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MODEL OF THE POTENTIAL BARRIER OUTSIDE THE SURFACE OF A CONDUCTOR WITH WALLS OF FINITE THICKNESS

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Tunneling effect of graphite is studied by atomic force microscopy. The tunneling current in the gap between a conductive tip and a newly cleaved graphite surface at a given voltage keeps almost constant when the gap-distance varies within 1 μm, which cannot be explained by the commonly accepted well model of the potential outside a conductor. Thus modification of the well model is made and a cup model, with a certain wall thickness of the cup, is proposed in the present work.

Keywords: Surface potential; atomic force microscopy; tunneling; potential well model; graphite.

1. Introduction

Electron tunneling e ect between two electrodes has been widely studied both theoretically and experimentally. Simmons[1] proposed a generalized formula for the electron tunneling e ect with a potential barrier of arbitrary shape between two electrodes over the full range from close-spaced metal–vacuum–metal tunneling e ect to field-emission tunneling. The current density J between two electrodes can be written as

$$J = \frac{e}{2\pi h(\beta L)^2}\left\{\varphi \exp(-A\varphi^{1/2}) - (\varphi + eV) \times \exp\left[-A(\varphi + eV)^{1/2}\right]\right\}, \quad (1)$$

where $A = \frac{4\pi\beta L\sqrt{2m_e}}{h}$, $\beta \approx 1$, V is the potential between the two electrodes m_e is the electron mass, φ is the average barrier height between the two electrodes above Fermi level, L is the potential thickness at Fermi level, which is approximately equal to the gap-distance or electrode separation, d.

Obviously, Eq. (1) predicts the strong dependence of J on L or d, which has been the basic principle of the scanning tunneling microscopy. The room temperature gold–vacuum–gold tunneling experiments within 2 nm of d performed by Teague[2] supported the formula. Young[3] experimentally confirmed Simmons' formula too with tungsten and platinum electrodes within 40 nm of d, but beyond this distance,

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J was almost independent of d, which apparently contradicts Simmons' formula. More than 30 years ago, this confliction had not been noticed (see Fig. 1 in Ref. 3). Here in our experiment, the tunneling current between a conductive tip and a graphite surface was measured, the result of which also contravenes Simmons' formula.

2. Experimental

The experiment was performed with Solver P47 atomic force microscopy (AFM) at room temperature. Silicon tips coated with conductive W_2C or TiN films were used for measuring the I–V curves. The force constants of the cantilever are 48, 11.5, 5.5, and 3 N/m, and the lengths are 90, 100, 130, and 200 μm, respectively. The curvature radius of the tip is around 35 nm. The sample is a highly oriented pyrolytic graphite (HOPG).

At first, the testing area on the surface of the newly cleaved HOGP was proved to be atomically flat by scanning the surface topography. Then the I–V curve was measured with d reduced from 1 μm till the tip touched the graphite surface (in this case there is still a gap distance no matter how small it is). The tunneling current keeps almost constant within the measuring range as shown in Fig. 1, which is hardly explained by Simmons' formula. Thus, further consideration is necessary.

3. Results and Discussion

Commonly a conductor was assumed to be a three-dimensional potential well with a plain bottom (Fermi level). The energy of the electron resting at the bottom of such a potential well is less than that of the vacuum level — the energy of electron resting infinitely far from the conductor surface. And the well depth, called work function, can be defined as the minimum energy to remove an electron from the Fermi level in a conductor to a point at infinite distance outside the surface.[4–9] In 1914, Schottky proposed an image potential,[10] which modified the well model. In the image potential theory, the corner of the mouth of the well was smooth and rounded rather than orthogonal, but the well shape of the potential was still kept,[11–18] as shown in Fig. 2(a). In his treatment, Schottky considered that the work function came from the attraction of an escaping electron to its image on the surface (image force). Most of the other calculations, thereafter, were based on the definition that the work function was the di erence in energy between a lattice with an equal number of ions and electrons and the lattice with the same number of ions but with one electron removed.[4,5] No matter what ways were used to calculate the work function, they all led to the well shape of the potential.

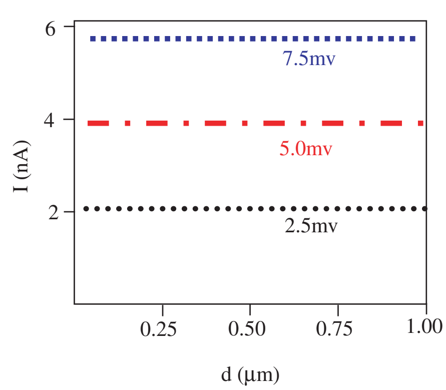

Fig. 1. Tunneling current with gap distance between a conductive tip and a newly cleaved graphite surface, measured by an AFM.

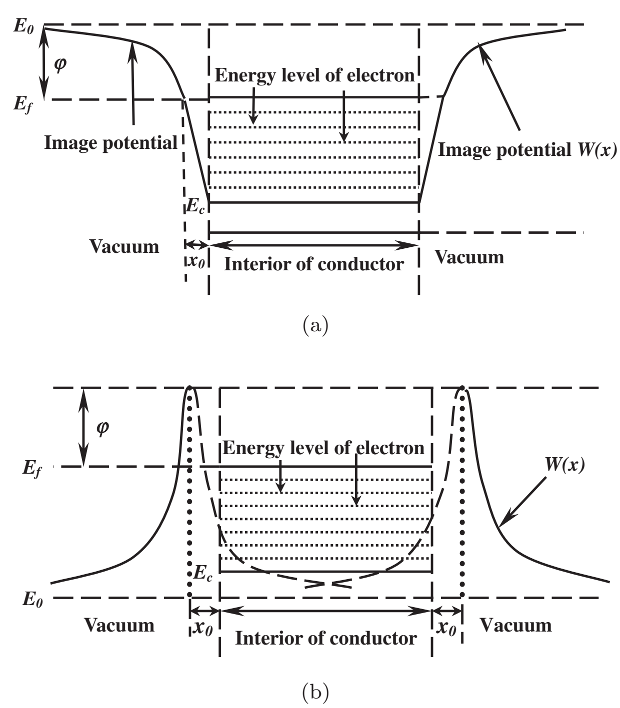

Fig. 2. Comparative illustration of the well model (a) and the cup model (b) for a conductor. E_0: vacuum level; E_f: Fermi level; E_c: bottom of conduction band; ϕ: work function; W: surface potential.

To explain our experimental results, however, the well shape of the potential has to be reconsidered. For a conductor, there is an electron gas, like a curtain, gathered nearby the surface of the conductor. When an electron passes through the curtain, the curtain may exert a repulsion force on the electron. If we simply assume this repulsion to be the main force exerted on the passing electron and ignore any other e ects, such as the core attraction to the electron, the well shape of the potential will be modified, as calculated in the following sections. Apparently, this simple assumption overemphasizes the e ect of the electron gas on the passing electron. And it is not correct actually if the other e ects are neglected. This kind of simplification, however, will definitely show an extreme condition when only the repulsion from the electron gas is considered. And it will be helpful to clearly understand the real shape of the potential outside a conductor.

Let us assume that the electron gas is a single-layer network, as shown in Fig. 3, which provides electrostatic resistance to prevent an electron, with a velocity of v, passing through it. Let $2l$ be the average diagonal length of one unit square of the electron network, x be the distance of the electron to the plane of the network. The force exerted by the electron network on the passing electron at point x will be given by

$$F_x = \frac{4Ke^2}{x^2 + l^2}\cos\alpha, \tag{2}$$

where K is constant. Here, only the four neighboring electrons of the unit square are considered to exert force on the passing electron.

As

$$\cos\alpha = \frac{x}{\sqrt{x^2 + l^2}}, \tag{3}$$

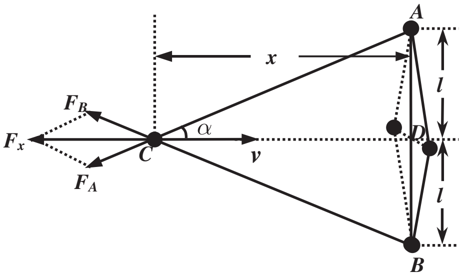

Fig. 3. Illustration of the forces exerted by a unit square of electron network on a passing electron at point C.

Eq. (2) can be changed into

$$F_x = 4Ke^2x(x^2 + l^2)^{-\frac{3}{2}}. \tag{4}$$

When $x = 0$ or $x = \pm\infty$, $F_x = 0$.

Let

$$\frac{dF_x}{dx} = 0 \quad \text{then } x_{\max} = \pm\frac{l}{\sqrt{2}}, \tag{5}$$

which means that the electron at the distance of $\pm\frac{l}{\sqrt{2}}$ from the plane of the network experts the maximum force.

Then an electron from $x = -\infty$ to x must do work $W(x)$ to overcome force F_x, therefore,

$$\begin{aligned} W(x) &= -\int_{-\infty}^{x} F_x dx = -4Ke^2\int_{-\infty}^{x} x(x^2 + l^2)^{-\frac{3}{2}}dx \\ &= \frac{4Ke^2}{\sqrt{x^2 + l^2}}\bigg|_{\infty}^{x} = \frac{4Ke^2}{\sqrt{x^2 + l^2}}. \end{aligned} \tag{6}$$

According to Eq. (6), the graph of $W(x)$ to x can be drawn as shown in Fig. 2(b). The graph is symmetrical to the plane of the network and presents the shape of a cup with a certain thickness of the wall, rather than a well.

The single-layer electron network is only an idealized model. If we further take into account of the other e ects on the passing electron, the graph of $W(x)$ to x may be much more complicated and definitely not symmetrical, but the basic shape like a cup will still be remained.

In terms of the well model previously mentioned, when two electrodes approach each other, it is quite understandable that the thickness of the potential barrier for an electron to go through is approximately equal to the electrode separation and the work function can be taken as the average barrier height from the Fermi level between the two electrodes. In the new cup model, however, the thicknesses of the potential barrier between the two electrodes will be dependent on the thickness of the cup walls because di erent electrodes may possess di erent thickness of the surface potential. To show it more clearly, we simply use a rectangular shape of the cup walls, which may not influence our analysis of the intrinsic nature of the phenomena. Suppose $d1$ and $d2$ are the thicknesses of the potential barrier of the two electrodes, respectively, d is the electrode separation and L is the potential barrier thickness between the two electrodes in Eq. (1). If $d1$ and $d2$ are both extremely small, even the two electrodes get into contact with each other (still keep a gap distance of several angstroms in this case), d is still larger than L, which is equal to ($d1 + d2$), as shown in Fig. 4(a). When d varies, L keeps constant. As a result, J is independent of d according to Eq. (1). If $d1$ and $d2$ are relatively large, the walls of the two potential barriers may be overlapped as shown in Fig. 4(b). In this case, d is equal to L, but smaller than ($d1 + d2$). When d varies within ($d1 + d2$), L varies too. Accordingly, J is strongly dependent on d according to Eq. (1). But when d varies beyond ($d1 + d2$), as shown in Fig. 4(c), L, which is ($d1 + d2$), keeps constant and does not change with d, which leads to the independence of J on d.

In the present experiments, the two electrodes are the sharp silicon tips coated with conductive W_2C or TiN film and graphite, respectively. For the sharp tip

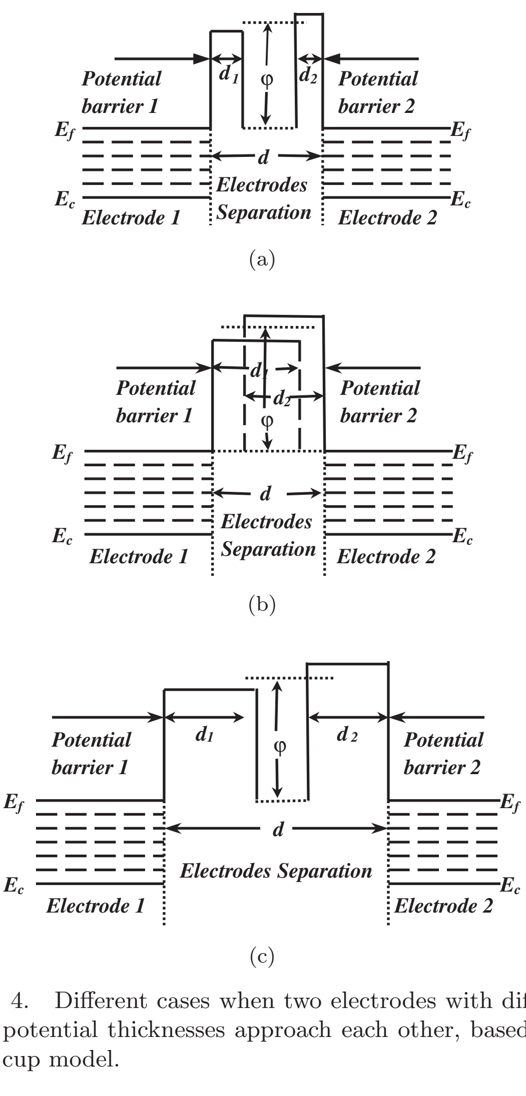

Fig. 4. Different cases when two electrodes with different potential thicknesses approach each other, based on the cup model.

coated with conductive compound, it is quite acceptable that it may have a small density of electron on the compound film surface, which leads to the smaller thickness of the potential cup wall. For the layer-structured graphite with relatively large layer spacing, a small electron density on the surface is also understandable, which may also present a small wall thickness. Accordingly, the present experiment with compound-coated tip and graphite corresponds to the case of Fig. 4(a), by which the real result is perfectly explained. In Young's experiment,[3] the two electrodes were pure metals, tungsten and platinum, which provide larger values of the wall thickness. The experimental result is just what Figs. 4(b) and 4(c) depict. Within a critical range of the electrode separation J is dependent on d, but beyond this range, J is independent of d. In Young's experiments, the critical range was 400 Å, which means the thickness of the wall of the potential cup for the tungsten–platinum system is about 200 Å. For the other previous measurement of the tunneling e ect, they all can be explained by the case of Fig. 4(b).

The well model means that an electron outside the conductor surface will return to the surface without any barrier. But the cup model predicts that an electron outside the conductor surface beyond the potential cup wall have to overcome a barrier to return to the surface, but within the cup wall the electron will return to the surface without any barrier. For metals, the thickness of the cup wall is probably in the order of a few hundreds of angstroms. Therefore, an electron beyond this range from the surface is di cult to return to the surface. By combining laser techniques with angle-resolved photoelectron spectroscopy, Hofer *et al.* observed that electron wave packet travels about 200 Å away from the surface into the vacuum and then returns with a period of 800 fs.[17,18] This experimental result coincides with the above cup model prediction.

According to the well model, the energy of an electron outside a conductor (vacuum level) is higher than the Fermi level in the conductor. But according to the cup model, the vacuum level is at the ground level, which is lower than the Fermi level in the conductor. As we know that the electrons in the conductor are confined inside the conductor by the surface potential barrier resulting in the formation of energy level in the conductor, and due to the Pauli's exclusion principle, the electrons in the conductor have to occupy the higher level up to Fermi level. But, the electrons outside the conductor do not have any confinement, so they should all occupy the ground level. Therefore, the vacuum level should be at the ground level rather than above the Fermi level. That means that our cup model but not the commonly accepted well model for a conductor is reasonable theoretically.

4. Conclusions

In order to explain the tunneling e ect of graphite, we modified the commonly accepted well model of the potential barrier for conductors, and a cup model with a thickness of the cup wall is proposed. The new model can also be applied to the results previously explained by the well model.

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