Friction law for atomic-scale contact assisted by atomistic simulations

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Abstract

Non-empirical law depicting how atomic-scale friction behaves is crucial to facilitate the practical design of tribosystems. However, progress in developing a practically usable friction law has stagnated because atomic-scale friction arises from the continuous forming and rupturing of interfacial chemical bonds and such interfacial chemical reactions are difficult to measure precisely in experiments. Here, we propose a usable friction law for atomic-scale contact by using atomistic simulations to correctly measure the interfacial chemical reactions of a realistic rough surface, and confirm its applicability to predicting how atomic-scale friction varies with temperature, sliding velocity, and load.
Friction is particularly important for reducing energy consumption because around 30% of the world’s energy is lost to friction\textsuperscript{1,2}. Generally, friction between two solids sliding relative to each other depends on not only the types of contacting materials but also external conditions such as temperature, applied load, and sliding velocity. Practically applicable friction laws that predict how these external conditions influence the friction force are crucial because they would benefit greatly the practical design of lubricating systems.

Conventionally, friction force \( F_f \) between two surfaces is proportional to the applied normal force \( F_N \). This linear relation between \( F_f \) and \( F_N \) is explained by the well-known Amontons’ law, which states that the real contact area \( A_{\text{real}} \) between two macroscale surfaces is generally proportional to \( F_N \)\textsuperscript{3,4}; thus, if the shear stress on \( A_{\text{real}} \) is reasonably assumed to be constant, then the linear relations \( F_f \propto A_{\text{real}} \propto F_N \) appear. Recently, however, with the advances in nanotribological experiments, it has been found that frictional behavior at nanoscale contact does not generally obey Amontons’ law\textsuperscript{5,6}. Instead, nanoscale friction behaves like a thermally activated process\textsuperscript{7}, and various analytical models have been established to explain the nanoscale friction data. For example, by treating nanoscale friction as a point-contact scheme in which a contacting atom is thermally activated to scan over a corrugated potential surface, successful predictions have been made regarding how the friction force of this contacting atom varies with temperature and scanning velocity, such as the Prandtl–Tomlinson (PT) model and its extended theories\textsuperscript{8–11}. Moreover, recent works have shown that nanoscale frictional behavior is dominated by the thermally activated formation of interfacial chemical bonds\textsuperscript{12}, and thus the corresponding \( F_f \) at nanoscale contact is proportional to the number of atoms that have interfacial chemical bonds\textsuperscript{13–15}. Based on the scheme in which interfacial chemical bonds are formed and ruptured repeatedly
during the friction, a recently proposed multi-bond analytical model of nanoscale friction offered a good interpretation of experimental data under various external conditions\(^{5,16-19}\).

However, even though the aforementioned works are unquestionably useful in understanding nanoscale friction partially, experimental insights into the thermally activated friction processes are far below what is needed in practice. To predict practically the atomic-scale friction, the crucial first step is to obtain the exact number of atoms having interfacial chemical bonds \((N_{ib})\) and the mean shear force per interfacial bond \((F_{ib})\), according to the detailed external conditions (applied normal force, sliding velocity, and environmental temperature), material properties (e.g., Young’s modulus and density), and surface morphology (determining the real contact area). Because both the forming and rupturing of interfacial bonds are chemical reactions, \(N_{ib}\) and \(F_{ib}\) can be calculated via the reaction rate theory by introducing several semi-empirical parameters such as the activation energy of interfacial bond formation, just like what the PT and multi-bond models have done. Once these semi-empirical parameters, material properties, and surface morphology are known, it is possible to predict how the external conditions affect the friction force at the atomic scale. Generally, exact values of these semi-empirical parameters should be extracted from experimental results of \(N_{ib}\) and \(F_{ib}\) at different surface temperatures as actually experienced by atoms in the real contact surface, because both the forming and rupturing of interfacial bonds are temperature-dependent processes. However, for experiments, \(N_{ib}\), \(F_{ib}\), and the real surface temperature are extremely difficult to be precisely measured even using the most advanced experimental instruments, although it is easy to experimentally obtain other required information such as applied loads, sliding velocities, Young’s modulus, and surface roughness. This lack of correct values for \(N_{ib}\), \(F_{ib}\), and the real surface temperature directly hinders the development and validation of a practically applicable friction law. In this paper, we propose that the interfacial
chemical reactions and real surface temperature could be monitored very effectively and precisely using the large-scale reactive molecular dynamics (MD) simulations with our previously developed high-accuracy reactive potentials\textsuperscript{20–22}. We aim to establish a practically and easily applicable friction law that can predict how the friction force varies with the external conditions at the atomic scale, based on the precisely measured $N_{ib}$, $F_{ib}$, and surface temperature from MD simulations.

\textbf{Results}

We use diamond-like carbon (DLC)\textsuperscript{23,24} as the test material because DLC is a widely used and studied solid lubricant. Fig. 1A shows the friction simulation model, in which two hydrogen-passivated DLC substrates with self-affine roughness\textsuperscript{25} are used to represent a realistic contact state. The rigid layer of the upper substrate is loaded with a normal force ($F_N$) and slid forcibly with a sliding velocity ($v$), while the rigid layer of the lower substrate is kept stationary. Temperature of the thermostat layers neighboring the rigid layers, which is regarded as the substrate temperature ($T_{sub}$), is controlled during the friction simulation. Obviously, the real temperature of contacting surface ($T_{real}$) is higher than $T_{sub}$ because of the frictional heat at the friction interface. Therefore, to obtain the exact $T_{real}$ and then understand how it influences the friction force and interfacial chemical reactions, we perform friction simulations with different $T_{sub}$ while keeping $F_N$ and $v$ unchanged. To obtain the accurate $T_{real}$ in MD, temperature distributions in the substrate depth direction are investigated, as exemplified in Fig. 1B where $T_{sub} = 300 \text{ K}$, $F_N = 675 \text{ nN}$, and $v = 100 \text{ m/s}$. Initially, temperature of the whole substrate is distributed homogeneously and is around 300 K; however, during friction, temperature increases with proximity to the friction interface. Here, $T_{real}$ is defined as the mean of the highest
temperature in the distribution profile, which is about 500 K higher than $T_{sub}$. Using this definition, we observe that the obtained $T_{real}$ increases almost linearly with increasing $T_{sub}$ (Fig. 1C). See the Supplementary Information for detailed simulation setups and discussions on $T_{real}$.

Fig. 1 Simulation setup and calculation of $T_{real}$. (A) Simulation model of two rough surfaces. Blue balls represent hydrogen atoms, while orange and red ones represent carbon atoms in the upper and lower substrate, respectively. (B) Temperature distribution of a typical friction simulation with $T_{sub} = 300$ K, $F_N = 675$ nN, and $v = 100$ m/s. (C) $T_{real}$ as a function of $T_{sub}$ under the same $F_N$ and $v$ as in (B).

The next task is to know how friction force ($F_f$) and interfacial chemical reactions are affected by $T_{real}$ in the MD simulations. Open squares in Fig. 2A show the MD-measured $F_f$ as a function of $T_{real}$, where an interesting mountain-type temperature dependence of $F_f$ appears. What is the origin of this $F_f$-$T_{real}$ relationship? At atomic scale, $F_f$ is essentially proportional to the total number of atoms having interfacial chemical bonds ($N_{ib}$)$^{13-15}$; thus, if $F_{ib}$ represents the mean shear force per interfacial bond, $F_f$ can be calculated by

$$F_f = \frac{N_{ib}F_{ib}}{2}$$  \hspace{1cm} (1)
where the product of $N_{ib}$ and $F_{ib}$ is halved because the upper and lower substrates are assumed to contain the same number of interfacial bonding atoms. Thus, we can now study how $T_{real}$ affects $N_{ib}$ and $F_{ib}$ separately. Figs. 2B and 2C show the results of $N_{ib}$ and $F_{ib}$ respectively as a function of $T_{real}$ which are directly measured from the MD simulations. Qualitatively, $N_{ib}$ increases whereas $F_{ib}$ decreases non-linearly with the increasing $T_{real}$, and hence the competition of the increasing $N_{ib}$ and decreasing $F_{ib}$ is suggested to be the origin of the mountain-type $F_f-T_{real}$ relationship.
Fig. 2 Friction simulation results. (A) $N_{ib}$, (B) $F_{ib}$, and (C) $F_f$ as a function of $T_{real}$ with $F_N = 675$ nN and $v = 100$ m/s.

Next, we discuss quantitatively how $T_{real}$ influences $N_{ib}$ and $F_{ib}$. For $N_{ib}$, because only the atoms in the real contact area have opportunities to form chemical bonds with their counterparts, $N_{ib}$ can be computed by multiplying the number of atoms in the real contact region ($2A_{real}(F_N)/A_{atom}$, where the real contact area $A_{real}(F_N)$ is a function of $F_N$ and $A_{atom}$ is the average surface area per atom) with the probability of forming an interfacial bond. As we have reported previously, this probability is affected by both temperature ($T$) and applied normal force ($F_N$), and can be computed by applying the reaction rate theory to the reaction of interfacial bond formation. Thus, the expression of $N_{ib}$ as a function of $T$ and $F_N$ is

$$N_{ib}(T, F_N) = \frac{2A_{real}(F_N)}{A_{atom}} \exp \left[ \frac{V_{atom}}{2E k_B T} \left( \frac{F_N}{A_{real}(F_N)} \right)^2 - \frac{\Delta U_{ib}}{k_B T} \right]$$  \hspace{1cm} (2)$$

where $V_{atom}$ is the average volume per atom, $E$ is the Young’s modulus, $k_B$ is the Boltzmann constant, and $\Delta U_{ib}$ is the activation energy of forming an interfacial bond. $A_{real}(F_N)$, $A_{atom}$, $V_{atom}$, and $E$ can be obtained directly if the material properties and surface morphology are known, but $\Delta U_{ib}$ still needs to be determined from experimental and/or simulation fitting (see the Supplementary Information for detailed discussion). In Fig. 2B, Eq. 2 reproduces the MD results of $N_{ib}$ very well if $\Delta U_{ib} = 0.0847$ eV and $T = T_{real}$ are used. Here it should be additionally but interestingly noticed that Eq. 2 with $T = T_{sub}$ could not fit the MD results whatever (Fig. S3 in the Supplementary Information), indicating that the one which truly dominates the thermally activated friction process is $T_{real}$ rather than $T_{sub}$ or the environmental temperature. Meanwhile, the lateral force of rupturing an interfacial bond, $F_{ib}$, could be correctly obtained by the multi-bond model
proposed by Urbakh’s group\textsuperscript{5,16–19}. However, Urbakh’s multi-bond model is too complex to be applied simply, because its analytical expression involves multiple hard-to-determine empirical parameters. Instead, $F_{ib}$ can be estimated by the simpler PT model because the thermally activated process of rupturing an interfacial bond can be regarded as the process of climbing a potential curve. Using a previous form\textsuperscript{9}, we have

$$F_{ib}(T, v) = F_c - \left[ \beta k_B \ln \left( \frac{bT}{v} \right) \right]^{\frac{2}{3}} T^{\frac{2}{3}}$$

(3)

where $\beta$ is potential curve corrugation of contact surface and is a function of the critical force ($F_c$). $b$ is a material- and system-dependent parameter as discussed exhaustively in the Supplementary Information. Here, only $F_c$ and $b$ as fitting parameters should be determined by comparing with the experimental/simulation results. By fitting Eq. 3 to the MD-measured $F_{ib}$ using $T = T_{real}$, we obtain $F_c = 2.006$ nN and $b = 1.000$. Thus, with the values obtained above for $\Delta U_{ib}$, $F_c$, and $b$, Eq. 1 succeeds to predict a mountain-type temperature dependence of the friction force, which matches the MD-measured $F_f$ perfectly (Fig. 2A).

It is also essential to precisely understand the frictional behaviors as well as the interfacial chemical reactions affected by different $F_N$ and $v$, and we expect Eqs. 1–3 (with the above extracted $\Delta U_{ib}$, $F_c$, and $b$) to be valid for describing the load and velocity effects. According to Eqs. 2 and 3, it is obvious that, if temperature is unchanged, $F_N$ and $v$ would only have influences on $N_{ib}$ and $F_{ib}$, respectively. Thus, to check the relationship between $N_{ib}$ and $F_N$ and assess the validity of Eq. 2, we perform friction simulations using the same model as that in Fig. 1A, by varying $F_N$ while keeping $T_{sub} = 300$ K and $v = 100$ m/s; thereafter, to study the $F_{ib}(v)$, simulations are performed by varying $v$ while keeping $T_{sub} = 300$ K and $F_N = 675$ nN. Open squares in Figs. 3A and 3B show the simulation results of $N_{ib}$ and $F_{ib}$ as a function of $F_N$ and $v$. 


respectively. Focusing on $N_{ib}(F_N)$ firstly, the measured $N_{ib}$ increases monotonically with $F_N$, and then we should confirm whether this relationship obeys Eq. 2 or not. Note that $T_{real}$ will increase with $F_N$ even though $T_{sub}$ is kept unchanged because larger applied load brings more frictional heat (Fig. S2A in the Supplementary Information). Obviously, to predict $N_{ib}(F_N)$, the exact values of $T_{real}$ must be taken into consideration; otherwise, for instance, if $T = T_{sub}$ is substituted into Eq. 2, the prediction (red line in Fig. 3A) differs greatly from the simulation results. However, if $T = T_{real}$ (which is obtained with respect to each $F_N$) is used, the prediction agrees with the simulation results very well (blue line in Fig. 3A). Meanwhile, for $F_{ib}(v)$, the MD simulations show a decreasing trend of $F_{ib}$ with increasing $v$. As with the load-induced change of $T_{real}$, increasing $v$ also cause a raise of $T_{real}$ because of the higher frictional heat (Fig. S2B in the Supplementary Information). Therefore, to correctly predict $F_{ib}(v)$, we must use the exact values of $T_{real}$; otherwise, for instance, the predicted $F_{ib}$ using $T = T_{sub}$ exhibits a positive correlation with $v$ (red line in Fig. 3B), which differs completely from the simulation results. However, if $T = T_{real}$ (which is obtained with respect to each $v$) is substituted to Eq. 3, the predictions show an agreement with the MD simulation results (blue line in Fig. 3B). Overall, the above results demonstrate that Eqs. 1–3 are indeed valid for describing nanoscale friction behavior under different applied loads and sliding velocities, but only if using the correct surface temperature rather than the substrate or environmental temperature.
Fig. 3 Validation of load and velocity effects. (A) $N_{ib}$ as a function of $F_N$ with $T_{sub} = 300$ K and $v = 100$ m/s. (B) $F_{ib}$ as a function of $v$ with $T_{sub} = 300$ K and $F_N = 675$ nN; note the use of a logarithmic coordinate for $v$ (abscissa).

Here, as a trial application of Eqs. 1–3, we predict how $F_N$ and $v$ affect the temperature dependence of $F_f$. In Fig. 2C, $F_f$ exhibits a mountain-like dependence on $T_{real}$ under constant $F_N$ and $v$. According to Eqs. 2 and 3, this temperature dependence of friction may be altered by $F_N$ and $v$ through their effects on $N_{ib}$ and $F_{ib}$, respectively. Fig. 4A shows the predicted $F_f$ as a function of $T_{real}$ under a constant $v$ of 100 m/s but different $F_N$. With increasing $F_N$, the $F_f-T_{real}$ curve moves upward entirely because of the increasing $N_{ib}$ with $F_N$, while the critical temperature corresponding to the maximum friction (referred as to $T_{max}$) remains unchanged. Regarding the velocity effect, Fig. 4B shows the predicted $F_f$ under a constant $F_N$ of 675 nN but different $v$. 
Herein we observe the entire shift-up of the curve with the increasing $v$ again, but interestingly the $T_{\text{max}}$ increases with increasing $v$, differing from the load effect. The above predicted trends, namely, that the sliding velocity changes $T_{\text{max}}$ whereas the applied load does not, agree qualitatively with previous experiments\textsuperscript{19,29}. This result helps the reduction of friction by choosing the proper temperature and sliding velocity, thereby benefiting greatly the practical design of lubricating systems.

![Diagram](image)

**Fig. 4** Effects of $F_N$ and $v$ on temperature dependence of $F_f$. (A) $F_f$ as a function of $T_{\text{real}}$ under a constant $v$ of 100 m/s but different $F_N$. (B) $F_f$ as a function of $T_{\text{real}}$ under a constant $F_N$ of 675 nN but different $v$.

We must also point out the limitations of Eqs. 1–3 for friction prediction. First, they are not available for the systems in which non-bonding interactions such as van der Waals are dominant.
Such systems include (i) atomic-scale contact of ultra-smooth surfaces (because surface adhesion becomes a dominant factor with decreasing surface roughness\textsuperscript{30,31}) and (ii) friction of two-dimensional materials such as graphene and MoS\textsubscript{2} (because friction of these materials stems mostly from the van der Waals interactions between neighboring layers). Second, Eqs. 1–3 may fail under extremely high or low temperatures, loads, and sliding velocities, as discussed exhaustively in the Supplementary Information.

Discussion

In summary, we succeeded in using large-scale reactive MD simulations to precisely monitor the real surface temperature and interfacial chemical reactions of DLC in a realistic rough-surface contact state. Based on the MD simulation results, we established a proper theoretical friction law to describe the atomic-scale frictional behavior and further predict how the friction force varies with temperature, sliding velocity, and applied load. Furthermore, we showed that the actual temperature of the contacting surface must be used in the proposed friction model to practically and correctly predict the friction force; otherwise, the predictive results may deviate greatly if the substrate or environmental temperature is used in the proposed friction law. This work could contribute greatly to understanding the fundamentals of friction and the practical design of lubricating systems.

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Data availability

All data needed to evaluate the conclusions are present in the paper and/or the Supplementary Information. Additional data are available from the authors upon request.

Acknowledgments

This research was supported by MEXT as “Exploratory Challenge on Post-K Computer” (Challenge of Basic Science - Exploring Extremes through Multi-Physics and Multi-Scale Simulations), JST CREST, JSPS Grant-in-Aid for Young Scientists (B) (Grant No. 17K14430), JSPS Grant-in-Aid for Scientific Research (C) (Grant No. 19K05380), and JSPS Grant-in-Aid for Scientific Research (A) (Grant No. 18H03751). We gratefully acknowledge the Center for Computational Materials Science (CCMS, Tohoku University) for the use of MAterials science Supercomputing system for Advanced MUlti-scale simulations towards NExt-generation - Institute for Materials Research (MASAMUNE-IMR) (Grant Nos. 18S0403 and 19S0506).

Author contributions

M.K. supervised the research. Y.W. conceived the main idea of this work, and then designed and performed the simulations. J.X. prepared the simulation code framework. The manuscript was written by Y.W. and revised by J.X., K.A., and M.K. All authors participated in the interpretation of the data and discussion of the manuscript.

Competing interests

The authors declare no competing interests.