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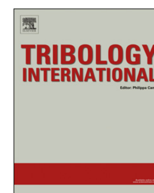

# Size and load dependence of nanoscale electric contact resistance

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ABSTRACT

Nanoscale electrical resistance between a platinum-coated atomic force microscope tip and highly oriented pyrolytic graphite surface is measured as a function of normal load and tip radius. These measurements are complemented by molecular dynamics simulations that relate load and radius to contact area. Simulation-predicted contact area and experimentally-measured resistance are used to calculate contact resistivity. The results show that the effect of load on resistance can be captured by the real contact area, while tip size, although in part captured by area, affects contact resistivity itself, potentially through interface distance. Our study provides new insight into the effect of load and geometry on nanoscale electric contact and, more significantly, highlights the role of atomic-scale contact features in determining contact resistance.

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## 1. Introduction

As demand for high density, high speed electronic and electromechanical devices continues to increase, implementation of true nanoscale structures has become critical for next generation electronics engineering [1–3]. However, although contact resistance is one of the major parasitic components in electronic devices, conduction at nanoscale contacts is not yet clearly understood [4]. Furthermore, electrical transport through nanoscale contacts often exhibits behavior deviating from that of conventional contacts [5,6]. This can be partially attributed to the fact that the dimension of contact is smaller than the characteristic Debye length, resulting in an enhanced electrical conduction [5,7]. Nanoscale structures also have discrete energy levels which, in turn, can result in unconventional electric behaviors.

Recently, single layer graphene (SLG) and multi-layer graphene (MLG) have been the focus of extensive research due to their unique properties, such as high electrical and thermal conductivity [8–11], very low friction [1,12,13] and the quantum hall effect [10,14,15]. Many studies have focused on electrical properties due to the wide applicability of SLG and MLG to various electronic and electromechanical devices [17–21]. Since contact resistance is a major factor limiting device scalability, reliability and performance in any electronic device [22–24], it is important to understand this behavior in graphene-based materials. Although there are quite a few studies on metal-SLG contact, little is known about the electrical properties of metal-MLG contacts [29]. Of the previous metal-MLG studies, several have focused on the effect of number of graphene layers on contact resistance [31,32,34]. Other studies revealed a pressure dependence of electrical conductance on a double layer graphene surface [33] and that conductance is affected by step edges observed on the surface of MLG [30,35,33]. These findings highlight at the critical role of the contact and its atomic-scale features in determining nanoscale resistance.

In this paper, we explore this important relationship between a nanoscale contact and its resistance by studying the electric contact between a platinum-coated AFM tip and highly oriented pyrolytic graphite (HOPG) surface. We measure the contact resistance with different size tips under various loads using the experiments, and then investigate the contact between tip and substrate using complementary simulations. The simulations are used to predict real and apparent contact area, and then this information is used with the resistance measured experimentally to calculate contact resistivity. The results are analyzed in terms of the ability of the two contact area definitions to capture the effects of load and tip size on resistance.

## 2. Method

An atomic force microscope (AFM; Model 5500, Agilent Technology) system was used to enable contacts between a conductive probe and a HOPG (Alfa Aesar) surface with controlled forces. HOPG with a thickness of 200 μm was used for the electrical characterization. To avoid significant contamination and/or oxidation of the surface, the surface was always cleaved using a blade razor before each measurement. The strong $sp^2$ covalent intralayer bonds and relatively weak van der Waals interlayer bonds in HOPG made a thin layer readily exfoliated [36]. To investigate the contact

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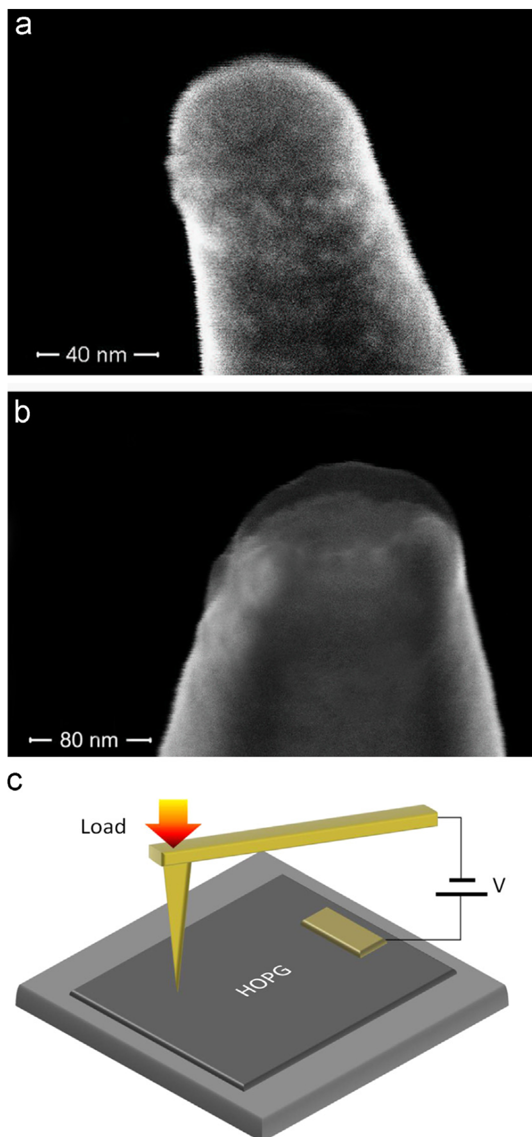


**Fig. 1.** Scanning electron microscope images of AFM tips with radii (a) 32 nm, (b) 77 nm, and (c) a simplified schematic diagram of the experimental setup.

area dependence, tips with two different apex radii (32 nm and 77 nm, shown in Fig. 1(a) and (b)) were prepared by depositing Pt on commercially available probes (Team Nanotec HSC Probe, NanoScience Instruments Inc.). The commercial probe was originally coated with tungsten carbide and its apex was in a hemispherical cone shape. Their nominal tip radii (the values specified by the vendor) were 20 nm and 40 nm. A dense Pt film was coated on the probes by a direct current sputter deposition scheme in an Ar pressure of 10 mTorr. The electrical characterization was conducted under ambient conditions at room temperature ($\sim$300 K). The forces applied by the cantilever (with a spring constant of 3.0 N/m) were in the range of 100–800 nN during the electrical measurement. The tip–substrate contact resistances were obtained using a semiconductor parameter analyzer (HP4145B). An illustration of the experiential setup is shown in Fig. 1(c). In this setup, electrical current was measured during a potentiodynamic sweep performed from 0 to 50 mV when the tip is in contact with the HOPG surface. We observed a consistent linear relationship between the bias and the current (data not shown) such that the contact resistance could be acquired by applying the Ohms law ($R = V/I$) with currents measured under any given bias; we used a

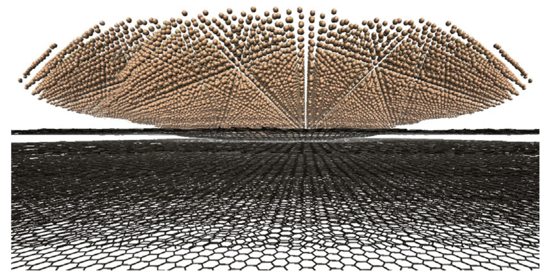

**Fig. 2.** Snapshot from a molecular dynamics simulation of the apex of a 32 nm radius AFM tip placed on a seven layer graphite substrate.

bias of 50 mV for this purpose. All sources of resistance except for that from the Pt–HOPG contact were found to be negligible ($< 15\ \Omega$) compared to the measured resistance which was in the range of kΩ. A capillary condensation of water from the ambient, which is usually called a meniscus, can be a medium for an alternative current path between the tip and the sample [37,38]. Considering a significantly higher resistance of the water meniscus than the Pt and HOPG contact, we also neglected this meniscus effect [31]. After the electrical characterization, the tip apex shape was examined using a field emission scanning electron microscopy as shown in Fig. 1. The tip was found to have maintained its apex shape throughout the measurement despite the mechanical and electrical stresses.

A complementary atomistic model described the near-contact region of the experimental system. As shown in Fig. 2, the model includes the apex of a Pt AFM tip and an adjacent graphite substrate. Seven graphene sheets were ABA-stacked, with an interlayer distance of 0.335 nm. Here we used 7 layers of graphene to represent the top layers of the HOPG thin film. The assumption is reasonable in light of a recent report showing that the transition to a bulk-like resistivity appears at 7–8 layers of graphene [34]. The atoms in the bottommost layer of graphite were fixed to model a supporting substrate and the atoms at one end of all the layers were fixed as well to prevent relative sliding. The boundaries were periodic in the $x-y$ plane (in the plane of the graphene sheets), and the boundary in the $z$-direction was formed by the fixed bottom layer of graphite and the rigid body of atoms at the top of the tip. The model tips had a hemispherical geometry and consisted of platinum atoms in a FCC structure, with the same radii as the experimental tips (32 and 77 nm). A constant external normal load was maintained on the atoms treated as a rigid body at the top of the tip. A Langevin thermostat was applied to the free atoms in the system to maintain a temperature of 300 K. The interatomic interactions within the tip and substrate were described via the Embedded Atom Method (EAM) potential and the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential [39] respectively, and the long range interactions between tip and substrate were modeled using the Lennard-Jones (LJ) potential (energy minimum 0.022 eV, zero-crossing distance 0.295 nm). The simulations were performed using LAMMPS simulation software [40].

## 3. Results and discussion

Fig. 3 shows the resistance measured with 32 and 77 nm radius tips under loads between 100 and 800 nN. For the 77 nm radius tip in Fig. 3(b), there are three sets of data. All resistances measured with the 77 nm tip are smaller than those measured with the 32 nm tip. Further, for both tips, resistance decreases monotonically with increasing load.

The potential sources of the measured resistance are the Pt-coated tip, the HOPG and the contact itself. The resistivity of

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