The Influence of Sliding Speed on the Friction Behavior of Silica Surface

Shang Gao, Li Hong Yang, Yi Gan, and Qiang Chen

ABSTRACT: Studies have shown that the relative sliding speed of the silicon-based material surface has an effect on its friction behavior. In this study, the molecular dynamics method was used to simulate the sliding of the SiO\textsubscript{2} surface at different speeds. This is to explore the internal mechanism between SiO\textsubscript{2} surface friction behavior and the relative sliding speed. First of all, this study constructed a 3D model of the SiO\textsubscript{2} friction surface and simulated the sliding process under two different environments of absolute dryness and full wetness. Then, the sliding of the SiO\textsubscript{2} surface at different speeds in dry and wet environments is simulated and verified the rationality of the simulation through experiments. The final results show that the lattice distortion and tribochemical reactions that occur on the SiO\textsubscript{2} surface of the material have varying degrees of influence on the friction behavior of the material surface. In the dry environment, the coefficient of friction of the SiO\textsubscript{2} surface increases with the speed. On the contrary, in the humid environment, the SiO\textsubscript{2} surface decreases as the speed increases. The analysis results found that the speed has varying degrees of influence on the lattice distortion and tribochemical reaction of the SiO\textsubscript{2} surface. Eventually, this study quantifies the effect of speed on SiO\textsubscript{2} surface tribochemical reactions and lattice distortion in two different environments.

1. INTRODUCTION

Silicon is an extremely common material. It is widely found in rocks, gravel, and dust. Silicon rarely exists in nature as a simple substance but in the form of complex silicate or silica. At present, silicon-based materials are mainly used in micromotors (MEMS),\textsuperscript{1,2} microbearings, accelerometers, and other equipment due to their excellent performance.	extsuperscript{3,4} However, at the same time, silicon-based materials still face many shortcomings, such as poor friction properties, low reliability, and easy wear, so they cannot be applied on a large scale. Generally speaking, reducing friction in the mechanical system can reduce energy consumption and extend the life of the system.\textsuperscript{5−13} Therefore, it is of great significance to understand the friction phenomenon in the movement of silicon-based materials and reveal its mechanism of friction.

In recent years, the research on friction behavior has also gone deep into the nanolevel due to advances in nanotechnology.\textsuperscript{14} A large number of researchers have discovered that the relative sliding velocity at the atomic scale has an important influence on the friction behavior of the material surface, which is different from traditional macroscopic tribology. Riedo and Gnecco\textsuperscript{15} found through FFM experiments that there is a proportional relationship between speed and the coefficient of friction when the speed is lower than a certain critical value. Han et al.\textsuperscript{16} determined the coefficient of friction of the SiO\textsubscript{2} surface at different sliding speeds and found that there is a proportional relationship between the coefficient of friction and speed, which is consistent with the experimental results of Riedo and Gnecco. However, Ge et al.\textsuperscript{17} research found that the friction coefficient of the surface of nano-SiO\textsubscript{2} at a faster speed decreases with the increase in speed. Therefore, how the speed affects the coefficient of friction of the SiO\textsubscript{2} surface and the quantitative relationship between the speed and the coefficient of friction is an issue that needs to be studied urgently.

At present, many scholars have analyzed the origin of SiO\textsubscript{2} surface friction.\textsuperscript{18−20} At the atomic scale, the frictional behavior and energy loss on the SiO\textsubscript{2} surface mainly come from the action of a mechanical force and tribochemical reaction during the sliding process. Due to the mechanical force on the SiO\textsubscript{2} surface, lattice distortion will be observed, and then, energy loss will be observed in the sliding process. Yeon et al.\textsuperscript{21} found that many siloxane bonds would be formed on the surface of SiO\textsubscript{2}. Li et al.\textsuperscript{22} found that the siloxane bond on the SiO\textsubscript{2} surface will break during the sliding process, and the rupture of the siloxane bond has an impact on the friction behavior of the SiO\textsubscript{2} surface. Relevant studies have shown that the degree of wear on the surface of silicon-based materials in an environment with air humidity ranging from 0 to 50% increases with the increase of RH.\textsuperscript{23,24} Yu et al.\textsuperscript{25} believe that the
increase in friction and wear is due to the tribochemical reaction on the silicon-based surface, which causes energy loss. Wang and Duan found that the friction performance of silicon-based materials under water lubrication conditions is also related to the dehydration reaction on the surface of the material. The dehydration reaction forms siloxane bonds and causes energy loss. Wang and Duan quantified the effect of dehydration and hydrolysis on the friction properties of SiO₂. Therefore, the surface friction coefficient of SiO₂ is closely related to the mechanical force and surface tribochemical reaction.

It can be seen that, in the sliding process, the mechanical action and tribochemical reaction on the SiO₂ surface with different sliding speeds are different, which affect the friction performance of the material surface. This article intends to use the ReaxFF-MD simulation method for molecular dynamics simulation. First, this study constructed a 3D model of the friction surface of SiO₂. Then, the relative sliding movement of the SiO₂ surface at different speeds in the dry and wet conditions is simulated. Then, we analyzed the effect of speed on the friction coefficient of the friction surface under dry and wet conditions. Next, we mainly discuss the influence of speed on the mechanical force on the SiO₂ surface and the influence of speed on the tribochemical reaction of the friction surface. Finally, we will quantify these influencing factors.

2. SIMULATION METHOD

The simulation in this paper is based on the molecular dynamics method. Molecular dynamics simulation is used to determine the force between atoms through the potential function after establishing the model. Then, by solving the Newtonian equation of motion of the system, the trajectory of the atom in the space can be obtained. Finally, the physical properties of the system are obtained by statistics.

The simulation object of this research is α-quartz glass. α-Quartz glass is a kind of special glass containing only a single component of silicon dioxide. It is an amorphous structure formed by silicon atoms and oxygen atoms connected by siloxane bonds. In a dry environment, the model is mainly composed of upper and lower parts. The size of the upper part is 15 Å × 15 Å × 15 Å, and the size of the lower part is 150 Å × 15 Å × 15 Å (as shown in Figure 1a below). In a wet environment, the model is divided into three parts: upper, middle, and lower parts in a humid environment. The middle part is a layer of water molecules with a thickness of 10 Å, and its density is 0.97 g/cm³. Then, water molecules are filled randomly, ensuring that the coverage rate of water molecules on the material surface of the lower half is about 90%. The size of the upper part is 15 Å × 15 Å × 15 Å, and the size of the lower part is 150 Å × 15 Å × 15 Å. In Figure 1, red is the H atom, blue is the Si atom, and white is the O atom. The green arrow is the direction of the load on the upper part. The red arrow is the direction of movement of the upper part.

The simulated force field adopts the SiO-ReaxFF force field developed by van Duin et al. in 2003 under dry conditions. On the other hand, the simulation in a humid environment uses the SiOH-ReaxFF force field developed by Larsson and others in 2013. The two friction surface sliding models set the same motion conditions under the two friction conditions of dry and wet. The smaller SiO₂ surface above moves at a constant speed along the positive x axis. Furthermore, by applying it with a force of 10 nN, the direction of the force is along the negative direction of the z axis. The larger SiO₂ friction surface below maintains its relative position unchanged. In the case of wet friction, the layer of water molecules should restrict its movement in the y direction. The simulations were performed under two different conditions with speeds of 10, 20, 30, 40, and 50 m/s.

The whole system adopts NVE to control temperature and pressure. The simulated temperature is set at 800 K by the Nose—Hoover thermal bath method, and the time step is 0.25 fs. During the sliding process, the applied load is 10 GPa. The pressure of the system is maintained at 1 atm by the Nose—Hoover algorithm, and the pressure is adjusted in the z axis direction. Molecular dynamics simulation is completed by Lammps.

3. RESULTS AND DISCUSSION

3.1. Coefficient of Friction. The friction performance of the material surface is usually expressed by the coefficient of friction. The calculation method of the coefficient of friction in this paper is

\[ \mu = \frac{F_x}{F_z} \]

The coefficient of SiO₂ surface friction at different speeds is shown in Figure 2 below. Figure 2a shows the coefficient of friction at different speeds in the dry environment. Figure 2b shows the coefficient of friction at different speeds in the wet conditions. To verify the rationality of the simulation results, a coefficient of friction measurement experiment was carried out. This experiment measured the coefficient of friction SiO₂. During the experiment, the sliding speed was 10 m/s and the applied load was 10 GPa, which was consistent with the simulation. The dry and wet coefficients of friction obtained in the experiment are shown in Figure 2c.d.

It can be seen from Figure 2 that the friction coefficient of the SiO₂ surface in different environments is affected by the sliding speed. In the case of dry friction, as the relative sliding speed increases, the coefficient of friction increases (as shown in Figure 2a). On the other hand, in the case of wet friction, its changing trend is opposite to that of dry friction. As the speed increases, the coefficient of friction decreases to a certain extent (as shown in Figure 2b). However, we found that the coefficient of friction between speeds of 10 and 20 m/s does not change much. Then, we simulated the coefficient of friction at speeds of 12, 15, and 18 m/s and then found that the coefficient of friction between speeds of 10 and 20 m/s has hardly changed, with only small fluctuations. As mentioned above, the friction behavior of the SiO₂ surface is mainly affected by surface mechanical forces and tribochemical reactions. The following will discuss the impact of speed on the above two factors and we will quantify them.
3.2. The Effect of Speed on the Lattice Distortion of SiO₂ Surface. The SiO₂ surface is subjected to mechanical force during the sliding process, so lattice distortion occurs. Lattice distortion is an unbalanced state of atomic state caused by external forces. Lattice distortion corresponds to the previous test experiments on friction and wear mechanisms, and it is also the main reason for the appearance of hillocks on the surface of quartz glass. We tracked some atoms in the sliding process and recorded their relative position changes. However, the hillock phenomenon was not observed in our simulations. We speculate that this is caused by the conditions set in the previous experiment that are not of the same order of magnitude.

Observation found that the relative position of these atoms changed drastically in this process, which is the phenomenon of lattice distortion. In the dry environment, at 120 ps, the SiO₂ surface is not subjected to mechanical forces, and the positions of the calibrated silicon atoms are shown in Figure 3. At 248 ps, the SiO₂ surface began to be subjected to mechanical forces. The position of silicon atoms and surrounding oxygen atoms began to change slightly. At 320 ps, due to the continuous mechanical force on the SiO₂ surface, the Si atom position changes significantly. Under humid conditions, the author also tracked the movement of some atoms. Then, we found that the SiO₂ surface also has lattice distortion under wet conditions. The lattice distortion process under water lubrication is similar to the previous one, but its relative position changes less.

To quantify the effect of speed on the friction behavior of the SiO₂ surface, we separately counted the number of atoms that undergo lattice distortion at different speeds in dry and wet environments, as shown in Figure 4. The way we judge whether the lattice distortion occurs is to judge based on the tracked atomic coordinate information. It can be seen from Figure 4a that, in the case of dry friction, as the speed increases, more silicon atoms undergo lattice distortion, which is consistent with the result that the coefficient of friction increases with the increase in speed. In the case of wet friction,
although there is the same trend, the speed has less influence on it. Under the wet conditions, the shear force on the friction surface can be greatly weakened due to the interaction between the layers of water molecules. Moreover, water is a common lubricant, so water can play a good lubricating effect. So, in the case of water lubrication, the shear force on the SiO₂ surface will be greatly weakened. Therefore, the velocity has little effect on the lattice distortion on the wetted surface.

3.3. The Effect of Speed on Surface Tribochemical Reactions. As mentioned above, in addition to the influence of mechanical force on the surface coefficient of friction, the tribochemical reaction on the surface also brings significant energy loss. Hydrolysis and dehydration reactions occur on the surface of silica when it comes into contact with water molecules. The surface of silica is composed of a large number of siloxane bonds. When the hydrolysis reaction occurs, the siloxane bond is broken. After the siloxane bond is broken, it combines with water molecules to form two hydroxyl groups, as shown in formula 1. Moreover, studies have found that the dehydration reaction occurs on the surface of SiO₂ after the hydrolysis reaction occurs, as shown in formula 2. The following will mainly discuss the hydrolysis reaction and dehydration reaction at different speeds in two environments.

\[
\text{Si} - \text{O} - \text{Si} + \text{H}_2\text{O} \rightarrow 2\text{Si} - \text{OH} \quad (1)
\]

\[
\text{Si} - \text{O} + \text{Si} - \text{OH} \rightarrow \text{Si} - \text{O} - \text{Si} + \text{H}_2\text{O} \quad (2)
\]

3.3.1. The Effect of Speed on the Hydrolysis Reaction. In a completely dry environment, there are no water molecules on the surface of SiO₂. Therefore, no hydrolysis reaction occurs and no energy loss is observed, which is also related to our simulation results. The energy loss in this case only comes from the lattice distortion caused by mechanical stress in an environment without water. The difference is that, in fully wet conditions, the SiO₂ surface is in contact with a large number of water molecules. Then, a hydrolysis reaction occurred, causing energy loss. The observed hydrolysis reaction is shown in Figure 5. At 100 ps, the initial stage of movement, there are a lot of water molecules around the surface of SiO₂, but no hydrolysis reaction occurs on the surface of SiO₂. Until 226 ps, the surface has begun to move, and we observe that the hydrogen atoms in the water molecules begin to approach the O atoms in SiO₂. At 330 ps, the siloxane bond is broken, and the nearby water molecule also breaks into an O atom and a hydroxyl group. Finally, they combine to form two hydroxyl groups.

To quantify the effect of speed on the hydrolysis reaction on the SiO₂ surface, we tracked some atoms and counted the number of atoms that undergo hydrolysis reactions at different speeds, as shown in Figure 6 below. We judge whether a hydrolysis reaction has occurred based on the change in the distance between the labeled atoms. For example, in Si—O—Si, the distance between Si atoms and O atoms is about 1.5 Å. When the hydrolysis reaction occurs, one bond will break to

![Figure 4. Lattice distortion in two environments at different speeds. (a) Lattice distortion at different speeds in a dry environment. (b) Lattice distortion at different speeds in a wet environment.](image)

![Figure 5. Schematic diagram of the hydrolysis reaction.](image)

![Figure 6. Hydrolysis reaction at different speeds.](image)
form two Si−OH, and their distance will become up 2 Å. Through this change in distance, we can judge whether the tribochemical reaction has occurred. It can be seen from Figure 6 that, as the relative sliding speed continues to increase, the number of silane bonds that undergo hydrolysis reaction shows a downward trend. However, at the same time, we also noticed that, when the speed is between 10 and 20 m/s, the rate of decrease of the hydrolysis reaction is smaller. This phenomenon also explains why there is no obvious fluctuation in the coefficient of friction within this range. Then, the hydrolysis reaction phenomenon decreased sharply, and the coefficient of friction began to change accordingly. When the final speed is higher, the hydrolysis reaction phenomenon no longer decreases, and the rate of the decrease of the coefficient of friction gradually decreases. Then, we simulated the movement with a speed of around 50 and found that the coefficient of friction was fluctuating and there was no obvious trend of change. This is consistent with the trend in Figure 6 and Figure 2b. Fewer silane bonds participate in the hydrolysis reaction to produce hydroxyl groups, which will reduce energy loss. This is reflected in the coefficient of friction as a decrease in the coefficient of friction. In the case of water lubrication, the energy loss caused by lattice distortion is very small. The energy loss mainly comes from the hydrolysis reaction caused by the tribochemical reaction. Therefore, the hydrolysis reaction is the main factor affecting the coefficient of friction. As the speed increases, the hydrolysis reaction decreases, which also explains the decrease in the coefficient of friction.

### 3.3.2. The Effect of Speed on Dehydration Reaction

Wang and Duan's research shows that, when water molecules are sufficient, the SiO2 surface will not undergo a dehydration reaction during the sliding process. In the simulation process of this article, we did not find the dehydration reaction on the surface of SiO2 in the dry environment and humid environment, which is consistent with Wang and Duan's research results. Therefore, the dehydration reaction did not affect energy dissipation in this study.

### 4. CONCLUSIONS

1. In different environments, speed has different effects on friction behavior. Under dry conditions, the coefficient of friction on the SiO2 surface increases with the increase of the relative sliding speed. Under wet conditions, the coefficient of friction on the SiO2 surface decreases with the increase of the relative sliding speed. The reason for this phenomenon is that speed has different effects on their surface mechanical action and tribochemical reaction.

2. In a dry environment, the main factor affecting the coefficient of friction of the SiO2 surface comes from the lattice distortion caused by mechanical stress. By counting the number of lattice distortions on the surface of SiO2 at different speeds, it is found that the faster the speed, the more atoms undergo lattice distortion, which will cause more energy loss. This is also the main reason for the increase in the friction coefficient of the SiO2 surface in dry environments. In the dry environment, no obvious tribochemical reaction was found on the SiO2 surface, so the tribochemical reaction of the SiO2 friction surface in the dry environment has no effect on the coefficient of friction.

3. In a humid environment with abundant water molecules, velocity has the same trend in the influence of lattice distortion of the SiO2 surface. However, due to the effect of the water molecule layer, this effect is small. In the case of sufficient lubrication, the water molecule layer between the two friction surfaces can greatly weaken the mechanical force received by the friction surface, and the lattice distortion is mainly caused by the mechanical force, so the speed has little effect on it. It is found through observation that, in a completely humid environment, the energy loss on the surface of SiO2 mainly comes from the hydrolysis reaction. Due to the abundance of water molecules on the surface, no dehydration reaction occurred on the SiO2 surface. The final statistics found that, as the speed increases, the hydrolysis reaction is suppressed, and energy dissipation is less. Therefore, the coefficient of friction has decreased.

### AUTHOR INFORMATION

**Corresponding Author**

Li Hong Yang — School of Mechanical Engineering, University of Shanghai for Science and Technology, Shanghai 200082, China; Email: lhyang@usst.edu.cn

**Authors**

Shang Gao — School of Mechanical Engineering, University of Shanghai for Science and Technology, Shanghai 200082, China; orcid.org/0000-0002-6574-7610

Yi Gan — School of Mechanical Engineering, University of Shanghai for Science and Technology, Shanghai 200082, China

Qiang Chen — School of Mechanical Engineering, University of Shanghai for Science and Technology, Shanghai 200082, China

Complete contact information is available at: https://pubs.acs.org/10.1021/acsomega.0c05897

**Notes**

The authors declare no competing financial interest.

**ACKNOWLEDGMENTS**

We are very grateful to Professor Yang, the editor, and the reviewers for their help with this article. It is because of their unremitting help that this article was born. Thank you very much.

**REFERENCES**

1. Kurkjian, C. R.; Krause, J. T.; Paek, U. C. Tensile strength characteristics of “perfect” silica fibers. *Le J. Phys. Colloq.* 1982, 43, C9-585–C9-586.

2. Bunker, B. C.; Rieke, P. C.; Tarasevich, B. J.; Campbell, A. A.; Fryxell, G. E.; Graff, G. L.; Song, L.; Liu, J.; Virden, J. W.; Mcvay, G. L. Ceramic Thin-Film Formation on Functionalized Interfaces Through Biomimetic Processing. *Science* 1994, 264, 48–55.

3. Patton, S. T.; Cowan, W. D.; Eapen, K. C.; Zabinski, J. S. Effect of Surface Chemistry on the Tribological Performance of a MEMS Electrostatic Lateral Output Motor. *Tribol. Lett.* 2001, 9, 199–209.

4. Sankar, A. R.; Lahiri, S. K.; Das, S. Performance Enhancement of a Silicon MEMS Piezoresistive Single Axis Accelerometer with Electroplated Gold on a Proof Mass. *J. Micromech. Microeng.* 2009, 19, 427–440.
(5) Demirri, S.; Boedo, S.; Grande, W. J. Conformity Effects on the Wear of Low-Speed, Large Aspect Ratio Silicon Journal Microbearings. Wear 2010, 268, 361–372.

(6) Bhushan, B. Nanotribology and Nanomechanics of MEMS/NEMS and BioMEMS/BioNEMS Materials and Devices. Microelectron. Eng. 2007, 84, 387–412.

(7) Eder, S. J.; Feldbauer, G.; Bianchi, D.; Chikah-Bayr, U.; Betz, G.; Vernes, A. Applicability of Macroscopic Wear and Friction Laws on the Atomic Length Scale. Phys. Rev. Lett. 2015, 115, No. 025502.

(8) Ribeiro, R.; Shan, Z.; Minor, A. M.; Liang, H. In Situ Observation of Nano-Abrasive Wear. Wear 2007, 263, 1556–1559.

(9) Yu, J. X.; Qian, L. M.; Yu, B. J.; Zhou, Z. R. Nanofrettting Behaviors of Monocrystalline Silicon (1 0 0) against Diamond Tips in Atmosphere and Vacuum. Wear 2009, 267, 322–329.

(10) Song, C.; Li, X.; Yu, B.; Dong, H.; Qian, L.; Zhou, Z. Friction-Induced Nanofabrication Method to Produce Protrusive Nanostructures on Quartz. Nanoscale Res. Lett. 2011, 6, 310.

(11) Zhang, L.; Tanaka, H. Atomic Scale Deformation in Silicon Monocrystals Induced by Two-Body and Three-Body Contact Sliding. Tribol. Int. 1998, 31, 425–433.

(12) Kaneko, R.; Umemura, S.; Hirano, M.; Andoh, Y.; Miyamoto, T.; Fukui, S. Recent Progress in Microtribology. Wear 1996, 200, 296–304.

(13) Tanaka, H.; Shimada, S.; Anthony, L. Requirements for Ductile-Mode Machining Based on Deformation Analysis of Monocrystalline Silicon by Molecular Dynamics Simulation. CIRP Ann. 2007, 56, 53–56.

(14) Egberts, P.; Carpick, R. Friction at the Atomic Scale. Physics 2013, 6, 102.

(15) Riedo, E.; Gnecco, E. Thermally Activated Effects in Nanofriction. Nanotechnology 2004, 15, S288.

(16) Han, X.-m.; Gao, F.; Song, B.-y.; Fu, R. Effect of Friction Speed on Friction and Wear Performance of Cu-Matrix Friction Materials. Tribology 2009, 29, 89–96.

(17) Ge, S.-R.; Wang, Q.-L.; Li, L.; Huang, X.-L. Tribological Behavior of Nano-TiO2 and Nano-SiO2 Filled Nylon Composites. Tribology 2004, 24, 152–155.

(18) Wang, Q.-h.; Zhang, X.-r.; Pei, X.-q. Study on the Friction and Wear Behavior of Basalt Fabric Composites Filled with Graphite and Nano-SiO2. Mater. Des. 2010, 1403–1409.

(19) Barnette, A. L.; Asay, D. B.; Kim, D.; Guyer, B. D.; Lim, H.; Janik, M. J.; Kim, S. H. Experimental and Density Functional Theory Study of the Tribochemical Wear Behavior of SiO2 in Humid and Alcohol Vapor Environments. Langmuir 2009, 25, 13052–13061.

(20) Bhushan, B.; Goldade, A. V. Measurements and Analysis of Surface Potential Change during Wear of Single-Crystal Silicon (100) at Ultralow Loads Using Kelvin Probe Microscopy. Surf. Sci. Acta 2000, 157, 373–381.

(21) Yeon, J.; van Duin, A. C. T.; Kim, S. H. Effects of Water on Tribochemical Wear of Silicon Oxide Interface: Molecular Dynamics (MD) Study with Reactive Force Field (ReaxFF). Langmuir 2016, 32, 1018–1026.

(22) Li, A.; Liu, Y.; Szlufarska, I. Effects of Interfacial Bonding on Friction and Wear at Silicon/Silica Interfaces. Tribol. Lett. 2014, 56, 481–490.

(23) Wang, X.; Kim, S. H.; Chen, C.; Chen, L.; He, H.; Qian, L. Humidity dependence of tribochemical wear of monocrystalline silicon. ACS Appl. Mater. Interfaces 2015, 7, 14785.

(24) Yu, J.; Kim, S. H.; Yu, B.; Qian, L.; Zhou, Z. Role of Tribochemistry in Nanowear of Single-Crystalline Silicon. ACS Appl. Mater. Interfaces 2012, 4, 1585–1593.

(25) Wang, M.; Duan, F.-L. Atomic-Level Wear Behavior of Sliding between Silica (010) Surfaces. Appl. Surf. Sci. 2017, 425, 1168–1175.

(26) Yeon, J.; He, X.; Martin, A.; Kim, S. H. Mechanochemistry at Solid Surfaces: Polymerization of Adsorbed Molecules by Mechanical Shear at Tribological Interfaces. ACS Appl. Mater. Interfaces 2017, 9, 3142–3148.

(27) Wen, J.; Ma, T.; Zhang, W.; Pssofogiannakis, G.; van Duin, A. C. T.; Chen, L.; Qian, L.; Hu, Y.; Lu, X. Atomic Insight into Tribochemical Wear Mechanism of Silicon at the Si/SiO2 Interface in Aqueous Environment: Molecular Dynamics Simulations Using ReaxFF Reactive Force Field. Appl. Surf. Sci. 2016, 390, 216–223.

(28) Yue, D.-C.; Ma, T.-B.; Hu, Y.-Z.; Yeon, J.; van Duin, A. C. T.; Wang, H.; Luo, J. Tribochemical Mechanism of Amorphous Silica Asperities in Aqueous Environment: A Reactive Molecular Dynamics Study. Langmuir 2015, 31, 1429–1436.

(29) So/rensen, M. R.; Jacobsen, K. W.; Stoltze, P. Simulations of Atomic-Scale Sliding Friction. Phys. Rev. B 1996, 53, 2101–2113.

(30) van Duin, A. C. T.; Strachan, A.; Steimann, S.; Zhang, Q.; Xu, X.; Goddard, W. A. ReaxFSSIO Reactive Force Field for Silicon and Silicon Oxide Systems. J. Phys. Chem. A 2003, 107, 3803–3811.

(31) Larsson, H. R.; van Duin, A. C. T.; Hartke, B. Global Optimization of Parameters in the Reactive Force Field ReaxFF for SiO2. J. Comput. Chem. 2013, 34, 2178–2189.

(32) Li, Y.-Z.; Chen, Y.-G.; Shi, Y.-L. The Effect of Quasiopericity on Lattice Distortion and Energy Gap in Spin–Peierls Model. Acta Phys. Sin. 2006, 55, 2539–2542.

(33) Song, C.; Li, X.; Cui, S.; Hong, H.; Yu, B.; Qian, L. Maskless and Low-Destructive Nanofabrication on Quartz by Friction-Induced Selective Etching. Nanoscale Res. Lett. 2013, 8, 140.

(34) Jia, J. H.; Zhou, H. D.; Wang, J. B.; Zhou, H.; Chen, J. M. A Comparative Investigation of the Tribological Behavior and Wear Mechanism of Bronze-Graphite Composite under Dry- and Water-Lubricated Sliding against Steel. Mocaxue Xuebao 2002, 22, 36–39.