of operation of the STM/AFM. This is in excellent agreement with the implications of equation (2). Ciraci *et al* [4] have computed the energy and force as functions of normal tip-sample distance for two different tip shapes (with no pedestal) and have obtained curves that are remarkably similar in shape to each other and to those in figures 1 and 3. However, they did not report any attempts to scale these curves or to fit them to a universal function. Such a scaling, should it succeed, would provide excellent independent corroboration of the results presented here.

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