



# Substrate effect on electrical conductance at a nanoasperity-graphene contact



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## ABSTRACT

The use of graphene for applications such as micro- and nano-scale electronic devices often involves incorporating the two-dimensional material onto various substrates. However, the effects of the substrate's mechanical properties on electrical contact conductance are not fully understood. Here, we explore these effects by measuring the conductance between a nanoscale probe and a single layer of graphene with three different levels of substrate support: no substrate, i.e. free-standing graphene, an elastic substrate, and a rigid substrate. These three systems are studied using conductive atomic force microscopy experiments complemented by molecular dynamics simulations using the electrochemical dynamics with implicit degrees of freedom method. In both experiments and simulations, at a given normal force, current increases as: rigid substrate < elastic substrate < no substrate. We demonstrate that the substrate support influences graphene/tip contact conductance through substrate's elasticity, which determines contact size, as well as through variability of interatomic distances in the contact, which contributes to the interface resistivity.

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## 1. Introduction

Graphene is a two-dimensional material that has gained significant attention due to its unique electrical, mechanical, thermal and tribological properties [1–4]. These properties enabled incorporation of graphene into many different applications, such as biosensors, electronic devices, electromechanical resonators and composites [5–10]. Often, the atomically thin nature of graphene requires depositing it on a substrate, which may in turn significantly affect the graphene's physical properties [11]. For example, an insulating substrate affects the in-plane carrier mobility of graphene, which may result in an increase of the electrical conductivity of the graphene [12]. The interactions between a substrate and graphene affects graphene's chemical reactivity [13,14], electronic properties [15,16], and shear strength and work of adhesion

[17]. In addition to changing graphene's intrinsic properties, a substrate can affect the properties of the contact between graphene and an adjacent material, such as electrical contact conductance [18].

The effect of a substrate on electrical contact conductance is of particular interest for applications such as microelectromechanical systems (MEMS) and nanoelectromechanical systems (NEMS), where nanoscale contacts between graphene and an adjacent material enable conduction within the device. Though MEMS involve multi-asperity contacts, their electrical transport may be extrapolated from single asperity contact experiments, traditionally performed using atomic force microscopy (AFM). Conductive AFM enables measurement of current flow through the contact formed by a nanoscale probe and the surface of interest in a controlled manner [19]. Previous studies using this approach have shown that electronic transport at an AFM tip-sample contact is determined largely by the magnitude of the applied normal force and the elastic and plastic responses of the material to that force [20,21]. Additionally, it was reported that defects in the contact can affect conduction [22]. For graphite specifically, studies have shown that contact resistivity can be dependent on the thickness of the graphite and topographic features induced by the substrate [23,24].

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However, there is a lack of understanding of how the mechanical properties of the substrate affect the conductance of a nanoscale contact between graphene and another electrically conductive material. In this study, we provide a detailed analysis of a substrate's contribution to the stable electrical contact between graphene and a conductive AFM tip.

We isolate the effect of the substrate by measuring conductance between a nanoscale conductive probe and graphene, where the single layer of graphene has three different levels of substrate support. The concept is illustrated in Fig. 1. The cases studied are: (a) no substrate, i.e. free-standing graphene, (b) an elastic substrate, and (c) a rigid substrate. These three systems are studied using conductive AFM experiments complemented by molecular dynamics (MD) simulations. In the experiments, current is measured using a doped ultrananocrystalline diamond (UNCD) tip in contact with free-standing graphene, graphene on polydimethylsiloxane (PDMS) and graphene on UNCD. In the complementary simulations, current is calculated using MD with the electrochemical dynamics with implicit degrees of freedom (EChemDID) method [25,26] for free-standing graphene, graphene on graphite and graphene on diamond. In both experiments and simulations, current is obtained as a function of normal force and the differences between the three cases are evaluated. The simulations allow further analysis of the origin of observed differences, in terms of the continuum concept of elasticity as well as local atomic-scale effects.

## 2. Methods

Electrical current flow as a function of normal force and voltage bias was measured for free-standing graphene, graphene supported by PDMS, and graphene supported by UNCD. The substrates were chosen from nonconductive materials to eliminate any possible cross conductivity contribution from the substrate. The hardness of substrate materials was measured with a Vickers hardness machine and found to be 49 GPa for the UNCD and 0.97 GPa for the PDMS. These results are comparable to values reported previously for these materials: UNCD (65–95 GPa [27]) and PDMS (1.57 GPa [28]). Therefore, the hard substrate was approximately 50 times harder than the soft substrate in these experiments. Statistically it has been shown that, the harder the substrate, the larger the elastic modulus [29,30]. Thus, the graphene supported by UNCD is expected to be the most rigid of the three cases.

To prepare the samples, single layer graphene was first chemical vapor deposition (CVD) grown on a copper foil and then transferred on the substrate of interest using 200 nm thick polymethyl(methacrylate) (PMMA) film. During the transfer, the copper was etched in a copper etchant (Sigma Aldrich) and the resulting graphene with the PMMA film on top was transferred to the substrate. The PMMA was removed using a warm acetone bath. Complete removal of the PMMA layer and the single-layer nature of the graphene film were confirmed using scanning electron microscopy (SEM) and Raman spectroscopy with a 534 nm green laser. For the

free-standing case, the graphene was transferred onto a silicon nitride substrate with 2  $\mu\text{m}$  diameter holes as shown in Fig. 2(a). For elastic substrate measurements, the monolayer graphene film was transferred onto a PDMS substrate as shown in Fig. 2(b). For rigid substrate measurements, the monolayer graphene film was transferred onto a UNCD substrate, as shown in Fig. 2(c), grown using Hot Filament UNCD synthesis technique [31].

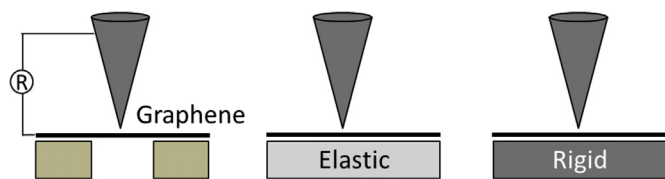
The samples were attached to the insulating quartz substrate using a ceramic paste and the grounding connection was made on the edge of the samples using a conductive silver paint. This geometry was created to allow the electrical current to travel from the tip to the graphene and then laterally across the graphene film to the contacting pads. The electrical resistance of the conductive pads was measured to be on the order of 1 Ohm, which is substantially lower than the contact resistance obtained from I-V curves measured in the experiments.

AFM measurements were performed using a Bruker Multimode AFM in contact mode with a conductive doped UNCD tip (Advanced Diamond Technologies, spring constant of  $\sim 0.3$  N/m, tip radius is  $\sim 20$  nm), shown in Fig. 2(d). High mechanical strength and wear resistance of the diamond tip allowed multiple tests to be performed without detectable changes of the tip radius. Interchangeability of the tip was also confirmed by performing several cycles of measurements in the following order: free-standing, PDMS, UNCD, PDMS and free-standing. The evolution of the electrical contact between the tip and graphene was tested in static mode while increasing the applied normal force. The maximum normal force was limited to 250 nN, which remained well below critical normal forces required for free-standing CVD grown graphene rupture (order of 2000 nN) or for inelastic deformation under AFM nano-indentation [32,33]. The applied bias voltage varied from  $-2$  V to 2 V and the maximum electrical current flow was limited to a maximum of 1  $\mu\text{A}$  to prevent local heating-induced failure of the tip and melting of the PDMS substrate.

To complement the experimental studies, we developed atomistic models of a diamond tip (radius 3 nm, height 2 nm) approaching three substrates: suspended monolayer graphene, eight-layer graphite, and monolayer graphene supported by a diamond substrate as shown in Fig. 3(a)–(c). These are comparable to the experimental systems shown in Fig. 2 except that, for the elastic substrate, instead of PDMS, the simulations used graphite for simplicity and model availability. Although the elastic modulus of graphite is not the same as PDMS, the elastic modulus of both materials is smaller than that of UNCD. Therefore, both graphite and PDMS represent an intermediate case between the unsupported free-standing graphene and the rigid diamond substrate.

The lateral dimensions of all model systems were 9.7 nm  $\times$  8.4 nm. The atoms in the top 0.4 nm of the tip were treated as a rigid body. The atoms at the both ends of the graphene layer along one of the lateral directions were fixed in order to constrain movement. The boundary in the other lateral direction was periodic. For the graphite substrate system, the bottom layer of graphene was fixed. For the graphene/diamond substrate system, the thickness of the diamond was about 1 nm and the atoms in the bottommost 0.2 nm of diamond were held fixed. The interatomic interactions were described by the ReaxFF force field with parameters reported in Ref. [34]. A Langevin thermostat was applied to all the non-constrained atoms in the directions perpendicular to the direction of tip movement to control the temperature at 300 K. The simulations were performed with LAMMPS [35] and the timestep was 0.25 fs.

The entire system was first relaxed for 5 ps with the tip 1.2 nm away from the surface until the potential energy of the system was stable. Then the tip was moved down at a speed of 10 m/s towards the surface. At different vertical positions, the tip movement was



**Fig. 1.** Schematic of the conceptual design. Current is measured for a nanoscale tip brought into contact with (a) free-standing graphene, (b) graphene supported by an elastic substrate and (c) graphene supported by a rigid substrate. (A colour version of this figure can be viewed online.)

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