Both atomic force microscopy (AFM) experiments and molecular dynamics (MD) simulation are carried out to investigate atomic stick-slip friction by sliding a Pt tip on an Au substrate. Efforts are taken to match the conditions for AFM experiment and MD simulation as closely as possible. The results show that AFM and MD provide consistent energetic parameters, which suggests that MD simulations can be reliably used to interpret energetic aspects of the interfaces. However, orders of magnitude differences in attempt frequencies are found, which indicates another challenge between the MD simulations and AFM experiments, i.e., the inertia gap.

INTRODUCTION

On clean crystalline surfaces, friction forces at the nano-scale often exhibit a “saw-tooth” pattern, known as atomic stick-slip. Atomic stick-slip is caused by unstable slip events, and can lead to significant energy dissipation. An understanding of its underlying mechanisms can eventually help elucidate friction in macroscopic contacts, which are comprised of numerous nano-scale asperity contacts. It can also help optimize the performance of micro- and nano-scale mechanical devices and components, where nano-scale friction can be a limiting factor. Thanks to the invention of atomic force microscope (AFM), in which a sharp tip approximating a single asperity is moved laterally over a sample substrate while the resulting friction force is measured, substantial advances have been achieved in understanding the mechanical behavior of single asperity friction, and several new techniques have been proposed to reduce or control friction.

One major challenge for AFM is the inability to access in situ information at the nano-scale buried interface between the tip and substrate, which plays a dominant role in controlling atomic-scale friction. Molecular dynamics (MD) simulation, as a powerful tool to describe how positions, velocities, and orientations of atoms evolve over time, has the advantage of directly observing the phenomena occurring in the buried interface and therefore has been widely applied to interpret AFM experimental results. In this paper, we will directly compare AFM and MD with optimally-matched conditions. Through the comparison, we reveal an important, yet largely overlooked challenge for correlation between AFM and MD: the inertia discrepancy, i.e., the difference between the massive AFM tip and a relatively light MD tip (due to computational limitations).

METHODOLOGY

Metal-metal contact between the platinum-coated tip and the gold (111) surface is investigated both by AFM and MD. Experimentally, the Au (111) surface is prepared by thermally evaporating gold onto freshly cleaved mica discs under high vacuum followed by annealing with a hydrogen flame in air resulting in unreconstructed (111) terraces. All measurements were performed under a clean and dry N₂ environment at room temperature.

In MD simulation, (111) surfaces are chosen as the contacting interface for both Pt tip (modeled as a truncated...
cone) and the Au substrate. All atoms are modeled by a Voter-Chen-style Embedded Atom Method. Due to the computational limitation of regular MD, there is a large speed gap between AFM and MD (see Figure 1(a)). We have implemented parallel replica dynamics (ParRep), an accelerated MD approach for infrequent-event systems, to reduce the gap between experimental and simulated atomic stick-slip speeds. The essential idea of ParRep is to view stick-slip as an infrequent event, i.e., most of the time the system resides in the “stick” state and the “slip” occurs infrequently and rapidly. We seek to speed up the “stick” process to reduce the computation time.

We replicate the system into copies, and minimize and randomize the copies to ensure they have independent trajectories. After a transition is identified in one copy, we stop all the processes and resume the process again at the next lattice site. In this way we can speed up the process with a boost factor up to.

RESULTS AND DISCUSSION
Friction at the nano-scale can depend very sensitively on a variety of parameters, e.g., materials, sliding direction, orientation, normal load, temperature, cantilever stiffness, speed, and so on.

To directly compare AFM and MD results, we made substantial efforts to optimally match the parameters used in experiments and simulations. Figure 2(a) shows the friction traces from an AFM experiment (left) and a MD simulation (right) with all parameters as close as possible, except speed. Both systems present the clear “saw-tooth”-like stick-slip traces with the same periodicity and similar maximum friction. To the best of our knowledge, it is the first time MD simulations have been brought this close to AFM experiments. Such optimal matching can provide rich physical information. Figure 2(b) demonstrates the variation of mean friction force with different speeds. Data for speeds between 1 nm/s and 1000 nm/s are obtained from AFM experiments and data for speeds between 0.005 m/s to 1 m/s are from ParRep MD simulations. We then fit the data to the analytical Tomlinson...
model with thermal activation (Equation 1) and the fitting parameters are shown in Table 1.

\[ F = F_c - \beta k_b T \ln \left( \frac{v}{v_c} \right)^{2/3} \]

Where \( F \) is friction, \( F_c \) is the friction force at zero temperature, \( \beta \) is the shape of the corrugation potential, \( k_b \) is Boltzmann’s constant, \( T \) is temperature, \( v \) is speed, \( v_c \) is the critical speed, \( f_o \) is the attempt frequency, and \( k_{tot} \) is the stiffness.

First, both the friction force at zero temperature \( F_c \) and the parameter determined by the shape of the corrugation potential \( \beta \) are reasonably consistent with those from the experiment. This suggests that the main features of the energetics of the stick-slip process can be captured by fully atomistic, or even effective low-dimensional models.

Second, there is a huge discrepancy (approximately six orders of magnitude) in the attempt frequency \( f_o \). The drastically different attempt frequencies can be interpreted by differences in vibrational characteristics due to widely differing effective inertias of low frequency modes. One can rationalize the relationship between the attempt frequency and the tip inertia through a spring-mass system, the smaller the mass, the larger the characteristic frequency of the spring mass system. Because of computation limitations, MD simulation can only simulate the tip apex of the AFM, which is very light and usually composed of thousands to millions of atoms in the simulation. Compared to the real “massive” AFM tip and cantilever, the MD tip is characterized by a much faster vibration frequency thus a much larger attempt frequency. This discrepancy poses another important challenge as well as opportunities to the nanotribology community.

**SUMMARY**

Optimal matching between AFM experiments and MD simulations has been pursued. The ParRep method is employed to reduce the driving speed in the MD simulations. The energetics of the stick-slip process can be captured by the MD simulations. However, due to the discrepancy in the effective inertia between MD and AFM, MD fails to capture the attempt frequency of AFM. Both the speed gap and inertia gap shown in Figure (3) motivate the introduction of new techniques such as transition state theory or multiscale methods to the rapidly developing field of atomic friction.

**ACKNOWLEDGMENTS**

This work was done in collaboration with Danny Perez and Arthur F. Voter at Los Alamos National Laboratory (LANL). We would like to thank Mr. Liang Guo for drawing the cartoons and are grateful to the National Science Foundation for its support via award CMMI-1068552 and CMMI-1068741.

**REFERENCES**


**Table 1 | Comparison between AFM and MD**

<table>
<thead>
<tr>
<th></th>
<th>( F_c (nN) )</th>
<th>( \beta (N^{1/2}/J) )</th>
<th>( f_o (GHz) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFM</td>
<td>0.55</td>
<td>( 3.0 \times 10^5 )</td>
<td>( 4.9 \times 10^5 )</td>
</tr>
<tr>
<td>MD</td>
<td>0.85</td>
<td>( 3.6 \times 10^5 )</td>
<td>40</td>
</tr>
</tbody>
</table>

![Figure 3 | Illustration of gaps between MD and AFM i.e., speed gap and inertia gap.](image-url)