Comment on "Interatomic Forces in Scanning Tunneling Microscopy: Giant Corrugations of the Graphite Surface"

In a recent Letter Soler *et al.*[1] describe giant corrugations observed in scanning tunneling microscopy (STM) studies of the basal plane of graphite and related layer materials. The amplitudes can be several times the size expected from the surface local density of states which controls normal STM imaging. This Comment is to discuss some limitations to the mechanism that they propose, and to suggest possible new STM image contrast sources.

Soler *et al.* make the two important observations that the amplitudes observed increase with decreasing tunnel-junction resistance, and that there exists[2] an "effective tunnel barrier" of 7.3 eV even when the vacuum barrier is completely quenched. Their conclusion is that when giant corrugations are seen, the tip and flat are acutally in contact. Elastic strains in the lattice near the tip must then be taken into account. As in our previous model[3] explaining anomalously low tunnel barrier heights, tip piezodisplacement becomes larger than tunnel-gap movement. Abraham and Clarke have recently confirmed[4] that very small barrier heights (measured from $\partial \ln I/\partial s$) are indeed seen when the corrugation height exceeds ~ 1 Å.

Soler *et al.*[1] calculate that a force of 10^{-8} N is applied across the contact and that the surface is depressed by 8 Å. It must be questioned whether their proposed single-atom contact (tip radius of 2 Å) can sustain such stresses. Two difficulties are as follows:

(1) The elastic energy stored in the contact is 4×10^{-18} N m (i.e., 25 eV). Half of this energy is localized within a few angstroms of the tip, because the total elastic energy at a radius r from the contact zone varies as $1/r^2$ even in anisotropic media. Only for perfect 2-D geometries such as line dislocations is the strain energy stored (logarithmically) over very large volumes. This very high local concentration of energy (a few electronvolts per atom) may be compared with the surface self-diffusion activation energy of tungsten of about 0.9 eV.[5] Some surface rearrangement of atoms is likely. Interstitial and other bulk defects, requiring typically 4 eV, might also appear. Note that when such inelastic strains occur, further energy is supplied by the loading force moving through the associated displacement.

(2) A simple estimate of the bond strains adjacent to the contact due to the hydrostatic pressure may be made from the bulk modulus. For single-atom contact and 10^{-8} N force, a value of $\approx 5\%$ is found even for the very rigid tungsten tip. Shear strains will be of the same order, while for the softer graphite they will be considerably higher. These strains exceed the theoretical lattice maxima; inelastic processes such as slip may therefore be expected.

The above observations lead to the conclusion that the actual contact area may be rather more than one atom wide. Other work on low-load indentation[3] also suggests this. The problem then arises—how is atomic lateral resolution obtained in the STM image?

Imaging a simple periodic structure does not strictly require a tunnel "beam" of single-atom width, but rather a fluctuation in total conductivity between tip and sample which varies in registry with unit lattice shear. A common feature of the layer materials discussed by Soler *et al.*[1] is a very easy shear along the basal plane. If there is a significant contact area as implied above, then the lateral tip movement will be most easily accomodated by sliding of planes just beneath the tip. The charge density increases at the minima in the graphite rings as the layer stacking shears out of its equilibrium (symmetry) position.[6] Shear over a complete lattice period therefore produces a single-cycle increase and decrease of the injected tunnel current. With a contact area a few atoms across, this process is likely to be coherent over the whole area. Thus a fluctuation in injected current occurs, as required, in registry with the lattice as the tip is rastered over surface. As an indication that this mechanism is reasonable, Binnig and Quate have recently shown[7] that STM-type images may be obtained in a "point-contact microscope," where a tip is merely loaded on a graphite surface and conductivity monitored during rastering.

An effect of the STM feedback loop in the results of Soler *et al.* will be to vary contact area. This explains the rather weak nonlinearity of corrugation observed compared to that expected from the Morse potential.

J. B. Pethica
Cavendish Laboratory
Cambridge CB3 0HE, United Kingdom

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[1] J. M. Soler, A. M. Baro, N. García, and H. Rohrer, Phys. Rev. Lett. **57**, 444 (1986).

[2] J. Tersoff, Phys. Rev. Lett. **57**, 440 (1986).

[3] J. H. Coombs and J. B. Pethica, IBM J. Res. Dev. **30**, No. 5, 455 (1986). See also G. Binnig, C. F. Quate, and C. Gerber, Phys. Rev. Lett. **56**, 930 (1986).

[4] D. Abraham and J. Clarke, in Proceedings of the Scanning Tunneling Microscopy Conference (STM '86) Santiago, Spain, July 1986, Surf. Sci. (to be published).

[5] S.-C. Wang and T. T. Tsong, Surf. Sci. **121**, 85 (1982).

[6] I. Batra, private communications, and work presented at STM '86 (see Ref. 4).

[7] G. Binnig and C. F. Quate, in STM '86 (see Ref. 4), Surf. Sci. (to be published).