

<https://doi.org/10.26599/FRICT.2026.9441284>

Research Article

The influence of tribochemical activity of silica abrasives on the atomic removal of sapphire

Hongguang Deng, Min Zhong, Meirong Yi, Jianfeng Chen, Xiaobing Li, Wenhui Xu*

School of Advanced Manufacturing, Jiangxi Key Laboratory of Light Alloy, Key Laboratory of Tribology, Nanchang University, Nanchang 330031, China

*Correspondence should be addressed to: flipreverse@126.com (Wenhui Xu)

Received: April 17, 2026; Revised: June 11, 2026; Accepted: July 6, 2026

© The Author(s) 2026.

Abstract: The tribochemical mechanism of active abrasives on sapphire was investigated by comparing the scratching behavior of Si and SiO₂ probes through atomic force microscopy (AFM) and ReaxFF molecular dynamics (MD). Experiments revealed that the SiO₂ probe, due to its higher chemical activity, was more sensitive to changes in load and sliding cycles. It exhibited significantly greater increases in wear depth and volume compared to the Si probe. Simulations demonstrated that more Si-O-Al bonds appeared on the contact region of SiO₂ and sapphire, enhancing tribochemical reactions and mechanical force transfer. This revealed the atomic-removal pathway: hydration layer softening, solid-phase chemical reaction, and mechanical stripping. This study provides important insights serving as a valuable guidance to deeply understand the chemical mechanical polishing of sapphire by silica

abrasives.

Keywords: SiO₂ abrasives; Tribochemical action; Nano wear; ReaxFF MD; Sapphire

1. Introduction

Sapphire is widely employed as window and substrate materials in the high-tech industry [1, 2]. The surface quality and subsurface damage have a direct impact on key product performance indicators such as lifespan and reliability [3]. However, due to its inherent properties (Mohs hardness 9, low fracture toughness), sapphire has become a typical difficult-to-machine material [4]. Chemical mechanical polishing (CMP) relies on chemical and mechanical interactions to be an efficient polishing method [5, 6]. CMP has been used to remove material from the sapphire surface and achieve atomic-level smooth surfaces [7, 8].

The sapphire CMP process is governed by a range of critical factors, most notably the abrasive particles, pads, and chemical additives. Abrasives are important contributors to excellent surface quality and high removal efficiency in sapphire CMP [9]. For example, Zhang et al. explored the action of alumina particles on sapphire CMP [10]. They believe that traditional alumina particles are prone to agglomeration, making it challenging to obtain an ideal surface. Tie et al. focused on the synthesis of CeO₂ particles and their impact on polishing, providing reference for subsequent applications [11]. Yang et al. investigated the influence of diamond abrasives concentration on the relationship between chemical reactions and mechanical wear, offering guidance to achieve optimal polishing parameters [12]. When cerium dioxide and nano-diamonds are combined with polystyrene, the sapphire MRR is 10–20% higher than that with single abrasives [13]. Compared with diamond and other

abrasives, SiO₂ particles have better polishing effects in sapphire CMP [14,15]. Therefore, SiO₂ abrasives are widely used in the field of sapphire polishing [16,17].

In traditional macro-scale CMP, it is usually assumed that each abrasive in the polishing solution exerts the same effect on the workpiece surface [18, 19]. However, in the actual CMP process, the force of each particle on the sample continuously changes, making it difficult to precisely control the indentation depth [20–22]. In addition, abrasives in CMP tend to aggregate due to their interactions. This results in random variations in the size of particles that contact the wafer surface during polishing. It can limit the improvement in surface quality [23–26]. Chemical reagents are typically added to the polishing solution to enhance the stability and dispersibility of abrasives [27–30]. However, the interplay of chemical components and particles makes it difficult to isolate the abrasive's chemical effect on sapphire CMP. It is generally believed that silica abrasives, with high tribochemical activity, can achieve better polishing performance in sapphire CMP [31]. Therefore, it is necessary to reveal the mechanism by which SiO₂ particles facilitate material removal in sapphire CMP at the micro scale. It helps to gain a deeper understanding of their influence on the atomic-removal behavior of sapphire.

Atomic force microscopy (AFM) has been employed to investigate microscale friction and wear on various material surfaces by utilizing the probe as an abrasive medium. This method can investigate a single abrasive's action on material removal. Shi et al. found that conical AFM probes could not only image workpiece surfaces but also serve a grinding function. It enables the removal of chemical products from sapphire surfaces [32]. To simulate the contact state between a single abrasive and a calcium fluoride wafer in CMP, a spherical silica probe was used for sliding friction experiments [33]. Xiao et al. conducted wear testing on silicon wafer surfaces using spherical diamond and silica probes [34]. They observed two distinct phenomena on the workpiece surface: protrusions and grooves. They suppressed or promoted wear on silicon chips. In aqueous solution, spherical silica probes were used for mechanochemical friction testing of single crystal silicon workpieces with three different crystal orientations [35]. The experimental results indicated that the

mechanochemical activation effect was stronger for Si(100) and Si(111) crystal planes. Spherical alumina probes were used for wear testing of gallium nitride surfaces, and experiments showed that the tribochemical reactions were closely related to water molecules [36]. Jiang et al. conducted microscopic wear experiments on pure iron surfaces using spherical silica probes in hydrogen peroxide solution [37]. The results showed that significant wear occurred on the material surface when glycine was added. AFM probe scratching has been proved to be a powerful tool to explore the effect of abrasives on polishing. However, few studies have reported on tribochemical testing between silica probes and sapphire.

Therefore, in this study, AFM was used to investigate the micro-wear behavior of SiO₂ abrasives on the sapphire surface. Simultaneously, AFM was employed to detect the morphology of the worn area to quantify parameters such as wear depth and volume. Furthermore, X-ray photoelectron spectroscopy (XPS) was utilized for the analysis of chemical products formed on the sapphire surface, facilitating the elucidation of the associated chemical reactions. Transmission electron microscopy (TEM) characterized the crystal structure change of sapphire. Moreover, ReaxFF MD was performed to reveal the bond formation and breaking at the interface between SiO₂ and sapphire caused by tribochemical action. It also elucidated the mechanical force transfer and the atomic-removal pathway. This research is beneficial to clarifying the tribochemical and removal mechanisms of SiO₂ abrasives during sapphire CMP from the micro and atomic level.

2. Experimental and simulation methods

2.1 Scratch experiment between sapphire and AFM tip

Scratching tests on the (0001) sapphire surface were performed by AFM (Dimension Edge, Bruker). Fig. 1 displays sapphire surface features (roughness Ra 0.26 nm). In deionized water, a spherical silica probe with a curvature radius of 300 nm was used to simulate the role of an individual particle in CMP. The AFM probe

cantilever's spring constant is 16 N/m. The curvature radius of the conical silicon tip is 20 nm, and the elastic coefficient is 6 N/m. The length of the SiO₂ and Si probe cantilever beams are 90 and 125 μm , the width is 40 and 35 μm , and the thickness is 2 and 1.75 μm , respectively. The torsional spring constant was calibrated using a standard grating with a wedge angle of 54.74°. The SiO₂-sapphire micro-wear system with AFM is shown in Fig. 2.

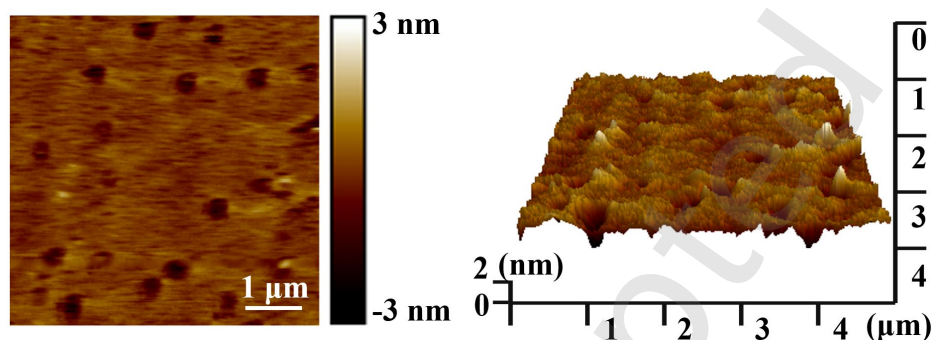


Fig. 1 Original sapphire surface's AFM image.

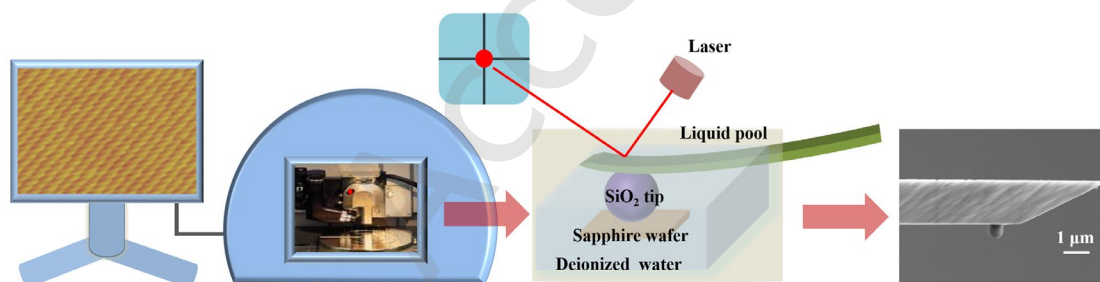


Fig. 2 Schematic diagram of SiO₂-sapphire micro-wear system with AFM.

2.2 ReaxFF MD between sapphire and abrasives

In contrast to traditional MD, ReaxFF MD effectively reveals chemical reactions during the scratching process through bond-level changes. It provides deeper insights into the tribochemical micro-removal mechanism between abrasives and sapphire. Figure 3 shows the ReaxFF MD models of monocrystalline silicon abrasives and amorphous silica abrasives rubbing against sapphire under the same load. Both models consist of three components: monocrystalline silicon (or amorphous silica) abrasives, H₂O, and the sapphire substrate. The dimensions of the two models are 53.1×33.5×65.58 Å. After two annealing cycles, silica transforms from crystalline to

amorphous [38]. The abrasive and sapphire substrate are divided into Newtonian layers and mobile rigid layers. The Newtonian layers of the abrasive and sapphire, combining the water molecules, constitute the reactive regions throughout the simulation.

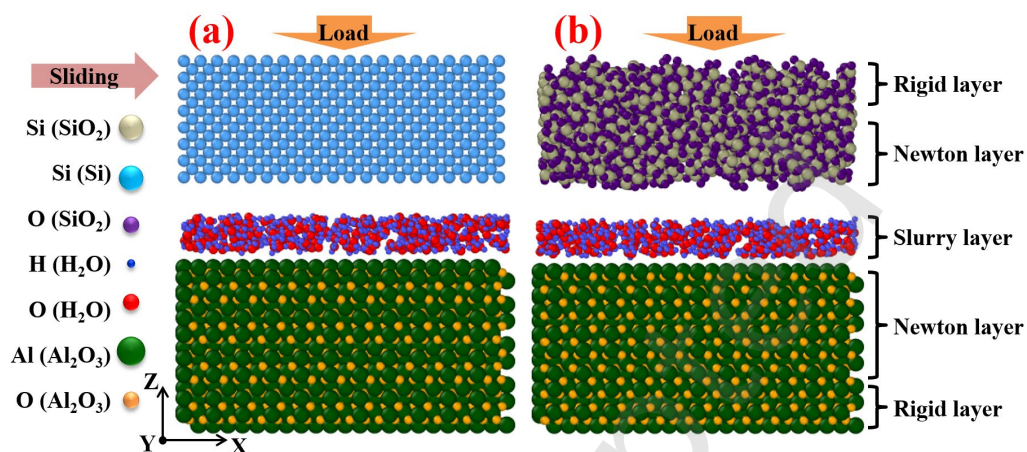


Fig. 3 ReaxFF MD models of sapphire scratching experiments: (a) Si; (b) SiO₂ abrasives.

The simulations are performed using LAMMPS, visualized with OVITO, and the output data are processed using Python scripts [39, 40]. Periodic and fixed boundary conditions are used along X-Y and Z, respectively. Appropriate reactive force fields are selected to describe interatomic interactions [41, 42]. The latest version of the reaction force field has been applied to describe the reaction process at the SiO₂-H₂O-Al₂O₃ interface [43]. The charge update method used in the simulation is QEq. Relaxation is performed before the simulation to verify the accuracy of the reactive force field. Radial distribution function (RDF) of the relaxed Al-O bonds is shown in Fig. 4. The peak position is close to the experimentally measured value [44]. This indicates that the selected reactive force field can accurately simulate the interactions between the substrate, H₂O, and abrasive particles. The simulation process is divided into three steps. First, the entire model is fully relaxed for 25 ps. Second, the abrasive moves downward at 100 m/s. When the pressure on the Newtonian layer of the sapphire substrate reaches 5 GPa, the downward motion is stopped, and the load is maintained constant. Third, the abrasives slide along the X-axis at 400 m/s for 150 ps.

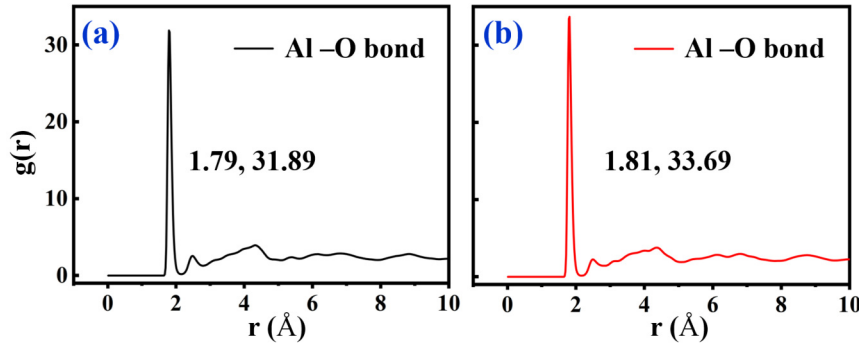


Fig. 4 Al-O bond RDF after model relaxation: (a) Si; (b) SiO₂ abrasives.

3. Results

3.1 Microscopic wear of sapphire surfaces as a function of sliding speeds

The SiO₂ probe sliding speed was set to 5, 10, 15, 20, and 40 $\mu\text{m/s}$, with 20 cycles of sliding. When sliding speeds increase, wear depth and volume gradually decline (Fig. 5). When loads of 1.76 and 3.52 μN are applied, the wear depth decreases by approximately 41% and 33%, respectively, as the sliding speed rises from 5 to 40 $\mu\text{m/s}$. This decrease in sapphire material removal may be attributed to the contact time. In Fig. 5(a), compared to a speed of 10 $\mu\text{m/s}$, the wear depth of sapphire slightly increases at 15 $\mu\text{m/s}$. This may be due to the synergistic effect of increased kinetic energy and reduced contact time of the probe at 15 $\mu\text{m/s}$. At this point, the effect of the former outweighs that of the latter, leading to an increase in atomic removal. As the sliding speed increases further, the effect reverses, resulting in a decrease in atomic removal. At a fixed load and scratching distance, reduced sliding speeds prolong the frictional interaction time between the probe and the sapphire, which in turn leads to a greater groove depth.

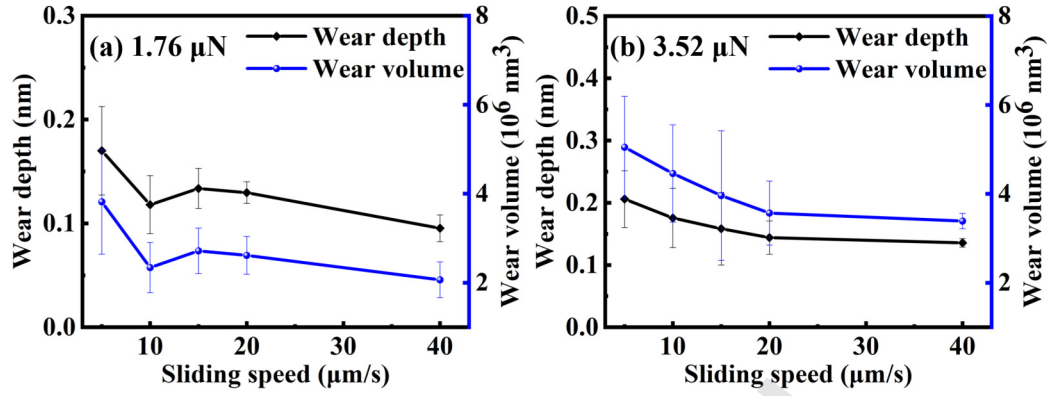


Fig. 5 Sapphire wear caused by SiO_2 probes vs. speeds.

Comparing the sliding results of Si [45] and SiO_2 probes, the wear depth of sapphire decreases to a greater extent in SiO_2 scratch tests. This phenomenon may be attributed to the chemical activity of SiO_2 itself, as understood from macroscopic CMP of sapphire. First, silica probe tips are prone to hydrolysis in deionized water, and hydroxyl groups readily form on the tip [46, 47]. Meanwhile, sapphire will also be hydroxylated in H_2O [48]. SiO_2 and sapphire remain in contact for a longer period at low speeds, allowing the hydroxyl groups on the tip and substrate to undergo dehydration condensation. It results in greater material removal from the sapphire surface. Additionally, SiO_2 abrasives are susceptible to chemical reactions with sapphire, generating a softer reactant Al_2SiO_5 , which promotes material removal from the sapphire surface [49]. Consequently, when it rises from 10 to 40 $\mu\text{m/s}$, the reduction of sapphire wear depth is more pronounced due to the enhanced chemical interactions at lower speeds.

3.2 Sapphire surface microscopic wear vs. sliding cycles

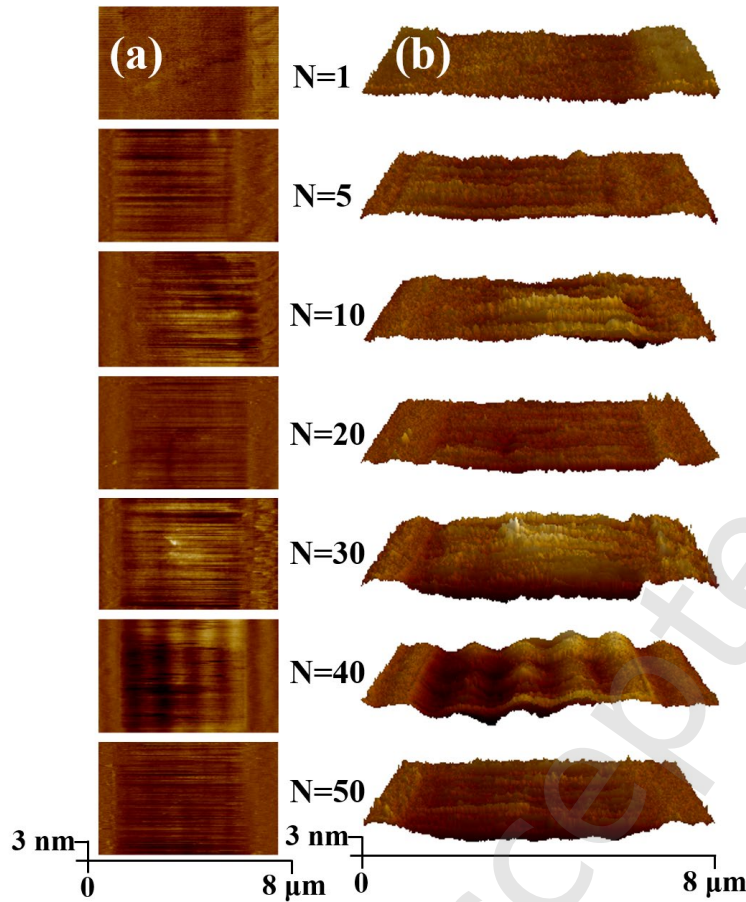


Fig. 6 Sapphire wear morphology vs. sliding cycles.

Sliding cycles were set to 1, 5, 10, 20, 30, 40, and 50. 17.60 μN and 10 $\mu\text{m/s}$ were applied to the silica probe. Figure 6 shows the two-dimensional and three-dimensional morphological characteristics of wear patterns on sapphire surfaces under different sliding cycles. Figure 7 exhibits the average cross-sectional profile, wear depth, and volume of the worn area. From Figs. (6–7), at 50 cycles, the scratched area on the sapphire surface is flatter and the material removal is more uniform. In Fig. 7(b), the wear depth and wear volume are shown to increase with increasing sliding cycles, reaching a steady state after 40 cycles. Under 1–50 cycles, wear depth and volume rise approximately 132% and 320%. Increasing sliding cycles results in a longer contact time. It allows more chemical reactions to occur, thereby promoting material removal. Therefore, more sliding cycles produce deeper and larger wear on sapphire.

Varying degrees of increments in wear depth and wear volume are primarily related to the spherical shape of the probe. During scratching, the contact of SiO_2 with

sapphire can be modeled as a sphere in contact with a plane. When the wear depth (h) is much smaller than the probe radius (R), the theoretical relationship between wear volume (W) and the wear depth (h) at a single contact point is $W \approx \pi \times R \times h^2$ [50, 51]. Therefore, the relationship of wear volume with depth is nonlinear. Consistent with this, the increase in wear volume is more than twice the increase in wear depth, as shown in Fig. 7.

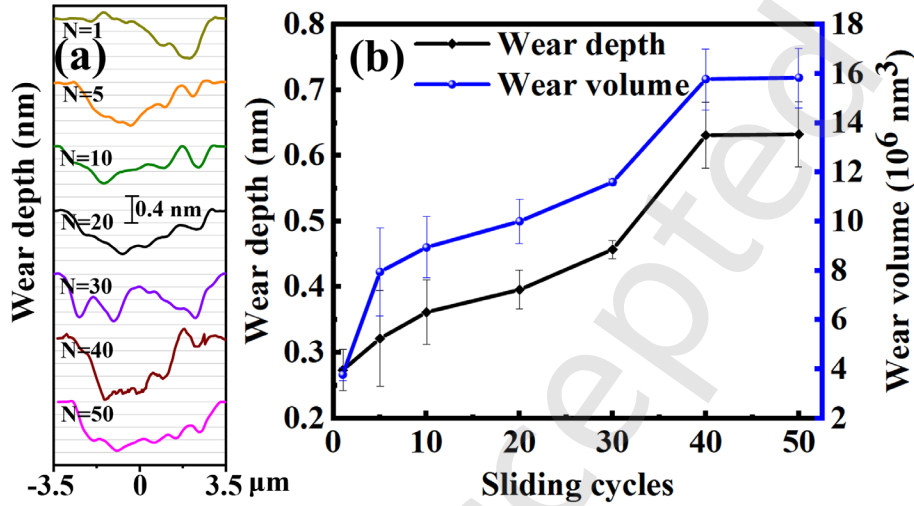


Fig. 7 Average cross-sectional profiles (a); wear depth and volume (b); vs. sliding cycles.

3.3 Microscopic wear of sapphire surfaces as a function of loads

The load applied to the silica probe were 1.76, 3.52, 7.04, 14.08, and 17.60 μN under 10 $\mu\text{m/s}$ and 50 cycles. Figure 8 presents the two-dimensional and three-dimensional morphological characteristics of sapphire surfaces under different loads. Figure 9 exhibits the average cross-sectional profiles, wear depth and volume of the worn area on the sapphire surface with loads. Both wear depth and wear volume increase with increasing loads. They increase approximately 294% and 433% when the load changes from 1.76 to 17.60 μN .

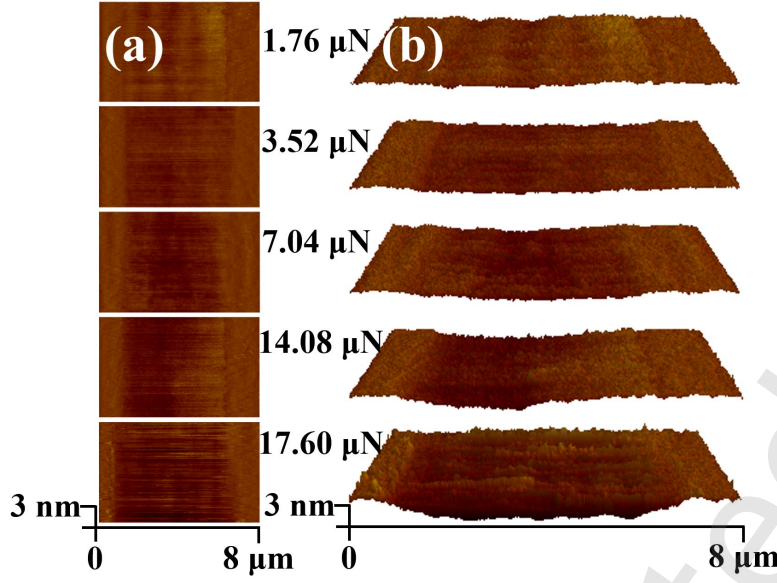


Fig. 8 Sapphire wear morphology vs. loads.

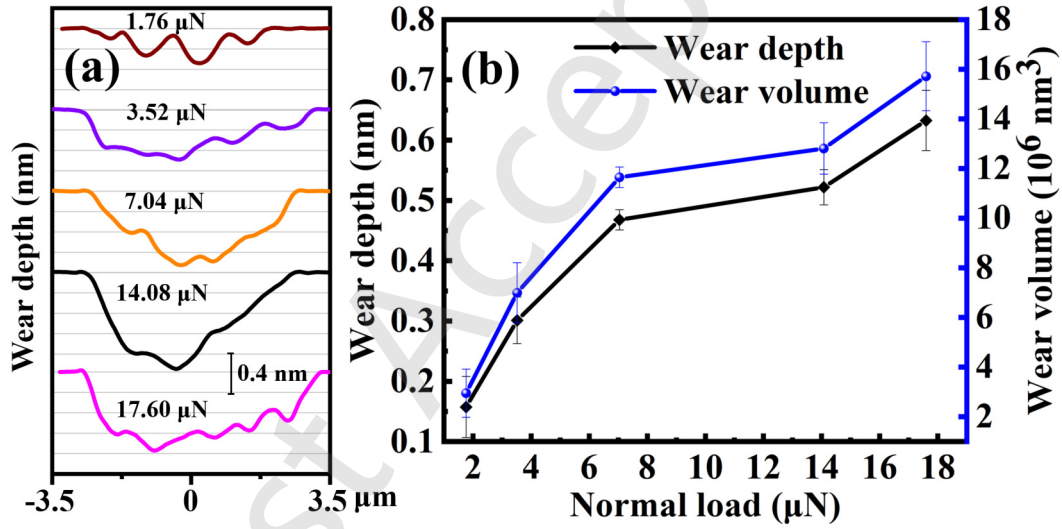


Fig. 9 Average cross-sectional profiles (a); wear depth and volume (b); vs. loads.

The contact pressure is strongly associated with loads. Hertz contact theory was used to calculate the pressure of probes on sapphire [52]. The following formulas give the maximum contact pressure $P_{\max}$ (Gpa) and the contact area A (μm^2).

$$P_{\max} = \frac{3(F_n + F_c)}{2A} = \frac{3(F_n + F_c)}{2\pi a^2} \quad (1)$$

$$a^3 = \frac{3R(F_n + F_c)}{4E_c} = \frac{3R}{4}(F_n + F_c) \left(\frac{1-\nu_1}{E_1} + \frac{1-\nu_2}{E_2} \right) \quad (2)$$

where F_n , a , F_c , R , and E_c are the normal load (μN), contact radius (μm), adhesion force (μN), tip radius (μm), and composite elastic modulus of the tip and sample (Gpa). ν_1 , ν_2 , E_1 , and E_2 are the Poisson's ratios and elastic modulus (Gpa) of the tip

and sapphire. The Hertz contact formula used in this work is applicable to smooth elastic ball-plane contacts considering adhesive forces. At the same time, the external load applied during the experiment was relatively low. The model assumes that the material is a homogeneous elastic body and does not take into account the gradient mechanical property changes of the surface chemical reaction layer.

Adhesion force between silica probes and the sapphire surface was measured, 74 nN (Fig. 10(a)). Then, the $P_{\max}$ and A were calculated and shown in Fig. 10(b). They increase with increasing loads. At the maximum load 17.6 μN , the maximum contact pressure is 5.41 GPa. This value is much lower than sapphire yield stress (10.4 GPa) [53]. It confirms that the use of Hertz contact theory is appropriate. Additionally, when the load changes from 1.76 to 17.60 μN , the $P_{\max}$ and A increase by 114% and 350%. From Figs. 9 and 10, the load-promoted micro-wear of the sapphire surface is found to arise from the coupled effects of contact pressure and contact area. As the contact pressure increases, the Al-O bonds in the sapphire crystal lengthen due to the increased external compressive stress. With the bigger contact area, more aluminum and oxygen atoms in sapphire bear external stress. Figure 11(a) shows the relationship between the lateral friction force and normal load. Friction force increases, revealing a strengthening in mechanical shear force.

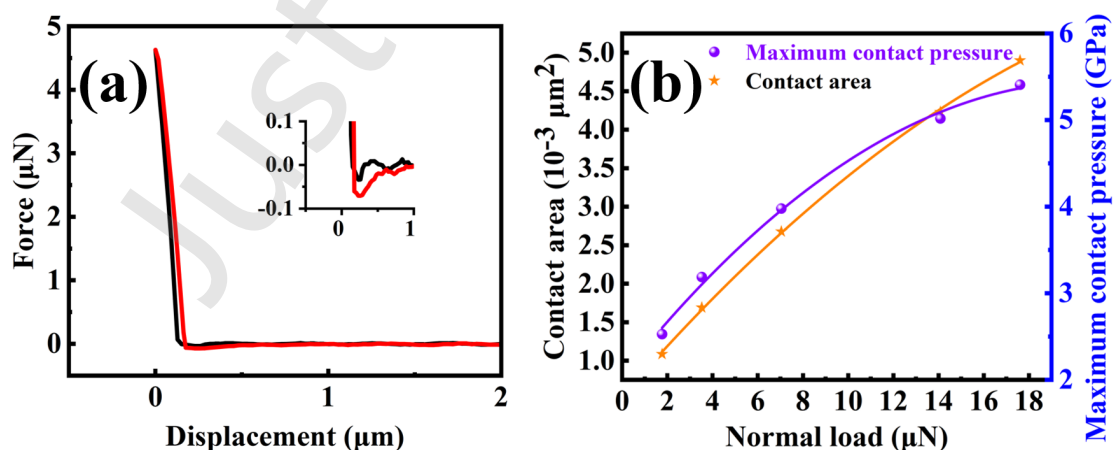


Fig. 10 Force curves of SiO₂ probe on sapphire surface.

Frictional dissipated energy is defined as the portion of mechanical energy irreversibly converted by the work of frictional force between two contacting surfaces during relative motion. This energy may cause deformation of the sapphire surface,

exacerbating material wear. The frictional dissipation energy is calculated using Eq. (3).

$$E = F_t \times 2 \times L \times n \quad (3)$$

where E is the frictional dissipation energy (J); F_t is the frictional force between probes and samples (μN); L is the scanning length (μm); and n is the number of scanning lines. When conducting nanowear experiments in contact mode using AFM, the probe completes forward scanning and reverse scanning along a predetermined scanning line in sequence. Although the direction of frictional force is opposite in the forward and backward directions, dissipated energy is a scalar and independent of the direction of motion. Here, the factor “2” originates from the reciprocating sliding mode: the AFM tip slides forward (distance L) and backward (distance L) during each wear cycle, both in contact with the sample surface. Thus the total sliding distance per cycle is $2L$, and the frictional dissipation energy needs to be multiplied by this coefficient. Figure 11(b) demonstrates how frictional dissipation energy relates to wear volume. At identical sliding distances, frictional dissipation energy is mainly related to frictional force. Thus, the Al-O bond becomes more prone to fracture due to the continuously increasing mechanical shear force. This facilitates the mechanical micro-removal of sapphire surface material. Consequently, wear depth and volume on sapphire grow as rising loads.

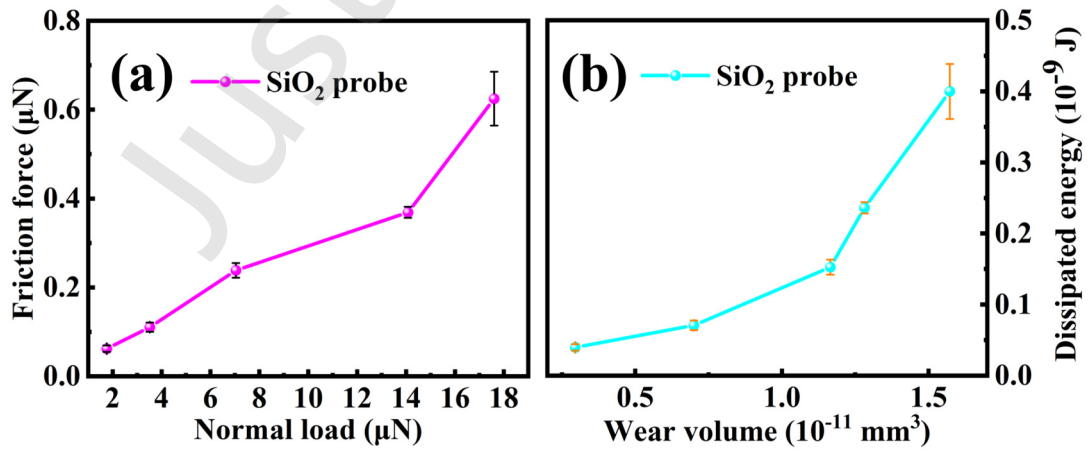


Fig. 11 Friction force between SiO₂ probe and sapphire under different loads (a); the relationship between frictional dissipation energy and wear volume (b).

Compared to silicon probes [45], under the action of silica probes, the increase in sapphire wear depth is greater as the load increases. This is likely due to the higher

chemical reactivity of silica abrasives with sapphire compared to silicon abrasives, which promotes easier material removal.

4. Discussion

4.1 Chemical reaction between SiO₂ abrasives and sapphire surface

To further elucidate roles of silica probes on sapphire micro wear, XPS is conducted on sapphire after scratch experiments under 17.6 μN and 10 $\mu\text{m/s}$. Figures 12(a) and 12(e) show the full spectra. Figures 12(b) and 12(f) exhibit peaks of Al. 74.20 and 74.07 eV are detected and attributed to $\text{Al}(\text{OH})_3$ and Al_2SiO_5 [54, 55], respectively. In Figs. 12(c) and 12(g), 530.43, 530.68, and 531.30 eV match Al_2O_3 , Al_2O_3 and Al_2SiO_5 [55-57], respectively. In Figs. 12(d) and 12(h), binding energy of 99.35 and 102.31 eV correspond SiO_2 and Al_2SiO_5 [55, 58], respectively. According to the XPS results, Al_2SiO_5 is detected on the scratched sapphire surface. This indicates that the material removal from the sapphire surface during the experiment is not solely attributable to mechanical wear but also involves tribochemical reactions. The reactions between sapphire and the silica probe in deionized water are given by Eqs. (4) and (5). Reference 59 clearly states that Al_2SiO_5 products are beneficial for material removal during sapphire polishing [59]. The reason is that the elastic modulus and hardness of Al_2SiO_5 (152 GPa, 6.6 Mohs) are lower than those of sapphire (426 GPa, 9 Mohs). When there is no chemical reaction, the hardness of sapphire (9 Mohs) is greater than that of SiO_2 abrasive grains (7 Mohs), making material removal difficult. However, the hardness of the chemical reaction products ($\text{Al}(\text{OH})_3$ and Al_2SiO_5) is much lower than that of the sapphire substrate [3]. Therefore, the material removal can be more easily achieved by scratching with the SiO_2 probe than Si probes [45].



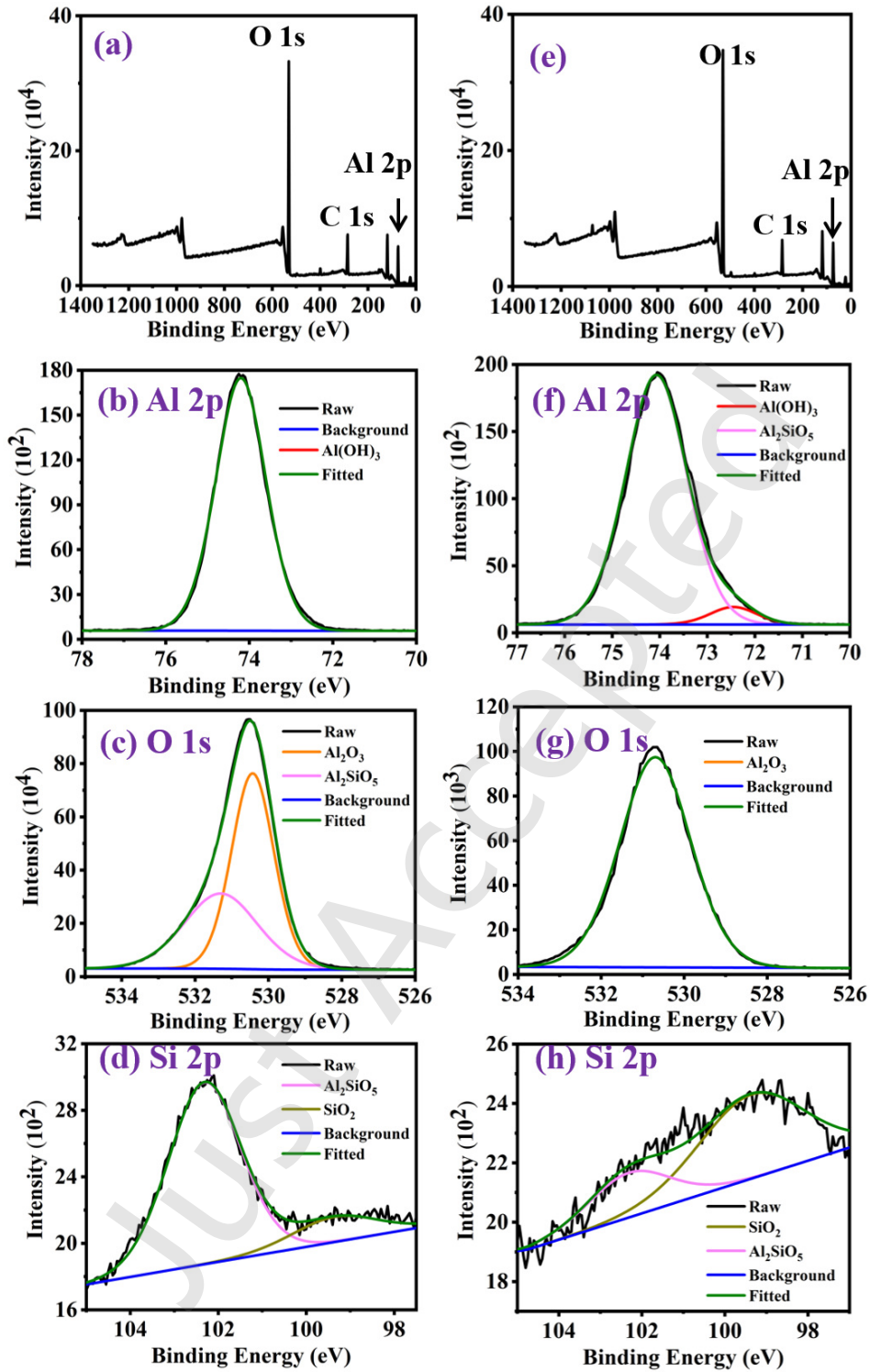


Fig. 12 XPS spectra of sapphire surfaces after scratching: (a-d) 30; (e-h) 50 sliding cycles.

The statistical analysis of Al, O, and Si elements in Fig. 12 reveals that the percentages of Al_2O_3 , $\text{Al}(\text{OH})_3$, Al_2SiO_5 , and SiO_2 change from 20.87%, 22.12%, 40.98%, and 0.18% in Figs. 12(a-d) to 73.74%, 0.51%, 16.97%, and 0.31% in Figs. 12(e-h), respectively. These quantitative XPS data depict the dynamic evolution of the

frictional interface of SiO₂ with sapphire from intense to inert reaction. Specifically, in Fig. 12(a), a strong chemical reaction occurs among the silica probe, sapphire substrate, and H₂O, leading to large amount of Al(OH)₃ and Al₂SiO₅ on the sapphire surface. In contrast, after an increased number of sliding cycles (Fig. 12(e)), there are much less Al(OH)₃ and Al₂SiO₅ on the sapphire surface. At this stage, the peak of intense tribochemical reactions on the sapphire surface has passed. The surface has shifted from generating large amounts of new reactants to consuming existing ones. In the overall scratch experiment between SiO₂ and sapphire, the initial intense tribochemical reaction generates Al₂SiO₅, resulting in a high initial wear rate. At this stage, the material removal mechanism is dominated by tribochemical wear. As the experiment progresses, the reduced reaction products and exposed sapphire substrate weaken the material removal. The scratching process transitions from a fast wear stage dominated by tribochemical reactions to a decaying wear stage with a lower growth rate.

4.2 TEM observation of sapphire wear

To reveal the impact of silica probes on the sub surface structural damage of sapphire, the cross-section of the scratched region was observed by TEM (Fig. 13(a)). Figures 13(b-d) are enlarged images of the corresponding dashed box area in Fig. 13(a). In Figure 13(b), a damage layer approximately 0.7 nm thick is present in the worn area. The distinct edges evidence a progressive lattice transition extending from the deposited gold layer, across the damaged subsurface, and into the sapphire matrix. Furthermore, a particularly bright region observed within the damaged layer indicates a lattice orientation that deviates markedly from that of the pristine sapphire matrix. Fast Fourier Transform (FFT) of Fig. 13(b) shows blurred and elongated spots in the central area. Based on the previous XPS analysis, this region is speculated to be an amorphous layer consisting of chemical reaction products and damaged matrix material. The high-resolution image of the damaged region is displayed in Fig. 13(c). FFT exhibits diffuse scattering and few distinct diffraction spots. It indicates the

presence of an amorphous structure and high-density dislocation regions in this area. The sapphire substrate high-resolution image is presented in Fig. 13(d). No lattice distortion is observed. Its Fourier transform shows a regular arrangement of lattice diffraction spots, demonstrating that this region is perfect single-crystal sapphire.

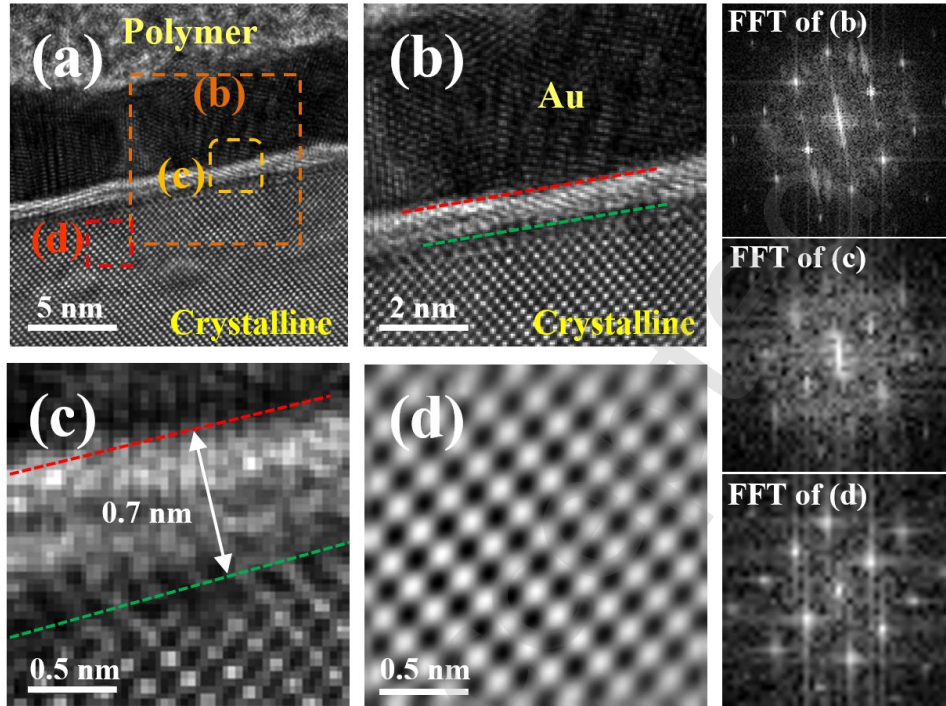


Fig. 13 TEM observation of sapphire wear area (a); high resolution images of the marked area (b-d).

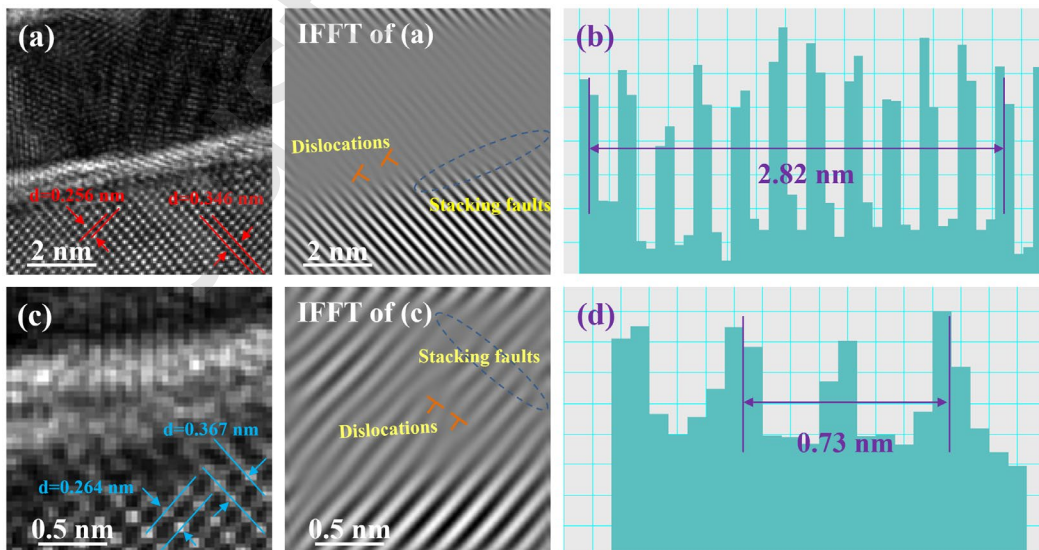


Fig. 14 Sapphire lattice fringe spacing in different regions.

To further observe the lattice damage, inverse FFT (IFFT) is performed on Figs.

13(b) and 13(c), as shown in Fig. 14. The IFFT images reveal that subsurface lattice damage in sapphire is manifested as numerous dislocations and a small number of stacking faults. Figures 14(b) and 14(d) display the lattice fringe images. The lattice fringe spacing of Fig. 14(a) is 0.256 nm and 0.346 nm, corresponding to the (1 0 -1 2) and (1 1 -2 1) crystal planes of sapphire, respectively. Their theoretical values are 0.254 and 0.345 nm. The measured spacing is consistent with the theoretical values. It indicates that the crystal structure in this region remains unperturbed and experiences negligible stress-induced effects. Crystallographic calculation determines the zone axis to be [5 -4 -1 -3]. Compared with Fig. 14(a), the (1 0 -1 2) plane spacing in Fig. 14(c) increases by approximately 3.1% (from 0.256 to 0.264 nm). It indicates that this region is subjected to significant tensile strain along the [1 0 -1 2] direction. Meanwhile, the (1 1 -2 1) interplanar spacing increases by approximately 5.5% (from 0.346 to 0.367 nm). It implies a more obvious change in lattice parameters along the [1 1 -2 1] direction. Such changes are typically accompanied by lattice distortion and local lattice rotation, which are characteristic of local strain. Overall, the closer the region is to the damaged layer, the more significant the change in interplanar spacing. It suggests that stress is more concentrated in this region and the crystal structure suffers more severe strain. These results reveal the distribution and evolution of lattice strain in sapphire during the wear process.

4.3 ReaxFF MD of the reaction between the abrasive and sapphire

Figures 15 and 16 show the states of the upper surface of the sapphire substrate and the bottom surfaces of Si and SiO₂ abrasives after full relaxation for 25 ps. The bottom surface of Si abrasives adsorbs significantly fewer water molecules than those of SiO₂ particles. Most water molecules are adsorbed onto the surfaces of Si or SiO₂ abrasives and the sapphire substrate via van der Waals force. A small portion are adsorbed via hydrogen bonding. In addition, water molecules can ionize, generating H⁺ and OH⁻ ions.

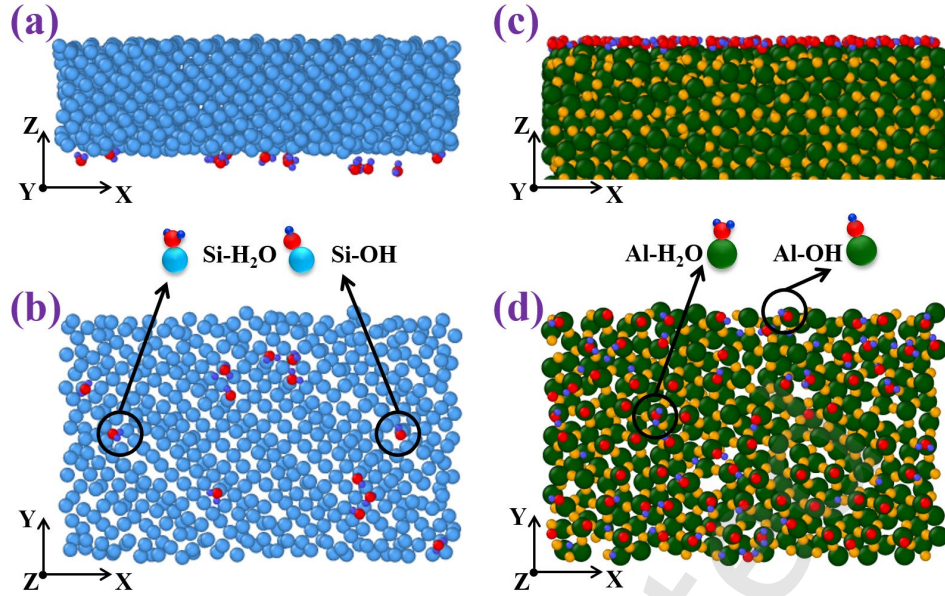


Fig. 15 Surface state of Si abrasives and sapphire substrate after relaxation.

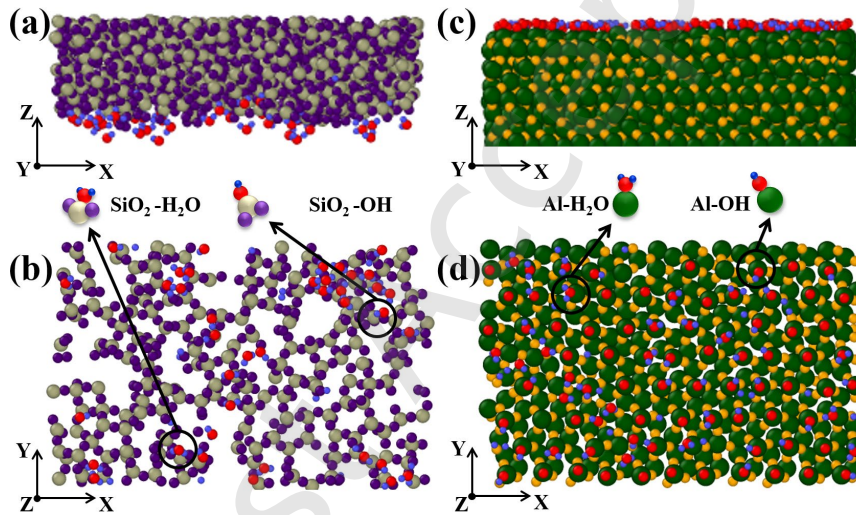


Fig. 16 Surface state of SiO₂ abrasives and sapphire matrix after relaxation.

With the aim of elucidating the adsorption and hydroxylation behavior of water molecules throughout the reaction course, statistical analysis was performed on the numbers of various species at each reaction stage, and the results are shown in Fig. 17. The number of Si-H₂O and SiO₂-H₂O complexes increase from 0 and stabilize at approximately 24. This indicates that the consumption of water molecules and their adsorption onto the abrasives and substrate are largely consistent between the two models. This also suggests that the concentrations of H⁺ and OH⁻ ions from water decomposition are roughly the same in both systems. The key difference is that the

number of Al-OH bonds with Si abrasives is only half of that with SiO₂ abrasives. Here, the oxygen in the Al-OH bonds originates from water molecules. This indicates that SiO₂ abrasives promote the formation of Al-OH bonds on the sapphire surface. Meanwhile, the direct adsorption of oxygen atoms from water molecules onto unsaturated Al³⁺ sites on the substrate represents the lowest-energy-barrier pathway for Al-OH bonds formation.

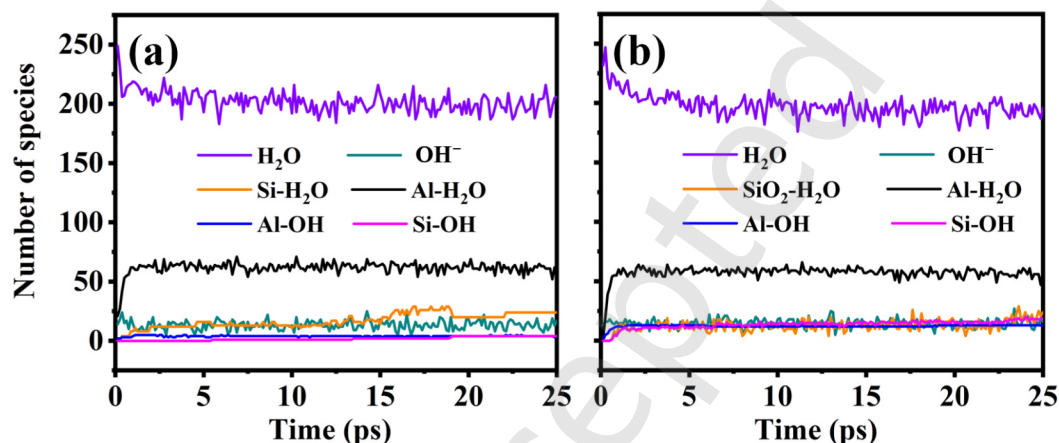


Fig. 17 Species numbers during the reaction process: (a) Si; (b) SiO₂ abrasives.

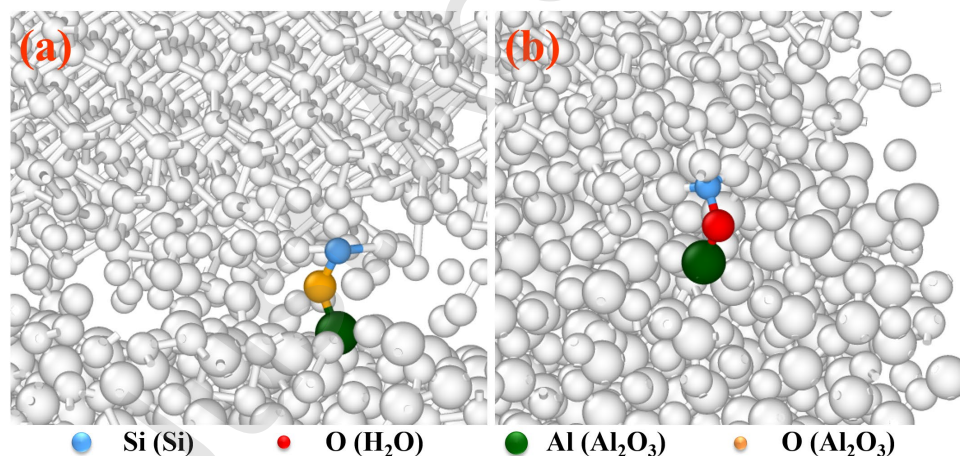


Fig. 18 Formation of bond bridges with Si abrasives scratching sapphire.

In addition, the number of Si-OH bonds in Si model is only one-quarter of that in SiO₂ model. This may be because the SiO₂ surface can effectively catalyze its own hydrolysis and hydroxylation, resulting in a higher surface OH density under the same conditions. The oxygen atoms in the Si-OH bonds of Si abrasives originate from water molecules. In contrast, for SiO₂ abrasives, the majority of oxygen atoms in the Si-OH bonds come from SiO₂ itself. Only a very small portion originate from water

molecules. The above reaction process demonstrates the chemical activity of SiO₂ abrasives. Compared with Si, the hydroxyl concentration on the SiO₂ abrasive's surface and sapphire substrate are higher in deionized water environment. The simulation results provide direct evidence for the AFM experiments. More chemical species are formed on sapphire using SiO₂ probes than Si.

To further elucidate the underlying mechanism governing the effects of deionized water and silica abrasive particles on sapphire substrate wear, the two ReaxFF MD models were analyzed with respect to bond bridge formation and substrate atom removal. As shown in Figs. 18 and 19, when Si or SiO₂ abrasives slide against the sapphire substrate, an interfacial bond bridge (Al-O-Si) forms in both models. This bond bridge can effectively transmit mechanical force from the abrasive particles, thereby enabling material removal. However, the oxygen atoms in the bond bridge originate from different sources depending on the abrasive type. For Si abrasives, they come from the sapphire and water molecules. For SiO₂ grains, they come from the sapphire, water molecules, and the silica abrasives themselves.

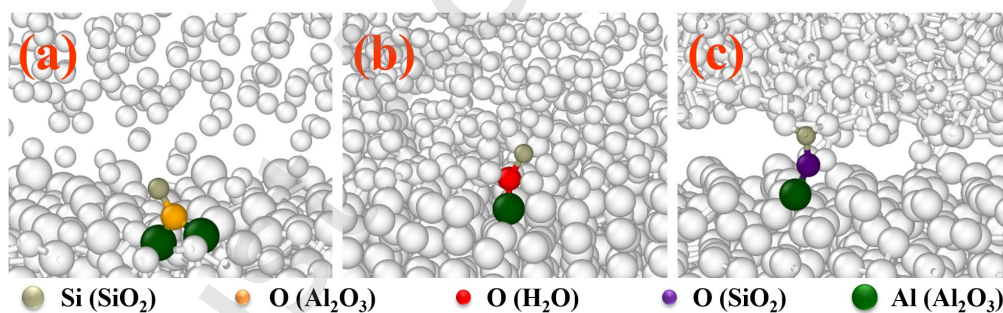


Fig. 19 Formation of bond bridges with SiO₂ abrasives scratching sapphire.

The numbers of Al-O-Si bond bridges formed with oxygen atoms from different sources were statistically analyzed. As shown in Fig. 20, O₁, O₂, and O₃ represent oxygen atoms from sapphire, H₂O, and SiO₂ abrasives. No Al-O₁-Si bond bridges form in the early stage of scratching, and the total number remains very small after scratching is completed. This indicates that water molecules adsorb onto the abrasives (both Si and SiO₂) and the sapphire substrate, forming Si-O₂H, Si-O₃H, and Al-O₂H bonds. When abrasives come into contact with the substrate, these bonds undergo dehydration condensation, forming Al-O₂-Si and Al-O₃-Si bond bridges. After the

abrasives have slid against the substrate for a period of time, O^{2-} sites appear on the substrate surface. They are not fully coordinated following the loss of Al atoms. Adjacent Si atoms can then combine with the O^{2-} sites to form Al-O₁-Si bond bridges. Numbers of Al-O₁-Si and Al-O₂-Si bond bridges in Fig. 20(a) are approximately 5 and 3. They are similar to the numbers of Al-OH and Si-OH bonds in Fig. 17(a). Similarly, in Fig. 20(b), Al-O₂-Si bond bridges grow continuously. It is consistent with the growth curve of Si-OH bonds in Fig. 17(b). Al-O₃-Si numbers are like those of Al-OH bonds shown in Fig. 17(b). These observations further demonstrate that Al-O-Si bond bridges are predominantly formed through the combination of Si-OH and Al-OH bonds.

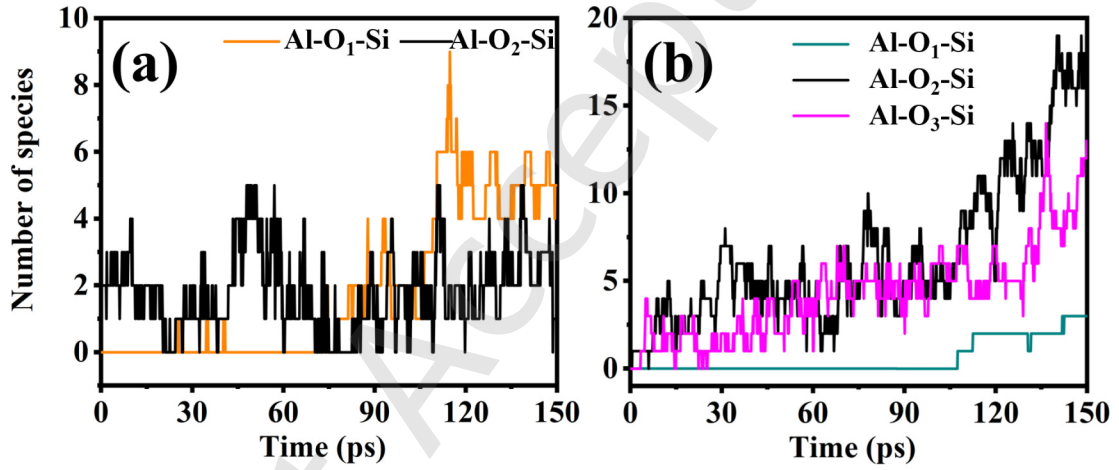


Fig. 20 The number of bond bridges present in the scratching: (a) Si; (b) SiO₂ abrasives.

A comparison of Figs. 20(a) and (b) reveals that the number of Al-O-Si bond bridges formed between Si abrasives and sapphire is much smaller than that formed between SiO₂ abrasives and sapphire. This phenomenon is attributable to the greater reactivity of SiO₂ relative to Si, with the silicon abrasives exhibiting a Si-OH bond count merely one-fourth of that found in silica particles. In addition, the number of Al-O₂-Si bond bridges in Fig. 20(a) fluctuates around an equilibrium value within 150 ps, showing no increasing trend compared with SiO₂ (Fig. 20(b)). This also indicates that silicon grains have lower activity.

In general, Al-O-Si formation promotes the atom removal of sapphire. However,

the promotion mechanism is not fully understood. In addition, the effects of silicon and silica abrasives on the removal of sapphire atoms may also differ. Therefore, it is essential to track the removal process of substrate atoms during scratching and visualize it via snapshots.

Figures 21 and 22 show the detach procedure of O and Al atoms from sapphire during sliding with Si and SiO₂ particles, respectively. For Si, at 0 ps, the O atom in Fig. 21(a) is labeled and found to be tightly connected to two Al atoms in the substrate. As scratching progresses, bond bridges form between Si grains and oxygen atoms. At 12 ps, the O atom is pulled from its original position, and the bond between it and Al in sapphire breaks. At 23 ps, O atoms have gradually risen with the movement of the abrasives and detached from the substrate surface. The Si and O atoms remain tightly connected through bonds. This phenomenon indicates that Al-O bonds are more prone to breakage than Si-O bonds. It is consistent with findings in the literature [60].

In terms of SiO₂, at 0 ps, the O atom in Fig. 22(a) is labeled and found to be closely connected to an Al atom in the substrate. At 95 ps, Si-O-Al bonds form between SiO₂ and Al atoms in sapphire, with oxygen atoms originating from water molecules. When the scratching process reaches 100 ps, the Si-O-Al bonds carry the O atom in the substrate away from its original position, causing it to rise gradually and be removed.

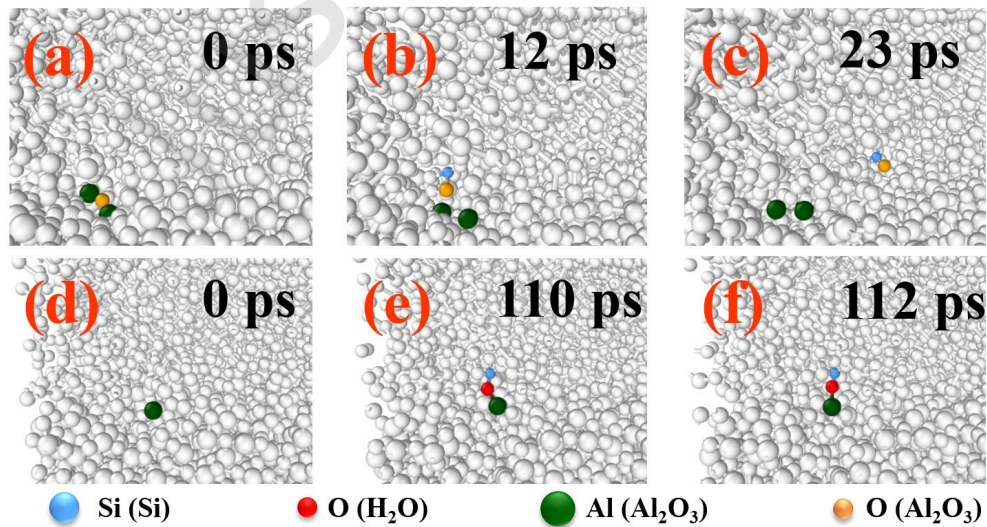


Fig. 21 The process of atomic removal during sapphire scratching by Si abrasives: (a-c) O; (d-f) Al.

A comparison of Figs. 21 and 22(d-f) reveals that the removal process of Al atoms is the same. Specifically, Si-O-Al bonds form between the abrasive particles and Al atoms in the substrate. Most oxygen atoms are provided by water molecules. When the abrasive particles slide, the interfacial mechanical shear force acts on Al atoms in sapphire through Si-O-Al bonds. It causes the atoms to gradually rise and eventually be detached by abrasives, achieving atomic removal.

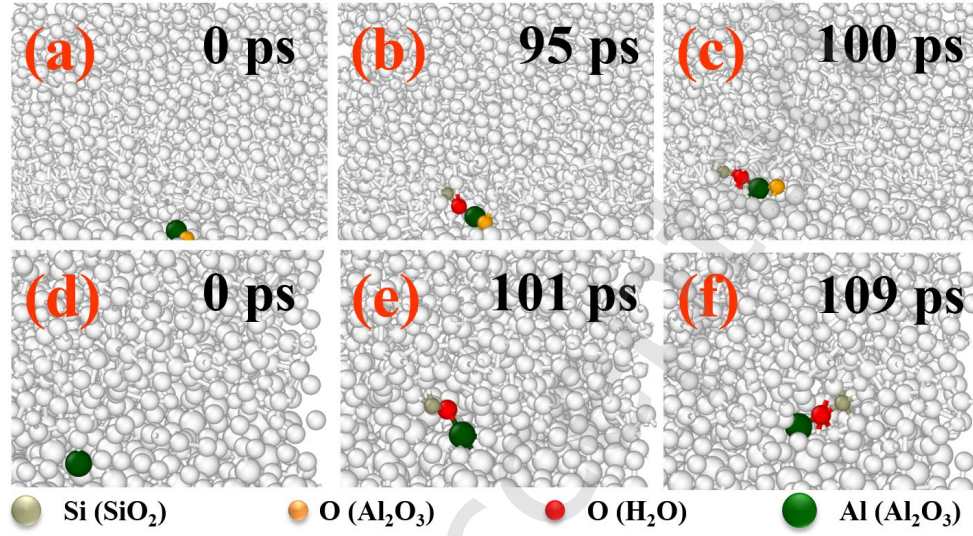


Fig. 22 The process of atomic removal during sapphire scratching by SiO_2 abrasives: (a-c) O; (d-f) Al.

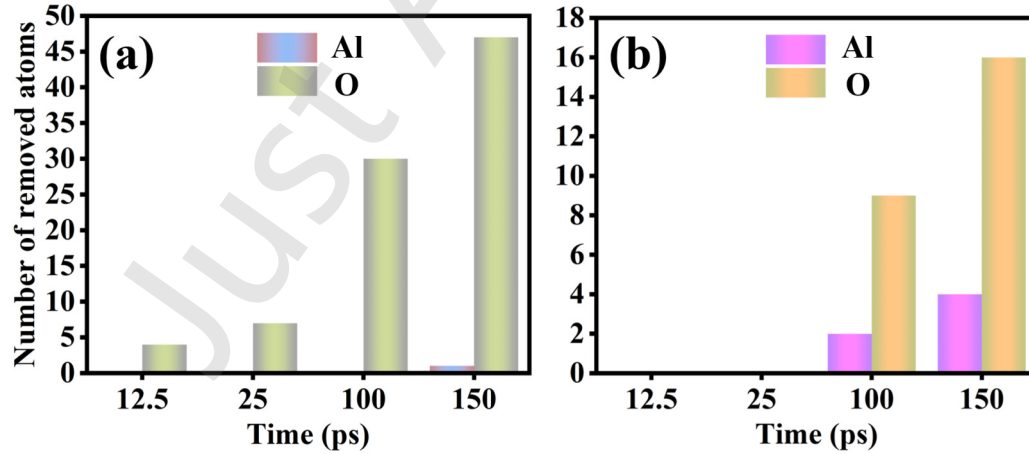


Fig. 23 Removed atoms from sapphire during the scratching: (a) Si; (b) SiO_2 abrasives.

For quantitative calculation of detached atoms, atoms with Z-coordinate values exceeding the sapphire substrate thickness ($26.27 \text{ \AA}$) are defined as removed. However, because Al and O atoms have different atomic radii, the numbers of removed aluminum and oxygen atoms are counted separately. Al atoms with

Z-coordinates exceeding 27.7 Å and O atoms exceeding 27 Å are considered removed. Figure 23 shows the number of removed atoms at four different time points. With Si abrasives, almost no Al atoms are removed within the first 100 ps. Notably, detached O atoms rises rapidly over time. With silica abrasive particles, neither Al nor O is removed during the first 25 ps. From 100 to 150 ps, the number of detached atoms increases continuously.

Based on Figs. 20-23, it can be concluded that Al atom detachment demands the assistance of Si-O-Al bonds. However, not all such bonds lead to Al atom removal from the substrate. The number of Si-O-Al bonds from SiO₂ abrasives is higher, and the number of Al atoms removed from the substrate is also higher. However, there is little correlation between the removal of substrate O atoms and the number of Si-O-Al bonds. In contrast, for Si grains with lower chemical activity, the number of O atoms removed is twice that for silica abrasives. This can be explained by Fig. 24. As shown in Fig. 24(a), the substrate O atoms removed at 73 ps are first labeled. Subsequently, snapshots show the state of the labeled O atom at 67 ps, 37 ps, and 0 ps in Fig. 24(a). When displayed in reverse chronological order, the atomic states reveal that O atoms are more likely to combine with H atoms from water to form water molecules and OH⁻ ions. According to mass conservation and Fig. 17(a), it can be inferred that as the scratching progresses, approximately 50 water molecules are consumed, while the total number of Si-OH, Al-OH, and OH⁻ ions is far less than 50. This indicates that the oxygen atoms in the consumed water molecules are exchanged with oxygen atoms in the substrate, forming water molecules in which the oxygen originates from the sapphire. The removal of O atoms from the substrate in this case is not caused by the chemical action of abrasive particles, but rather by the action of water molecules. Therefore, the amount of detached Al atoms from sapphire better reflects the influence of the differing chemical activities of Si and SiO₂ abrasives on sapphire atomic removal.

In summary, ReaxFF MD simulations have demonstrated that SiO₂ abrasives exhibit higher chemical activity than Si abrasives. Due to the high chemical activity, more Si-O-Al bonds are generated at SiO₂-sapphire interfaces during the scratching

process. The Si-O-Al bond transmits mechanical force to the sapphire substrate, resulting in a greater number of Al atoms being removed under the same load and sliding speed compared with Si abrasives. These simulation results support the experimental and XPS observations in the above sections.

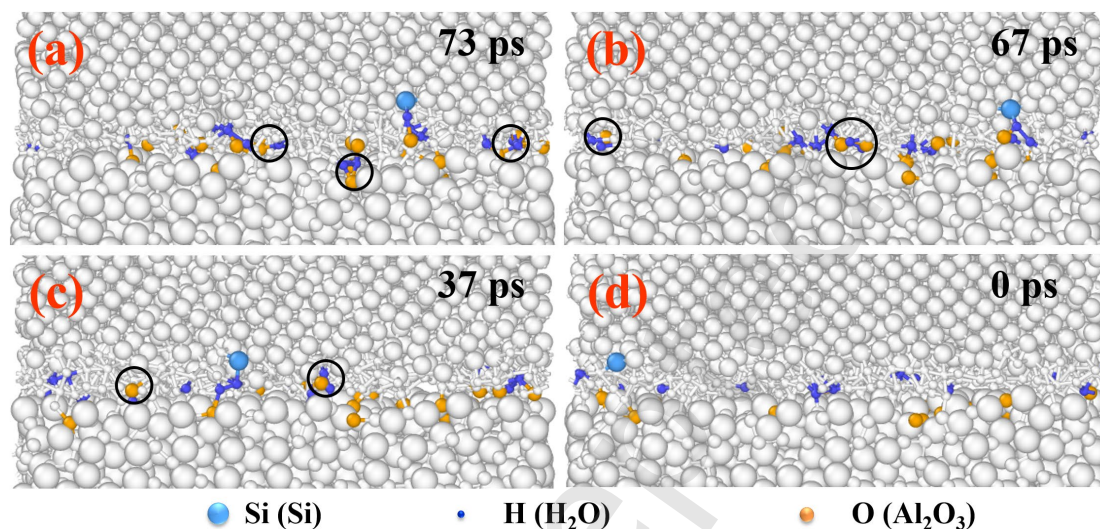


Fig. 24 The states of removed O atoms during the process of Si scratching at different time.

5. Conclusions

The effect of SiO₂ active abrasives on the micro wear of sapphire under different sliding speeds, sliding cycles, and loads is studied using AFM. The frictional chemical reactions present during the scratch experiment are analyzed by XPS detection and ReaxFF MD. At the same time, the sapphire wear region is explored through TEM. The conclusions are as follows:

1) Under the constant load, silica probes in deionized water at low sliding speeds are more likely to generate chemical products when scratching the sapphire surface, generating higher material removal. Consequently, higher sliding speeds lead to a significant decrease in wear depth of sapphire.

2) With sliding cycles changing from 1 to 50, sapphire wear depth and volume increase by approximately 132% and 320%, respectively. With the load rising from 1.76 to 17.60 μ N, the SiO₂-sapphire contact area increases by 350%, and the maximum

contact pressure increases by 114%. The combined effect of contact area and pressure results in the growth of approximately 294% in wear depth and 433% in wear volume.

3) The XPS analysis of scratched sapphire shows that Al_2SiO_5 is generated at SiO_2 -sapphire interfaces. During scratching, tribochemical products are removed, causing an acceleration of material removal.

4) ReaxFF MD simulations verify that SiO_2 abrasives are more active than Si. The higher concentration of hydroxyl groups exists on the SiO_2 surface particles after reaction with deionized water. Most of the oxygen atoms in the Si-OH bonds on SiO_2 originate from the abrasives themselves. In addition, this is also reflected in the number of Si-O-Al bonds generated during scratching. The bonds formed by SiO_2 particles are nearly four times those of Si abrasives.

5) The removal of O atoms from the sapphire substrate during scratching is closely related to the action of water molecules. The removal of Al atoms is more strongly associated with Si-O-Al bonds. This indicates that, compared with O atom removal, Al atom removal is more representative of the difference in chemical activity between Si and SiO_2 particles. More Si-O-Al bridge bonds lead to greater mechanical force transmitted to the sapphire surface, resulting in increased atomic removal.

These findings provide insights into the role of the chemical activity of SiO_2 abrasives in the atomic removal of sapphire in H_2O . It helps understand the polishing mechanism of sapphire CMP more deeply.

Acknowledgements

This work was supported by the National Natural Science Foundation of China (No. 92580119), and Jiangxi Province Key Laboratory of Light Alloy (2024SS Y05031).

Declaration of Interests

The authors declare that they have no competing interests.

References

- [1] Zhu G Q, Liu Y J, Ming R, Shi F, Cheng M J. Mass transfer, detection and repair technologies in micro-LED displays. *Science China Materials* **65**(8): 2128–2153 (2022)
- [2] Wang Y H, Liang Z Q, Zhao W X, Wang X B, Wang H. Anisotropic cutting mechanisms on the surface quality in ultra-precision machining of R-plane sapphire. *Appl Surf Sci* **622**: 156868 (2023)
- [3] Chu J N, Ren J T, Liu C L, Zhang C P, Zhu B Y, Chen X. The performance of a novel nano-SiO₂ dispersion solutions for the chemical-mechanical polishing of sapphire. *Appl Surf Sci* **709**: 163831 (2025)
- [4] Xu Y C, Peng C, Zhan Y J, Wang Q T. Machining performance and material removal mechanism of sapphire with novel polishing slurry. *Appl Surf Sci* **671**: 160756 (2024)
- [5] Shi X L, Chen G P, Xu L, Kang C X, Luo G H, Luo H M, Zhou Y, Dargusch Matthew S, Pan G S. Achieving ultralow surface roughness and high material removal rate in fused silica via a novel acid SiO₂ slurry and its chemical-mechanical polishing mechanism. *Appl Surf Sci* **500**: 144041 (2020)
- [6] Morinaga H. Origin and innovations of CMP slurry. *Ecs J Solid State Sc* **13**(7): 74006 (2024)
- [7] Zou Y D, Niu X H, Zhan N, Liu J H, Li X J, He C, Dong C X, Zhou J W. Effect of amino acid complexing agents on chemical mechanical polishing performance and action mechanism of C-plane sapphire: Combining experiments and theoretical calculations. *Mater Chem Phys* **316**: 129066 (2024)
- [8] Li X J, Zou Y D, Niu X H, Jia Y Q, Zhan N, Liu J H, He C, Dong C X, Shi Y H. Exploring the effectiveness of polyhydroxy complexing agents in sapphire chemical mechanical polishing: Combining experiments and theoretical calculation. *Tribol Int* **199**: 110042 (2024)
- [9] Wang S, Ruan J H, Xiao S H, Deng Q F, Zhao T C. Orthogonal experimental study on the influence of machining parameters on flat lapping of sapphire substrate. *Aip Adv* **14**(1): 15020 (2024)
- [10] Zhang W, Lei H, Liu W Q, Zhang Z F, Chen Y, Hu X G, Ye X S. Effect of

- EDTA-modified alumina composite abrasive on the CMP performance of sapphire substrate. *Mater Chem Phys* **312**: 128651 (2024)
- [11] Tie M W, Wang Y F, Zhang C, Huang X B. Classification, performance and recycling of ceria-based materials used for chemical mechanical polishing. *Nanoscale* **18**(11): 5638–5666 (2026)
- [12] Yang S Y. Atomic-scale insights into the abrasive concentration effects on 6H-SiC removal in CMP. *Tribol Int* **214**: 111277 (2026)
- [13] Zhou C, Xu X Y, Dai L, Gong H M, Lin S T. Chemical-mechanical polishing performance of core-shell structured polystyrene@ceria/nanodiamond ternary abrasives on sapphire wafer. *Ceram Int* **47**(22): 31691–31701 (2021)
- [14] Zhou M F, Zhong M, Xu W H. Novel model of material removal rate on ultrasonic-assisted chemical mechanical polishing for sapphire. *Friction* **11**(11): 2073–2090 (2023)
- [15] Zhang W, Lei H, Liu W Q, Zhang Z F. Effect of the carboxyl group number of the complexing agent on polishing performance of alumina slurry in sapphire CMP. *Ceram Int* **49**(9): 13687–13697 (2023)
- [16] Li X J, Zou Y D, Niu X H, Jia Y Q, Zhan N, Liu J H, He C, Dong C X, Shi Y H. Exploring the effectiveness of polyhydroxy complexing agents in sapphire chemical mechanical polishing: Combining experiments and theoretical calculation. *Tribol Int* **199**: 110042 (2024)
- [17] Zou Y D, Niu X H, Zhan N, Liu J H, Li X J, He C, Dong C X, Shi Y H. Chemical-mechanical synergies effects of multi-purpose pH regulators on C-, A-, and R-plane sapphire polishing. *Tribol Int* **195**: 109603 (2024)
- [18] Xia G, Wang Z R, Yao Q Y, Sun P, Guan H J, Wang Y G, Fan C, Bian D, Zhao D, Zhao Y W. Modeling of material removal rate considering the chemical mechanical effects of lubricant, oxidant, and abrasive particles for aluminum chemical mechanical polishing at low pressure. *Wear* **530-531**: 205023 (2023)
- [19] Wang L, Zhou P, Yan Y, Hou C Y, Guo D M. Micro-scale contact behavior and its effect on the material removal process during chemical mechanical polishing. *Tribol Int* **156**: 106831 (2021)

- [20] Luo Q F, Lu J, Tian Z G, Jiang F. Controllable material removal behavior of 6H-SiC wafer in nanoscale polishing. *Appl Surf Sci* **562**: 150219 (2021)
- [21] Luo Z, Zhang Z Y, Zhao F, Fan C, Feng J Y, Zhou H X, Meng F N, Zhuang X Y, Wang J M. Advanced polishing methods for atomic-scale surfaces: A review. *Materials Today Sustainability* **27**: 100841 (2024)
- [22] Xu Y C, Peng C, Wang N C, He J F, Zhan Y J, Wang Q T. Study on the polishing performance and mechanism of sapphire wafers by different types of degradable surfactants. *Surfaces and Interfaces* **52**: 104915 (2024)
- [23] Luo X Y, Yang W, Qian Y. Fixed abrasive polishing: The effect of particle size on the workpiece roughness and sub-surface damage. *The International Journal of Advanced Manufacturing Technology* **115**(9-10): 3021–3035 (2021)
- [24] Ding R Y, Lei H, Chen C D, Zhang Z F. Preparation of the Nanodiamond@SiO₂ Abrasive and its Effect on the Polishing Performance of Zirconia Ceramics. *Ecs J Solid State Sc* **11**(6): 64002 (2022)
- [25] Ma Q, Niu X H, Zhou J K, Liu Z L, Wang M Q, Song S B, Wu Z, Hu B, Li J H, Hong J. Recent advances in design and preparation of abrasives for chemical mechanical polishing of hard-brittle materials. *Journal of materials chemistry. C, Materials for optical and electronic devices* **14**(11): 4248–4428 (2026)
- [26] Xu Y C, Fan Z C, Yang D R, Tian Z G Wang Q T, Zhan Y J, Chen B S. Enhanced polishing performance and tribo-chemical removal mechanism of sapphire wafers under gas-assisted CMP (GA-CMP). *J Mater Process Tech* **346**: 119087 (2025)
- [27] Zeng N Y, Zhao H D, Liu Y L, Wang C W, Luo C, Wang W T, Ma T D. Optimizing of the colloidal dispersity of silica nanoparticle slurries for chemical mechanical polishing. *Silicon-Neth* **14**(13): 7473–7481 (2022)
- [28] Wang W T, Zhang B G, Shi Y H, Zhou D K, Wang R. Improvement in dispersion stability of alumina suspensions and corresponding chemical mechanical polishing performance. *Appl Surf Sci* **597**: 153703 (2022)
- [29] Gao S, Hu B Y, Song X, Dong Z G, Kang R K. Dispersal mechanism of different dispersants and its effect on performance of 4H-SiC polishing slurry. *Ceram Int*

51(3): 3943–3952 (2025)

- [30] Xu X Y, Wu Y J, Ning H L, Xiao B, Huo J R, Xie D, Wang C Y, Liu X L. Microscopic interaction mechanism between surfactants and SiO₂ abrasives and its performance in sapphire polishing. *Ecs J Solid State Sc* **14(10)** (2025)
- [31] Doi K. T, Aida H, Ohnishi O, Yin S H, Ren Y H. Challenges of future high-precision polishing methods for hard-to-process materials by the fusion of environmental control and plasma technology. *Diamond and Abrasives Engineering* **42(06): 637–649 (2022)**
- [32] Shi X L, Xu L, Zhou Y, Zou C L, Wang R R, Pan G S. An in situ study of chemical-mechanical polishing behaviours on sapphire (0001) via simulating the chemical product-removal process by AFM-tapping mode in both liquid and air environments. *Nanoscale* **10(42): 19692–19700 (2018)**
- [33] Guo J, Gong J, Shi P F, Xiao C, Jiang L, Chen L, Qian L M. Study on the polishing mechanism of pH-dependent tribochemical removal in CMP of CaF₂ crystal. *Tribol Int* **150: 106370 (2020)**
- [34] Xiao C, Li J, Guo J, Zhang P, Yu B J, Chen L, Qian L M. Role of mechanically-driven distorted microstructure in mechanochemical removal of silicon. *Appl Surf Sci* **520: 146337 (2020)**
- [35] Xiao C, Deng C B, Zhang P, Qian L M, Kim S H. Interplay between solution chemistry and mechanical activation in friction-induced material removal of silicon surface in aqueous solution. *Tribol Int* **148: 106319 (2020)**
- [36] Guo J, Gao J, Xiao C, Chen L, Qian L M. Mechanochemical reactions of GaN-Al₂O₃ interface at the nanoasperity contact: Roles of crystallographic polarity and ambient humidity. *Friction* **10(7): 1005–1018 (2022)**
- [37] Zhong X, Chen Y S, Jiang L, Li W H, Qian L M. Synergistic effect of oxidation and complexation on the material removal of pure iron at the nanoscale. *Wear* **524-525: 204771 (2023)**
- [38] Fogarty J C, Aktulga H M, Grama A Y, van D A C T, Pandit S A. A reactive molecular dynamics simulation of the silica-water interface. *The Journal of chemical physics* **132(17): 174704 (2010)**

- [39] Stukowski A. Visualization and analysis of atomistic simulation data with OVITO—the Open Visualization Tool. *Model Simul Mater Sc* **18**(1): 15012 (2010)
- [40] Aktulga H M, Fogarty J C, Pandit S A, Grama A Y. Parallel reactive molecular dynamics: Numerical methods and algorithmic techniques. *Parallel Comput* **38**(4-5): 245–259 (2012)
- [41] Hoover W G. Canonical dynamics: Equilibrium phase-space distributions. *Physical review. A, General physics* **31**(3): 1695–1697 (1985)
- [42] Ostadhossein A, Kim S Y, Cubuk E D, Qi Y, van D A C T. Atomic insight into the lithium storage and diffusion mechanism of SiO₂ /Al₂O₃ electrodes of lithium ion batteries: ReaxFF reactive force field modeling. *The Journal of Physical Chemistry A* **120**(13): 2114–2127 (2016)
- [43] Zhang S C, Zhong M, Li X B, Yi M R, Chen J F, Xu W H. Tribo-chemical atom removal in sapphire chemical mechanical polishing: Insight from ReaxFF MD and experiments. *Tribol Int* **213**: 111088 (2026)
- [44] Young M J, Bedford N M, Yanguas G A, Letourneau S, Coile M, Mandia D J, Aoun B, Cavanagh A S, George S M, Elam J W. Probing the Atomic-Scale structure of amorphous aluminum oxide grown by atomic layer deposition. *Acs Appl Mater Inter* **12**(20): 22804–22814 (2020)
- [45] Deng H G, Zhong M, Yi M R, Li X B, Chen J F, Xu W H. Friction and chemical action of deionized water on microscopic wear of sapphire surface. *Tribol Int* **214**: 111320 (2026)
- [46] Dhere S L, Latthe S S, Kappenstein C, Pajonk G M, Ganesan V, Rao A V, Wagh P B, Gupta S C. Transparent water repellent silica films by sol–gel process. *Appl Surf Sci* **256**(11): 3624–3629 (2010)
- [47] He H T, Qian L M, Pantano C G, Kim S H. Mechanochemical wear of soda lime silica glass in humid environments. *J Am Ceram Soc* **97**(7): 2061–2068 (2014)
- [48] Argyris D, Ho T, Cole D R, Striolo A. Molecular dynamics studies of interfacial water at the alumina surface. *The Journal of Physical Chemistry C* **115**(5): 2038–2046 (2011)

- [49] Vovk E A, Budnikov A T, Dobrotvorskaya M V, Krivonogov S I, Dan K Y. Mechanism of the interaction between Al_2O_3 and SiO_2 during the chemical-mechanical polishing of sapphire with silicon dioxide. *Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques* **6**(1): 115–121 (2012)
- [50] Spiegel M R. "Mathematical handbook of formulas and tables, in schaum's outline series". McGraw–Hill, 1992.
- [51] Simonsen A C, Hansen Per Lyngs, Klösgen Beate. Nanobubbles give evidence of incomplete wetting at a hydrophobic interface. *J Colloid Interf Sci* **273**(1): 291–299 (2004)
- [52] Carpick R W, Ogletree D F, Salmeron M. A general equation for fitting contact area and friction vs load measurements. *J Colloid Interf Sci* **211**(2): 395–400 (1999)
- [53] Gu X S, Zhao Q L, Wang H, Xue J M, Guo B. Fundamental study on damage-free machining of sapphire: Revealing damage mechanisms via combining elastic stress fields and crystallographic structure. *Ceram Int* **45**(16): 20684–20696 (2019)
- [54] Hess A, Kemnitz E, Lippitz A, Unger W, Menz D H. ESCA, XRD, and IR characterization of aluminum-oxide, hydroxyfluoride, and fluoride surfaces in correlation with their catalytic activity in heterogeneous halogen exchange-reactions. *J Catal* **148**(1): 270–280 (1994)
- [55] Zhang Z L, Jin Z J, Guo J, Han X L, Mu Q, Zhu X L. A novel chemical mechanical polishing slurry for yttrium aluminum garnet crystal. *Appl Surf Sci* **496**: 143601 (2019)
- [56] Xie W X, Zhang Z Y, Liao L X, Liu J, Su H J, Wang S D, Guo D M. Green chemical mechanical polishing of sapphire wafers using a novel slurry. *Nanoscale* **12**(44): 22518–22526 (2020)
- [57] Chastain J, King R C. "Handbook of x-ray and ultraviolet photoelectron spectroscopy". Perkin-Elmer Corporation, 1992.
- [58] Sarapatka T J. Xps study of light-induced effects on pd-Si and pd-SiO₂-Si

interfaces. *J Electron Spectrosc* **58**(3): 233–245 (1992)

[59] Liu X H, Zhong M, Xu W H. Molecular dynamics study of sapphire polishing considering chemical products. *Ecs J Solid State Sc* **12**(12): 124002 (2023)

[60] Wang Z J, Sohn I. Effect of substituting CaO with BaO on the viscosity and structure of CaO-BaO-SiO₂-MgO-Al₂O₃ slags. *J Am Ceram Soc* **101**(9): 4285–4296 (2018)

Just Accepted