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Atomistic study of lateral contact stiffness in friction force microscopy

H. Gao [a], Y. Dong [b], A. Martini [a,*]

[a] University of California – Merced, 5200 North Lake Road, Merced, CA 95343, USA
[b] The University of Akron, 302 E Buchtel Ave., Akron, OH 44325, USA

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ABSTRACT

The effective stiffness of a friction force microscope tip–substrate system is an important parameter that describes the relationship between lateral force and elastic deformation. In this study, we use a multi-spring model to simplify the system, where two contributions, the tip apex stiffness and the lateral contact stiffness, are discussed in detail. Molecular dynamics simulations are used to characterize stiffness by simulating a tip apex subject to shear or sliding over a substrate surface. The results show that, although the height of the tip apex and tip–substrate orientation affect the various stiffness contributions, the contact itself dominates the overall compliance.

1. Introduction

The advent of the friction force microscope (FFM) [1,2] has enabled quantitative measurements of atomic-scale friction, adhesion and wear. For a typical FFM, a nanoscale tip mounted to a cantilever slides over a substrate surface and the corresponding friction force can be measured by detecting the torsional bending of the cantilever through an optical method. Atomic-scale friction is recognized as a very sophisticated process that is affected by many factors, such as material properties, normal load, temperature, velocity, contact area etc. [3]. To simplify this complex system and provide a means of understanding observed trends, reduced-order, single asperity models have been introduced. The Prandtl–Tomlinson (PT) model [5,6] is the most successful and influential model used for this purpose. In this model, the total energy consists of two parts: tip–substrate interaction energy and elastic energy. The interaction between tip and surface is described by a sinusoidal corrugation potential and the elastic contribution is described by a linear spring. This model provides a quantitative description of the relationship between atomic-scale friction and stiffness.

The effective stiffness of a FFM is determined by contributions from multiple components in the system. To capture this effect, initially, a two-spring model was proposed to differentiate the elastic contributions of the tip and contact from that of the cantilever [7]. This relationship is illustrated schematically in Fig. 1(a). Based on this concept, the effective stiffness (k_{eff}) can be written as

$$1/k_{eff} = 1/k_l + 1/k_t, \tag{1}$$

where k_l denotes the lateral stiffness of the cantilever, and k_t denotes tip–contact stiffness. Reported values for effective stiffness are typically on the order of 1 N/m [8–13]. Typical values of the lateral stiffness of the cantilever usually fall into the range of tens to hundreds of N/m, which correlates with the material properties as well as the geometrical features of the cantilever [14–16]. The estimates of k_{eff} and k_l with Eq. (1) suggest that k_t should be on the order of 1 N/m, which is consistent with an estimate reported previously [17,18–20]. To further characterize k_t, we use an enhanced model that separates the tip-contact stiffness further into three contributions: the main body of the tip, k_b, the nano-sized tip apex, k_a, and the lateral contact stiffness (subsequently referred to simply as contact stiffness), k_c [3]. A schematic of the four-spring system is shown in Fig. 1(b). In this model, the tip–contact stiffness can be expressed as

$$1/k_t = 1/k_b + 1/k_a + 1/k_c. \tag{2}$$

The stiffness of the main body of the tip (k_b) has been reported to be on the same order as the stiffness of cantilever [15]. Since both k_l and k_b are an order of magnitude larger than k_{eff}, Eqs. (1) and (2) can be rewritten as

$$1/k_{eff} = 1/k_a + 1/k_c. \tag{3}$$

Physically, this expression indicates that the effective stiffness of the system will be determined by either k_a or k_c.

Direct quantitative measurement of contact stiffness in experiment is difficult due to the small size scale and the sensitivity of this parameter to material and operating conditions. This suggests a model-based approach. We first evaluate the possibility

* Corresponding author. Tel.: +1 209 228 2354.
E-mail address: amartini@ucmerced.edu (A. Martini).

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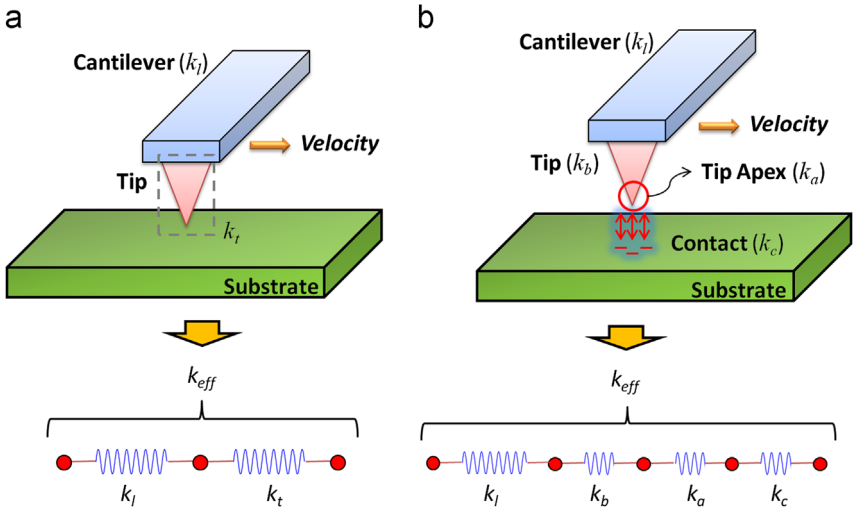

Fig. 1. Schematics of the (a) two-spring and (b) four-spring model systems.

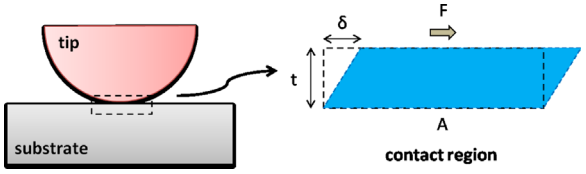

Fig. 2. Schematic of tip–substrate continuum contact where the top surface of the contact region (dashed frame) is displaced a small distance.

of simply using continuum mechanics. Consider a continuum representation of the contact shown in Fig. 2. For this system, shear stress (τ) is the lateral force (F) applied divided by a contact area (A), $\tau = F/A$. Strain can be expressed as $\varepsilon = \delta/t$, where δ is the relative displacement of the contact area, and t is the thickness of the contact region (shown in Fig. 2). Stress and strain are related by Hooke's law, $\tau = G\varepsilon$, where G is the shear modulus. Hence, according to the above expressions, we have $F = GA\delta/t$. The contact stiffness k_c can then be defined as the ratio of the lateral force to the relative displacement: $k_c = F/\delta$. By substituting the above expression for F into the expression for k_c, we deduce

$$k_c = GA/t \tag{4}$$

We can analyze this expression by evaluating its predictions with estimated magnitudes of the parameters. For example, if we assume that $k_c = 1$ N/m, $t = 1$ nm, and $G = 50$ GPa, the contact area will be 0.02 nm^2, which is unrealistically smaller than the projected area of a single atom. On the other hand, if we take $A = 100$ nm^2 and keep the other two parameters constant, then $G = 0.01$ GPa, which is much smaller than any solid tip or substrate material. Thus, reasonable approximation of any three of the parameters leads to an unphysical prediction of the remaining parameter. This result indicates that continuum mechanics cannot be used in the calculation of nanoscale contact stiffness.

To address this issue, we here introduce molecular dynamics (MD) simulation, which explicitly captures atomic-scale phenomena. This approach enables quantification of contact and apex stiffness independently and therefore provides a means of understanding effective stiffness in general. The effects of tip height and tip–substrate surface orientation are also investigated. We show that the tip–substrate interaction is the smallest and therefore determines the effective stiffness of the system. Finally, we evaluate the model stiffness in the context of the PT model and its relationship to experimentally-observed stick-slip friction and effective stiffness.

2. Methodology

We implement a molecular dynamics simulation of a copper (tip apex) – aluminum (substrate) system using LAMMPS software [4]. Two models will be studied in this work: (1) a tip apex sliding on a substrate and (2) a tip apex subject to shear. In both cases, the truncated cone shaped tip apex has major and minor radii of $R_1 = 6$ nm and $R_2 = 0.6$ nm and maximum total height $H_0 = 8.5$ nm. Varied tip apex heights, i.e. 0.25 H_0, 0.5 H_0, 0.75 H_0 and H_0, are also modeled. In our simulations, we do not explicitly model tip rotation (that may be caused by the twisting of the cantilever in an experiment) based on the assumption that its effect on stiffness will be small at low normal loads. The temperature is held at 0 K throughout the simulation to enable us to isolate configuration-determined stiffness from dynamic effects. The embedded-atom method [21] is used to describe the atomic interactions with previously-reported model parameters [22].

The first model is shown in Fig. 3(a). The dimensions of the substrate are $10 \times 10 \times 2$ nm^3, where sliding occurs on the (111) plane. The bottommost layers of the substrate are held fixed, and the topmost and bottommost few layers of the tip act as rigid bodies. There is a zero external normal load applied and the tip apex moves on the top surface of the substrate with a constant speed of 10 m/s. The overall lateral force is defined as the force on the top rigid layers of the tip, while the contact force is calculated directly from the interaction force between tip apex atoms and substrate atoms. The corresponding effective and contact stiffness can be obtained by measuring the slope of the force–distance curves.

We also investigate the mechanical properties of the tip apex alone, as shown in Fig. 3(b). In this model, we fix the top rigid layers of tip apex and move the bottom rigid layers at a speed of 10 m/s. We measure the lateral force on the bottom rigid layers. Then the tip apex stiffness is calculated from the slope of the force and distance curve.

3. Results and discussions

First, to characterize tip apex stiffness (k_a), we isolate the tip apex from the substrate. We displace the bottommost layer of the tip apex laterally (δ), and measure shear force (F). Fig. 4 shows F (blue solid circles) increases with δ for the tip model with $H = H_0$.