

Mechanisms of surface and subsurface damage of silicon wafers induced by external stress during nano-polishing

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ARTICLE INFO

Handling Editor: Dr P. Vincenzini

Keywords:

Silicon wafer
Molecular dynamics
Nano-polishing
Surface friction damage
External stress damage mechanism

ABSTRACT

The variation in external stress during nano-polishing of silicon wafers inevitably leads to surface friction defects and subsurface damage. To reveal the underlying relationship between the changes in external stress and the evolution of surface and subsurface damage in silicon wafers, this study utilizes molecular dynamics methods, combined with the Weierstrass-Mandelbrot three-dimensional rough surface theory. A molecular dynamics geometric model of the silicon wafer's rough surface is constructed using a spring loading mechanism. By analyzing atomic interactions within the simulation system and the stability of external stress controlled by the spring mechanism, a stable molecular dynamics simulation system is established. Through a multi-dimensional analysis of surface roughness, friction force, and shear strain, the effect mechanism of external stress on the evolution of surface and subsurface damage in silicon wafers is revealed. The results show that, with increasing external stress, the surface roughness of the silicon wafer changes non-linearly, reaching a minimum roughness of 6.310 nm, where structural damage is minimized. Shear strain extends along the $\langle 110 \rangle$ and $\langle 1-10 \rangle$ crystal directions, and dislocations slip along the shear strain direction, evolving into "V"-shaped dislocations that cause micro-damage, with a minimum damage layer thickness of 4.0 nm. This study reveals the stress damage mechanism of nano-polished silicon wafers at the microscopic scale and explains its macroscopic friction mechanical behavior.

1. Introduction

Silicon wafers are fundamental materials in semiconductor device manufacturing. They are made from single-crystal silicon and possess a stable crystal structure. Silicon wafers exhibit excellent thermal stability, good electrical conductivity, and high mechanical strength. These properties make silicon wafers indispensable in various applications, including integrated circuits (ICs), microelectromechanical systems (MEMS), power semiconductor devices, and high-efficiency crystalline silicon solar cells [1–4]. Despite these excellent properties of silicon wafers, various technical issues arise during processing, which may affect wafer quality and the performance of final devices. During polishing, any insufficient or excessive polishing can cause microscopic defects on the wafer surface [5–6], such as scratches or pits. Additionally, mechanical stress and heat generated during polishing can lead to

wafer deformation, warping, or even cracking [7–8]. These factors impact both the polishing outcome and the overall quality of the wafer. Mechanical polishing technology offers high material removal efficiency; however, it is prone to introducing scratches and residual stress, making it suitable primarily for preliminary processing. To address these macro defects, chemical mechanical polishing (CMP) technology is proposed and widely applied in high-precision surface processing [9–11]. This method combines the dual effects of chemical corrosion and mechanical friction. By using polishing liquids with micron or nano-abrasives, CMP softens the wafer surface material through chemical reactions and removes the material through mechanical force, thereby enhancing surface smoothness and reducing roughness. While CMP can significantly improve surface quality, its processing may still induce structural defects, such as silicon wafer warping and subsurface cracks, due to external stress. These defects are challenging to detect

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<https://doi.org/10.1016/j.ceramint.2025.05.203>

Received 17 February 2025; Received in revised form 12 May 2025; Accepted 13 May 2025

Available online 14 May 2025

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using conventional methods, and their formation mechanisms have yet to be fully understood. Nano-polishing focuses on the material removal behavior in CMP at the nanoscale, aiming to uncover its microscopic mechanisms. Therefore, this study examines atomic-level removal behavior under the influence of mechanical abrasives in the CMP process, employs molecular dynamics techniques to simulate the interaction process on the silicon wafer surface under various process parameters, and provides a detailed analysis of how external stress affects the evolution of surface and subsurface damage.

Molecular dynamics methods are widely used in studying the microevolution of materials. With the development of polishing technology, many scholars at home and abroad have researched and explored the mechanism of sub-surface damage of wafers in the polishing process. Wang et al. [12–13] used reactive molecular dynamics (ReaxFF MD) to investigate material removal and damage mechanisms on silicon surfaces during the CMP. The results showed that the oxide layer on the silicon surface played an important role in wear. This was mainly achieved by the insertion of oxygen atoms into the surface, rather than by the formation of Si-O-Si bridge bonds, which enhanced the material removal rate. Yan et al. [14] performed low-speed diamond grinding of single-crystal silicon. Phase transformation and dislocation behavior under high pressure were considered. A subsurface damage mechanism model for ductile-mode machining of silicon was proposed. It was found that the subsurface damage mechanism of silicon was related to the applied pressure during processing. Li et al. [15–16] studied the damage mechanisms of single-crystal silicon at varying grinding speeds and depths. Results showed the maximum height of grinding chips did not consistently increase with grinding speed. When the damage layer thickness reached half of its original thickness, further grinding led to the formation of new damage structures and an increase in damage layer thickness. Nguyen et al. [17–18] investigated the effects of sliding, rolling, and oscillating motions of diamond abrasives on the nano-structural characteristics of silicon substrates. Their findings revealed that the rolling motion resulted in the highest number of atoms removed, the optimal oscillating motion yielded the lowest convex surface height, and the sliding motion produced the lowest surface roughness. Both sliding and rolling motions were found to significantly affect the material removal rate (MRR) of the silicon substrate. Si et al. [19] examined the atomic-level removal mechanisms of single-crystal silicon during CMP. Simulations revealed that, at a scratch depth of 1 nm, a thicker silicon layer was removed through chip formation, resulting in an amorphous layer. In contrast, at a depth of 0.1 nm, only a single atomic layer was removed, producing a well-ordered crystal surface. The atomic layer removal mechanism was proposed, where material is removed layer by layer during CMP through the removal of single atomic layers. Existing research mainly uses traditional molecular dynamics (MD) or ReaxFF MD methods to explore the effects of polishing depth, speed, method, and water oxidation on the surface and subsurface damage mechanisms of silicon, making progress in these areas. However, studies on the evolution of subsurface damage in silicon wafers under gradient external stress are still limited, particularly in terms of the impact of stress gradients on the micro-damage evolution. Therefore, this study employs molecular dynamics methods to experiment with gradient external pressures and investigates the impact of external pressure on the material removal mechanisms of silicon wafers during polishing.

To explore the impact of external pressure on material removal mechanisms during chemical-mechanical polishing of silicon wafers, a molecular dynamics model is established for polishing rough silicon wafer surfaces with silica abrasives, incorporating random rough surfaces. Gradient polishing pressure experiments are designed to achieve models with high surface quality based on surface roughness variations. The friction force, stress-strain behavior, and dislocation propagation in models with lower surface roughness are analyzed. The influence of polishing pressure on the material removal mechanisms of silicon wafers and the evolution of subsurface damage is investigated. This approach

provides a microscopic explanation for the macroscopic mechanical behavior of polished silicon wafers, examines the mechanical properties of silicon wafers under varying stress conditions, and offers theoretical support for material design and optimization.

2. Establishment of Molecular Dynamics Model for silicon wafer nano-polishing

2.1. Establishment of physical model of SiO₂ abrasive polishing silicon wafer

To investigate the factors influencing material removal mechanisms during the polishing of rough silicon wafer surfaces, a molecular dynamics model is established for the nanoscale polishing of rough silicon wafers with silica abrasives. Compared with diamond, this study uses silicon dioxide as an abrasive because the hardness of silicon dioxide is similar to that of silicon wafers, which can avoid surface damage, achieve high-precision flatness, and has good dispersion stability and low cost, so as to accurately simulate the precision polishing behavior of silicon wafers during nano-polishing [20]. The details of the molecular dynamics model for polishing rough silicon wafer surfaces with silica abrasives are illustrated in Fig. 1.

The model represents the friction process between silica (SiO₂) abrasives and the rough surface of a silicon (Si) wafer at the nanoscale, with dimensions of 35 nm × 30 nm × 14 nm. The silicon wafer work area is divided into four regions: an outer blue boundary layer, a green temperature-controlled layer, a light orange Newtonian layer, and a light purple measurement zone. The boundary layer, with a thickness of 0.5 nm, absorbs stress waves and boundary effects generated in the system. Fixed boundary layers effectively reduce boundary effects. The temperature-controlled layer, with a thickness of 1 nm, maintains system temperature within a specified range through heat exchange. The Newtonian layer, with a thickness of 12.5 nm, allows atoms to follow Newton's second law, simulating the mechanical behavior of actual materials. A 30 nm × 8 nm × 12.5 nm region within the Newtonian layer is selected as the measurement zone. To ensure the stability of the abrasives, virtual atoms are connected to the abrasives with different elastic coefficients in the x, y, and z directions. Specifically, the elastic coefficients are 64 N/m in the x and y directions and 26 N/m in the z direction. Higher stiffness in the x and y directions helps reduce vibrations of the abrasives, minimizing the impact of vibrations on the forces applied to the abrasive atoms. The focus of this study is on the evolution of surface and subsurface damage in silicon wafers under external stress conditions, rather than the wear and deformation of SiO₂ abrasives. Therefore, atomic interactions within the abrasives are neglected, and SiO₂ abrasives are treated as rigid bodies [21]. The SiO₂ abrasive particle is placed 1 nm from the silicon wafer surface, and an external force F is applied to the particle. This induces a frictional interaction between the abrasive and the rough surface of the silicon wafer. Fig. 1(a) shows the crystal structure of SiO₂, where Si atoms form a stable tetrahedral structure with four O atoms through covalent bonds. Fig. 1(b) depicts the diamond cubic crystal structure of Si, where each Si atom is connected to four neighboring Si atoms. Fig. 1(c) illustrates the 3D morphology of the rough surface of the silicon wafer model. Molecular dynamics simulations reveal atomic interactions between SiO₂ abrasives and the silicon wafer surface, the impact of surface roughness on friction behavior, and the conversion of energy and migration of material during friction. Quantitative analysis of these microscopic mechanisms aids in understanding and optimizing tribological performance at the nanoscale.

Table 1 presents the parameter values for the molecular dynamics model of SiO₂ abrasive nano-polishing of silicon wafers. The silicon wafer workpiece contains 697,244 atoms, while the SiO₂ abrasive has a radius of 5 nm and contains 21,033 atoms. During the entire simulation process, the Langevin thermostat is applied to regulate the temperature of the thermostat layer at 298 K, in conjunction with the NVE ensemble.

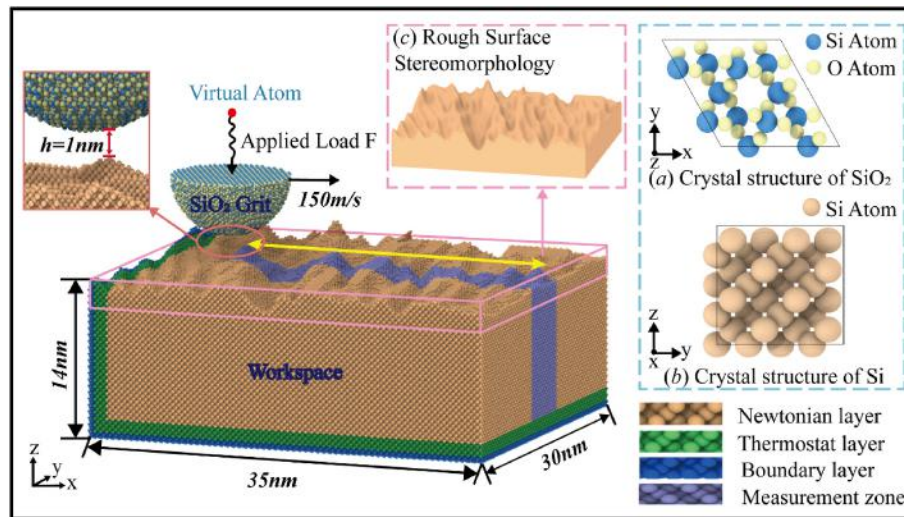


Fig. 1. Molecular dynamics model of silicon dioxide abrasive polishing a rough silicon wafer surface. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

Friction between the Newton layer and the abrasive generates heat, which is then transferred to the thermostat layer for dissipation. Periodic boundary conditions are applied in all three dimensions. The simulation time step is set to 1 fs, with a polishing distance of 22.5 nm and a polishing direction of $\langle 100 \rangle$, moving in the positive x direction. The polishing speed is chosen as an ultra-high rate of 150 m/s, polishing depth of 2.6 nm. External load pressures applied are 0, 20, 40, ..., 140, 160, and 180 nN. Detailed parameter values are listed in Table 1.

2.2. Creation of random rough surface

To accurately reflect the surface damage of silicon wafers during actual precision machining, and to address the unclear methods for generating random rough surfaces in molecular dynamics simulations, the Weierstrass-Mandelbrot (W-M) fractal surface [22] is utilized to generate the random rough surface model of the silicon wafer. The detailed process of model creation is illustrated in Fig. 2, which shows the principle and procedure for forming the random rough surface model of the silicon wafer.

The principle of the W-M fractal random rough surface is based on self-similarity, where the roughness characteristics exhibit similar distribution patterns at different scales. As depicted in Fig. 2(a), random rough surface types are illustrated. The roughness parameters R_a and S_a represent two-dimensional and three-dimensional surface roughness, respectively. These parameters quantify the extent of surface undulations. R_a denotes the average roughness measured along the x-axis direction, while S_a indicates the average roughness over the entire

three-dimensional surface. R_a is calculated as the average of the absolute values of height deviations within the measurement length. The measurement procedure involves first obtaining the surface profile by measuring along a specified direction. A reference line, usually the arithmetic mean line, is then established to compute height deviations. The height deviation of each point on the profile from the reference line is determined. Finally, the average of the absolute height deviations over the entire measurement length is computed to derive R_a . The specific calculation formula is as follows [23]:

$$R_a = \frac{1}{l} \int_0^l |Z(x)| dx \quad (1)$$

Where l is the measuring length and $Z(x)$ is the surface height deviation at position x .

S_a represents the arithmetic mean of the absolute heights of all sampling points on the three-dimensional surface and is used to characterize surface roughness. The calculation process includes the following steps: First, regular sampling is performed on the 3D surface of the silicon wafer using OVITO to extract the spatial coordinates of all surface atoms within the measurement region, and the surface height $Z(x_i, y_i)$ at each sampling point is recorded. Next, the extracted coordinate data are imported into MATLAB to construct a surface height matrix, which serves as the basis for subsequent calculations. Finally, a custom MATLAB script is employed to calculate the surface roughness S_a based on the discrete formula for three-dimensional surface roughness. The specific formula is given as follows [24]:

$$S_a = \frac{1}{MN} \sum_{i=1}^M \sum_{j=1}^N |Z(x_i, y_j)| \quad (2)$$

Where M , N are the number of surface sampling points in the x and y directions, respectively, $Z(x_i, y_j)$ is the surface height at (x_i, y_j) , and $|Z(x_i, y_j)|$ is the absolute value of the surface height at (x_i, y_j) . In machining, by measuring and analyzing S_a of the workpiece surface, the effect of the machining process can be evaluated to ensure that the product quality meets the standards.

The process of generating the three-dimensional random rough surface is illustrated in Fig. 2(b). First, Gaussian white noise waveforms are generated, as shown in Fig. 2(b₁), to replicate the surface's random characteristics. Then, the spectral distribution of the Gaussian white noise is calculated based on key parameters, including the fractal dimension D_s , wavelength λ , and the maximum number of frequency components n_{max} . Finally, waveforms with different frequencies are

Table 1

Parameters of molecular dynamics model for SiO₂ abrasive nano-polishing of silicon wafer.

Simulation parameters	Simulation parameter values
Silicon wafer workpiece size (nm)	35 × 30 × 14
Number of atoms in silicon wafer workpiece	697244
SiO ₂ abrasive grain radius (nm)	5
Number of SiO ₂ abrasive atoms	21033
Simulated temperature (K)	298
Ensemble selection	NVE
Timestep (fs)	1
Polishing distance (nm)	22.5
Polishing direction	$\langle 100 \rangle$
Polishing speed (m/s)	150
Polishing depth (nm)	2.6
External loads (nN)	0, 20, 40, ..., 140, 160, 180

superimposed to construct a self-similar three-dimensional fractal surface. The mathematical formulation of the W-M three-dimensional fractal random rough surface is expressed as follows:

$$Z(x, y) = \sum_{n=0}^N G_n \cos[2\pi\lambda^n(x \cos \theta_n + y \sin \theta_n) + \varphi_n] \quad (3)$$

In the equation, $Z(x, y)$ is the height of the three-dimensional surface, G_n is the amplitude of the n th frequency component, λ_n is the wavelength of the n th frequency component, θ_n is the azimuth of the n th frequency component, φ_n is the phase of the n th frequency component, and n_{max} is the number of maximum frequency components. By selecting different parameters, three-dimensional surfaces with different roughness and fractal characteristics can be generated. The fractal dimension D_s is a parameter that describes the complexity of the surface, usually $2 < D_s < 3$, and D_s is determined to be 2.8. The wavelength λ is a parameter related to the surface roughness, which determines the detail scale of the surface, and λ is 1.05. The maximum number of frequency components n_{max} determines the fineness of the surface generation, and n_{max} is 80. Fig. 2(b₂) is a W-M three-dimensional fractal random surface generated according to the above parameters. The specific random rough surface is obtained by filling Si atoms with LAMMPS software, as shown in Fig. 2(c) LAMMPS random rough surface morphology. The atomic coordinates of the surface measurement region of the silicon wafer workpiece are extracted using OVITO software. The extracted coordinate data are then imported into Matlab, where the three-dimensional surface roughness formula is applied for calculation. The resulting surface roughness S_a of the generated random rough surface model of the silicon wafer is 13.070 nm. The W-M three-dimensional fractal random rough surface model provides important theoretical and computational tools for understanding and analyzing complex surface morphology, and is of great

significance for materials science and engineering applications.

2.3. Selection of potential function

In molecular dynamics simulations, the potential function governs the interactions between atoms or molecules, influencing the system's energy and dynamic behavior. It describes atomic interactions, including attractive and repulsive forces, as well as multi-body interactions such as bonding, angles, and dihedrals. These forces determine particle trajectories, thereby affecting the overall system dynamics. The complexity and accuracy of the potential function directly impact the reliability of the simulation results. Consequently, different material systems require different potential functions. In this study, a mixed potential approach is employed: the SW potential is used for the interaction between silicon atoms in silicon wafers, the Tersoff potential describes Si-O interactions in silica abrasives, and the LJ potential is applied to model the interactions between silicon atoms in the wafer and oxygen and silicon atoms in the silica abrasive.

The Stillinger-Weber (SW) potential [25] is widely used to model silicon crystals due to its ability to effectively describe covalent interactions between silicon atoms, capture three-body and many-body effects, and provide the computational efficiency and accuracy required for large-scale simulations. The choice of the SW potential ensures the accuracy of the simulation results, particularly when addressing complex phenomena such as the mechanical properties, thermodynamic behavior, and phase transitions of silicon wafers. The potential includes both two-body and three-body interactions, which are used to accurately model the lattice structure of silicon. The total energy is expressed as:

$$E = \sum_i \sum_{j>i} \phi_2(r_{ij}) + \sum_i \sum_{j \neq i} \sum_{k>j} \phi_3(r_{ij}, r_{ik}, \theta_{ijk}) \quad (4)$$

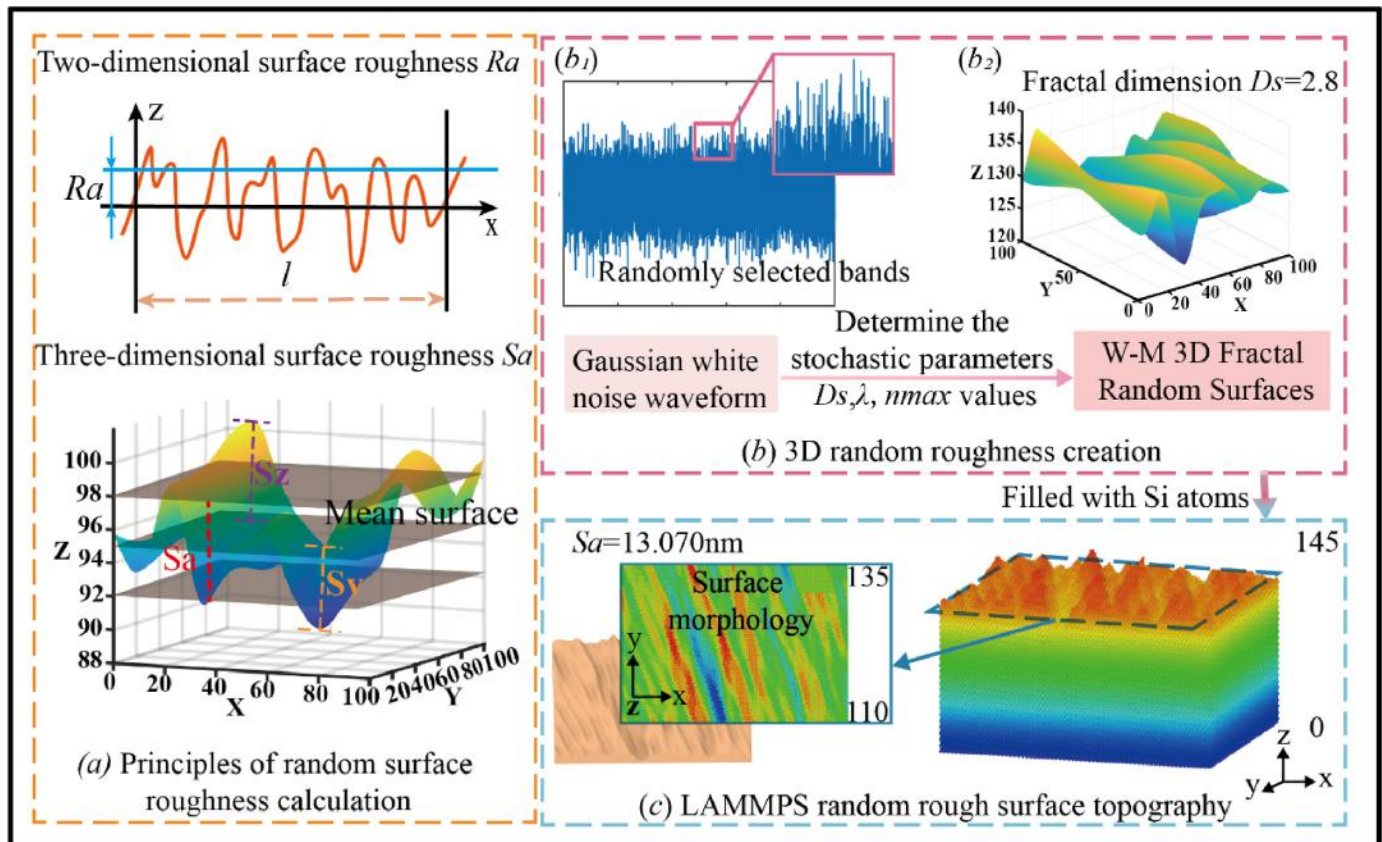


Fig. 2. Formation principle and establishment process of random rough surface model of silicon wafer. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

$\varphi_2(r_{ij})$ is two-body interaction potential, depends on the distance r_{ij} between two atoms i and j , its parameters directly affect the bonding strength and elastic properties of the bond. $\varphi_3(r_{ij}, r_{jk}, \theta_{ijk})$ is the three-body interaction potential, depends on the distances r_{ij} and r_{jk} between atoms i and j , k , and the angle formed by atoms i , j , and k θ_{ijk} , it plays a key role in lattice stability, phase transition and fracture behavior. Reasonable setting of potential function parameters is crucial for accurately characterizing the microstructure of silicon wafers. The specific parameter settings of the silicon wafer SW potential function are shown in Table 2.

The Tersoff potential is selected to describe the atomic interactions in the silicon dioxide abrasive, as it can accurately model the covalent bond interactions in silicon dioxide, particularly the interactions between silicon-silicon and silicon-oxygen. It captures many-body effects, the formation and breaking of chemical bonds, and the material behavior under high-temperature conditions. Furthermore, the Tersoff potential [26] has been extensively validated in simulating complex materials such as silicon dioxide, demonstrating its reliability and accuracy in describing the interactions between abrasives and workpieces. The Tersoff expression is given as:

$$E = \sum_i E_i = \frac{1}{2} \sum_{i \neq j} V_{ij} \quad (5)$$

$$V_{ij} = \frac{1}{2} \sum_{i \neq j} f_c(r_{ij}) [f_R(r_{ij}) + b_{ij} f_A(r_{ij})] \quad (6)$$

Where E is the binding energy, r_{ij} is the distance between atom i and atom j , f_c is the cutoff function, f_R and f_A are the repulsive and attractive terms respectively, which limit the scope of interaction. b_{ij} is the bond order factor, b_{ij} is the bond order factor, reflecting multi-body effects, especially the angle dependence. These parameters can accurately capture the interaction forces between Si-O atoms in silicon oxide by describing the local environment and multi-body interactions of the material, thereby affecting the stress-induced subsurface damage mechanism of silicon wafers during nano-polishing.

The Lennard-Jones (LJ) potential [27] is chosen to describe the interactions between silicon atoms in the silicon wafer and the silicon atoms, as well as the oxygen atoms, in the silicon dioxide abrasive. This choice is due to its ability to effectively capture the weak van der Waals forces between these materials, particularly the short-range interactions between surface atoms. While the Tersoff potential is effective in describing the covalent bond interactions in silicon and silicon dioxide abrasives, the LJ potential complements it by accounting for the weak interactions and short-range attractions at the interface. Additionally,

Table 2
Parameters of SW potential energy function for interacting atomic pairs.

Potential parameter value	Si-Si-Si
ϵ [eV]	2.1683
σ [Angstroms]	2.0951
a	1.80
λ	21.0
γ	1.20
$\cos\theta_0$	-0.3333
A [eV]	7.0496
B [eV]	22.5

Table 3
Lennard-Jones potential energy function parameters for interacting atomic pairs.

Interatomic interactions	ϵ [eV]	σ [Å]
Si-O	0.0001	2.95
Si-Si	0.0017	3.2

the LJ potential offers advantages in computational efficiency. The expression for the LJ potential is given as:

$$V_{LJ} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (7)$$

In formula (7), ϵ represents the potential well depth, which determines the strength of the interaction between atoms and affects the material's damage resistance and interface bonding characteristics. σ is the atomic spacing at zero potential energy, which determines the stable atomic spacing and directly affects the formation and expansion of dislocations. r is the distance between atoms, which regulates the range of van der Waals forces and thus affects the micromechanical response of the material. The specific parameter settings are shown in Table 3.

3. Silicon wafer polishing pressure gradient simulation experiment

To study the effect of different polishing pressures on the damage and material removal mechanisms of silicon wafers with rough surfaces during silica abrasive polishing, ten sets of nano-polishing experiments with varying pressures are designed. The surface damage distribution and subsurface damage evolution of silicon wafers are systematically studied using visualization analysis techniques. Fig. 3 presents the surface damage characteristics and roughness variation trends under gradient external stress conditions, aiming to reveal the impact mechanism of external stress on the polishing process.

Fig. 3(a) shows the effect of stepwise external stress (0–180 nN) on surface roughness. Fig. 3(b) presents the evolution of surface roughness (S_a) under different stress conditions. As the external stress increases, roughness (S_a) decreases initially, reaching a minimum value of $S_a = 6.310$ nm at approximately 60 nN. Further increases in stress lead to a subsequent rise in roughness. This process can be divided into four distinct stages: the initial stage (0–40 nN), where the surface microstructure remains stable and roughness changes minimally, indicating only slight compression or elastic deformation; the decrease stage (40–60 nN), where significant plastic deformation occurs, increasing atomic layer interactions and flattening surface protrusions, which significantly reduces roughness; the increase stage (60–160 nN), where continued stress increases lead to surface pits and indentations, causing roughness to rise, mainly due to atomic layer instability under excessive stress, forming microscopic indentations; the high-pressure stability stage (160–180 nN), where roughness stabilizes or increases slowly, indicating the formation of a more stable deformation structure with minimal roughness change.

To further explore the impact of gradient external stress on subsurface damage of silicon wafers, the evolution characteristics of subsurface damage under different external stress conditions are systematically analyzed. The distribution pattern and evolution mechanism of subsurface damage under gradient external stress are revealed. Fig. 4 shows the subsurface damage analysis of silicon wafer polishing experiments under gradient external stress conditions.

Fig. 4(a) shows the changes in friction force (F_z) and stress-strain distribution under varying external stresses. Fig. 4(a₁) demonstrates that friction force increases with friction distance and rises significantly under higher stress, indicating surface wear and smoothing, which increases the contact area and, in turn, increases friction force. Under high stress, significant plastic deformation may occur, further increasing friction force. Fig. 4(a₂) illustrates the stress-strain distribution under different external stress conditions. Particularly under high-pressure conditions, the strain concentration region expands, forming double-V dislocation rings and other complex dislocation structures, indicating strong shear deformation. As external stress increases, atomic layer interactions and sliding intensify, forming complex dislocation structures and enlarging the stress concentration region, which influences the material's friction behavior. Fig. 4(b) shows changes in dislocation

quantity and type on the material surface under various external stresses, as well as their relationship with atomic phase transitions. Fig. 4(b₁) shows that dislocation quantity increases with external stress, especially at high stress levels, where the increase is more pronounced, indicating a significant enhancement of atomic layer interactions. Fig. 4(b₂) further examines the evolution of dislocation types. As stress increases, the material surface transitions from primarily ordinary dislocations to complex dislocation structures, such as double-V dislocation rings, indicating significant localized shear deformation under high pressure. This leads to increased relative displacement between atomic layers, forming a complex dislocation network. In conclusion, when external stress is 60 nN, the surface roughness reaches its minimum value of $S_a = 6.310$ nm. The surface exhibits smooth morphological changes, friction force remains stable, and dislocation quantity begins to rise but does not increase significantly. The surface is primarily in the initial plastic deformation stage, without the formation of a large-scale dislocation network, and the microstructure remains relatively stable. Therefore, 60 nN is considered the optimal external stress during the polishing process.

4. Results and analysis of polishing pressure on silicon wafer surface damage and material removal

4.1. Effect of applied external pressure on atomic removal from rough surfaces

Surface roughness is a key parameter for evaluating the quality of polished silicon wafer surfaces, as it effectively reflects surface flatness. To quantitatively assess surface roughness, OVITO is employed to extract the atomic coordinates of the wafer surface, and the S_a value is subsequently calculated in MATLAB based on the principles of three-dimensional roughness evaluation. Additionally, the influence of external pressure on surface roughness is investigated by analyzing the corresponding surface morphology contour maps. Fig. 5 illustrates the effect of external pressure on both the surface roughness and morphology of the silicon wafers.

As shown in the surface roughness curve under applied external stress in Fig. 5(a), with the increase in applied external stress, the surface roughness S_a of the silicon wafer exhibits a distinct nonlinear trend. When the applied normal stress is $P = 0$ nN, the surface roughness is at its highest, with a value of $S_a = 9.661$ nm. As the external stress increases to 60 nN, the roughness significantly decreases to the minimum value of 6.310 nm. Further increasing the external stress to 120 nN and 180 nN causes the roughness to rise again, reaching 6.975 nm and 8.178 nm, respectively, showing a trend of first decreasing and then increasing. This change trend indicates that external stress has a significant regulatory effect on the surface atomic structure. At $P = 0$ nN, the surface atoms are loosely arranged, with noticeable local protrusions and depressions, leading to higher roughness. At $P = 60$ nN, the surface atoms tend to become more compact due to elastic compression and local plastic slip, resulting in a smoother surface and a significant decrease in S_a . As the external stress continues to increase, the stress exceeds the threshold of the local bonding energy, triggering atomic rearrangement that induces surface warping and piling, causing the roughness to rise again. Fig. 5(b) shows the average height curves of the polished surface. The trend in average height is the opposite of the roughness trend, forming an inverted “V” shape. At $P = 60$ nN, the average height is highest, at 119.19 Å. This suggests a nonlinear relationship between applied pressure and surface morphology. Fig. 5(c) compares surface roughness maps under four different pressures. These maps visually show height distribution, with red and blue areas representing raised and recessed regions, respectively. At 0 nN, the surface shows significant peaks and valleys, resulting in higher roughness. At $P = 60$ nN, the polished surface has fewer recessed areas compared to the other pressures, with no significant peaks. The surface appears overall smooth, consistent with the lowest roughness observed in Fig. 5(a).

Conversely, at $P = 120$ and 180 nN, the ratio of recessed to raised areas is about 1:2, with noticeable peaks and surface undulations. The changes in surface morphology under different pressures can be attributed to atomic rearrangement and interactions caused by external forces. In summary, when $P = 60$ nN, the external stress effectively reduces the surface roughness and optimizes the surface morphology. However, when the external stress further increases and exceeds the stress tolerance of the local structure, atomic disorder and local accumulation occur, leading to an increase in surface roughness. Therefore, the external stress regulates the nonlinear response characteristics of surface structural evolution within a certain range.

To provide a clearer understanding of the changes in surface atomic removal, the removal patterns are explained through variations in the number of abrasive particles. Fig. 6 illustrates the changes in the number of amorphized atoms under different pressures during the polishing process.

Fig. 6(a) shows the trend of the number of “other” type atoms during polishing under different pressure conditions. As the polishing distance increases, the number of “other” type atoms rises, influenced by stress-induced atomic migration, local bond breakage, and lattice reconstruction. Under low external stress conditions, plastic deformation dominates, with dislocation slip and shear band formation leading to atomic amorphization and lattice instability, which promotes a rapid increase in “other” atoms. However, as the external stress increases, the removal mechanism shifts from plastic flow to brittle fracture, and the material removal mode transitions from continuous wear to microfracture, suppressing the accumulation of lattice distortion and slowing the generation of “other” type atoms. Within the 0–5 nm polishing distance range, the abrasive particles are in the indentation area. The movement of the particles to the right resembles the indentation unloading process. Fig. 6(b) displays the trend of “other” type atoms in the silicon wafer model during unloading-like processes under different pressures. In the initial stage, the number of “other” type atoms increases rapidly, reaching a peak before decreasing slowly. After 5 nm, in the pure friction polishing zone, the growth rate of “other” type atoms accelerates. In the unloading-like process, as shown in the structural analysis maps at the peaks for pressures A–D, the first peak occurs at 1.8 nm for 0 nN, and at 2.25 nm for pressures of 60 nN, 120 nN, and 180 nN. At this stage, as the particles move, surface atoms experience tangential forces along the x-axis, causing atomic bonds to break and changes in the lattice structure, which leads to an increase in “other” atoms. After reaching the peak, the number of “other” type atoms gradually decreases. This decrease is due to the elastic recovery of atoms in the indentation area, bond restoration, and structure reformation. Additionally, because of the surface’s unevenness, abrasive particles settle in lower areas, reducing damage to the atomic structure. Fig. 6(c) illustrates the changes in “other” type atoms during pure friction polishing. The enlarged section of the curve shows that at 16 nm, the trend of “other” type atoms changes under four pressures. Before 16 nm, the number of “other” type atoms increases with polishing distance and decreases with increasing pressure. After 16 nm, although the number of atoms continues to increase, the growth rate significantly slows down at 60 nN. Analysis of the crystal structure maps shows that at 60 nN, the number of “other” type atoms is lower compared to the other pressures, indicating less structural damage in the material. This suggests that appropriate pressure helps reduce material damage. As pressure increases, atomic interactions intensify, leading to greater structural damage and an increase in “other” type atoms. However, the rate of increase slightly diminishes with higher pressure, indicating that material damage tends to saturate within a certain pressure range.

4.2. Effect of applied external pressure on the subsurface

To evaluate wafer quality, besides surface roughness, subsurface damage is also a critical factor affecting material performance. By analyzing the subsurface damage in silicon wafer specimens, the optimal pressure condition for maintaining high quality can be determined.

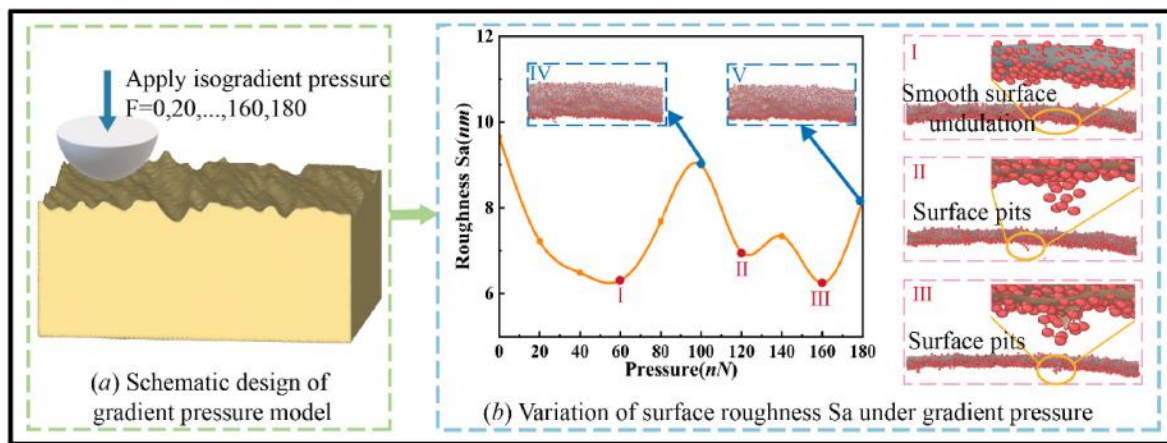


Fig. 3. Surface damage analysis of silicon wafer polishing experiment under gradient external stress. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

Fig. 7 illustrates the variations in dislocation number and length, as well as the evolution of dislocations under different pressures.

Fig. 7(a) illustrates the variation in the total number of dislocations under four different pressure conditions. Overall, dislocation numbers increase with the polishing distance under all pressure conditions. This phenomenon occurs because, as the polishing distance increases, abrasive particles accumulate around the primary abrasive, generating a reactive force. Consequently, the normal load on the surface rises, causing subsurface stress concentration and leading to the nucleation and propagation of dislocations. A significant fluctuation in dislocation numbers is observed at a polishing distance of 14.25 nm. Analyzing dislocation evolution, Fig. 7 I shows two types of dislocations: $1/3\langle 1-100 \rangle$ and Other, with Other-type dislocations being predominant and exhibiting clear ring formations. This indicates dislocation expansion and slip in the region, which makes it prone to crack formation. Fig. 7 II and III also display two types of dislocations: $1/3\langle 1-210 \rangle$ and Other. Dislocation numbers and lengths are greater in Fig. 7 III than in Fig. 7 II, indicating more extensive plastic deformation and severe subsurface damage at 120 nN, which significantly degrades silicon wafer performance. Although Fig. 7 IV shows no dislocations, the subsurface morphology indicates the presence of slip planes and cracks, which also impact wafer performance. Under 60 nN pressure, dislocation numbers fluctuate within a narrow range after a polishing distance of 14.25 nm. Fig. 7(b) shows the change in dislocation length under different pressures. Before a polishing distance of 16.65 nm, dislocation lengths generally increase, reflecting plastic deformation due to stress accumulation. After reaching 16.65 nm, dislocation lengths decrease at 60 nN and 120 nN, indicating stress release or recovery to a more stable state. The sudden change in dislocation length is analyzed using the cloud maps of dislocation types and lengths at points A-D. At point A, a valley is observed with a polishing distance of 15.75 nm, where dislocation lengths increase thereafter. Fig. 7 A shows changes in dislocation types and lengths, with three dislocations of type Other at 15.75 nm, and a type change to $1/3\langle 1-100 \rangle$ at 15.9 nm. The longest dislocation also changes from Other to $1/3\langle 1-210 \rangle$. This indicates an increase in Other-type dislocation lengths and the formation of small ring-like dislocations after breaking. At point B under 60 nN, dislocation lengths peak and then gradually decrease. Fig. 7 B shows all dislocations change types, with all becoming Other at 17.25 nm and then changing to $1/3\langle 1-100 \rangle$ and $1/3\langle 1-210 \rangle$ at 17.4 nm. The length of the ring dislocations also decreases, consistent with the data curve, indicating structural stabilization after reaching the peak. Points C and D, both at peak positions, show a faster reduction in dislocation length at 120 nN. In both cases, no change in dislocation types is observed. At 120 nN, dislocation numbers and lengths decrease, while at 180 nN, dislocation breakage and length reduction are evident. In summary, at 60 nN, dislocation numbers

increase steadily with polishing distance, with lengths gradually shortening and transitioning to a more stable state through elastic-plastic deformation.

The relationship between dislocations and phase-changing atoms is interdependent. Dislocation movement and expansion can induce phase transformations, while changes in crystal structure due to phase transitions can influence dislocation behavior and distribution. To assess subsurface damage in silicon wafers under various pressures, the evolution of crystal structure is analyzed from the perspective of atomic phase changes. Fig. 8 illustrates the changes in crystal structure under different external pressure conditions.

Fig. 8(a) shows the distribution of hexagonal diamond structure atoms under different external stresses (0 nN, 60 nN, 120 nN, and 180 nN), clearly presented as a bee swarm plot. At external stresses of 60 nN and 180 nN, the distribution of hexagonal diamond structure atoms is compact and relatively low, while at 0 nN and 120 nN, the distribution is more dispersed and higher. The number of hexagonal diamond structure atoms is counted along the current trajectory at intervals of 0.75 nm within a total polishing distance of 22.5 nm. Each data point represents the number of hexagonal diamond atoms at a specific polishing depth. The distribution density of these points reflects the evolution of the hexagonal diamond structure. Sparse distribution indicates significant changes in atom types and unstable crystal structure. In contrast, dense distribution shows minor changes in atom types and a more stable crystal structure. As the external stress increases, the number of hexagonal diamond structure atoms fluctuates markedly, indicating a phase transition or structural reorganization of atomic structures under stress. This is likely due to crystal distortion induced by external stress, altering atomic distances and triggering a transformation from hexagonal diamond to other crystal structures. Analyzing the number distribution curves further, under 60 nN and 180 nN, the fluctuation range of hexagonal diamond structure atoms is relatively smooth, showing a gradual increase. In contrast, under 0 nN and 120 nN, the number of hexagonal diamond atoms decreases as polishing distance increases, exhibiting larger fluctuations, consistent with the trends shown in the bee swarm plot. By comparing the changes in subsurface damage in silicon wafers under 60 nN and 180 nN external stresses, variations in the material's internal crystal structure are analyzed. As shown in Fig. 8(b), under 60 nN external stress, the thickness of the subsurface damage layer decreases with increasing polishing distance. At 16.5 nm, the maximum subsurface damage thickness is 4.3 nm, while at 22.5 nm, it decreases to 4.0 nm. Under 180 nN external stress, the subsurface damage layer thickens as polishing distance increases. At 16.5 nm, the maximum subsurface damage thickness is 4.0 nm, while at 22.5 nm, it increases to 4.5 nm. This suggests that under 60 nN external stress, atomic rearrangement occurs, leading to elastic deformation and a reduction in

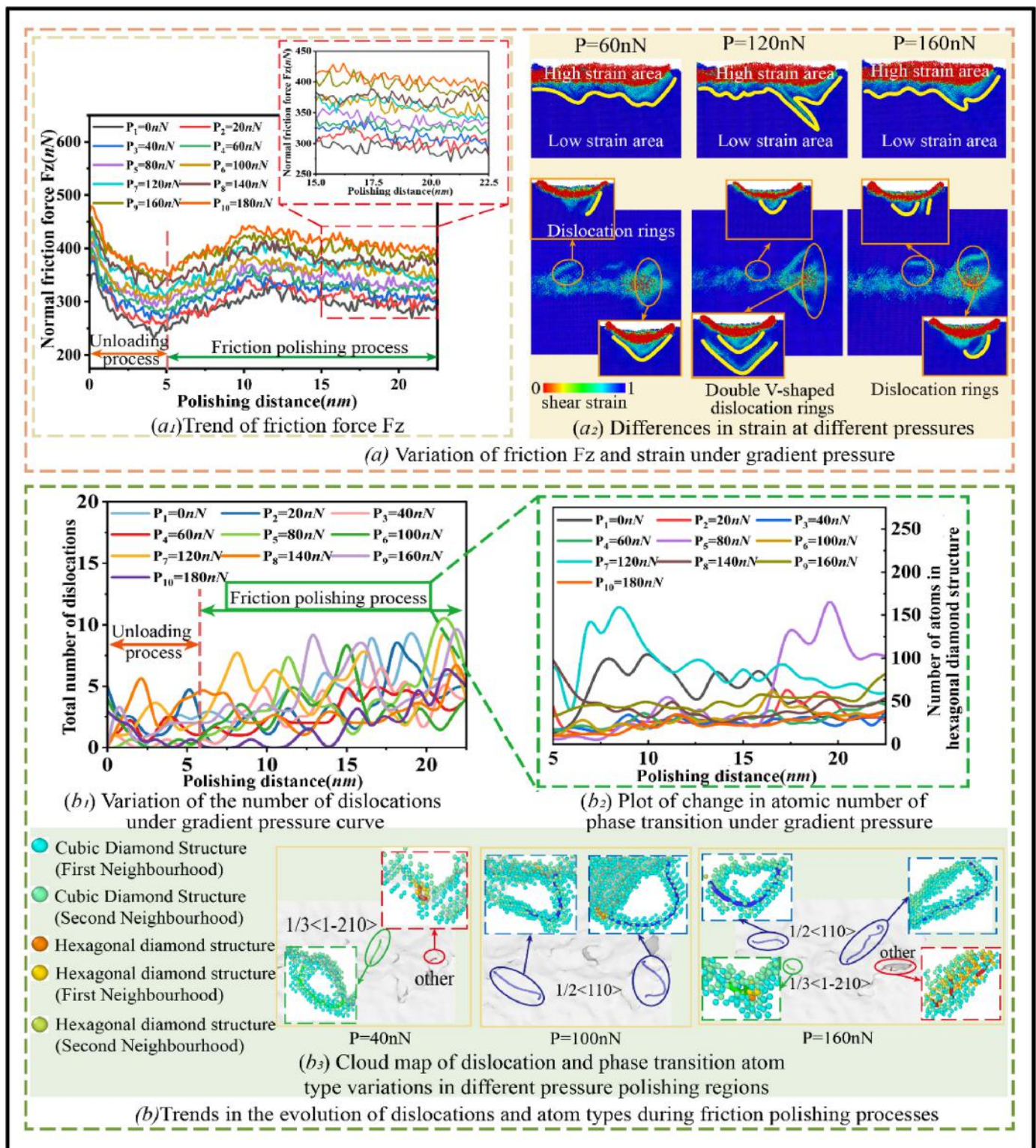


Fig. 4. Subsurface damage analysis of silicon wafer polishing experiment under gradient external stress. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

damage layer thickness, which has a reduced impact on material performance. The formation of the damage layer may be associated with atomic phase transitions, where stress-induced crystal structure changes lead to atomic rearrangements, forming new phases or defect structures. Comparing the changes in dislocations and phase transition atoms (red circles) and analyzing the top-down view of subsurface dislocations and phase transition atom distribution in Fig. 8(c) provides further insight.

Under 60 nN external stress, some atoms in the left red box transition from cubic diamond to hexagonal diamond structure, and the number of hexagonal diamond structure atoms increases with polishing distance. Concurrently, a $1/3\langle 1-100 \rangle$ dislocation type is generated. In the right box, some hexagonal diamond atoms transition back to cubic diamond, causing dislocation changes. Two $1/3\langle 1-210 \rangle$ dislocation lines, represented by green dislocations, either disappear or shorten, and Other-

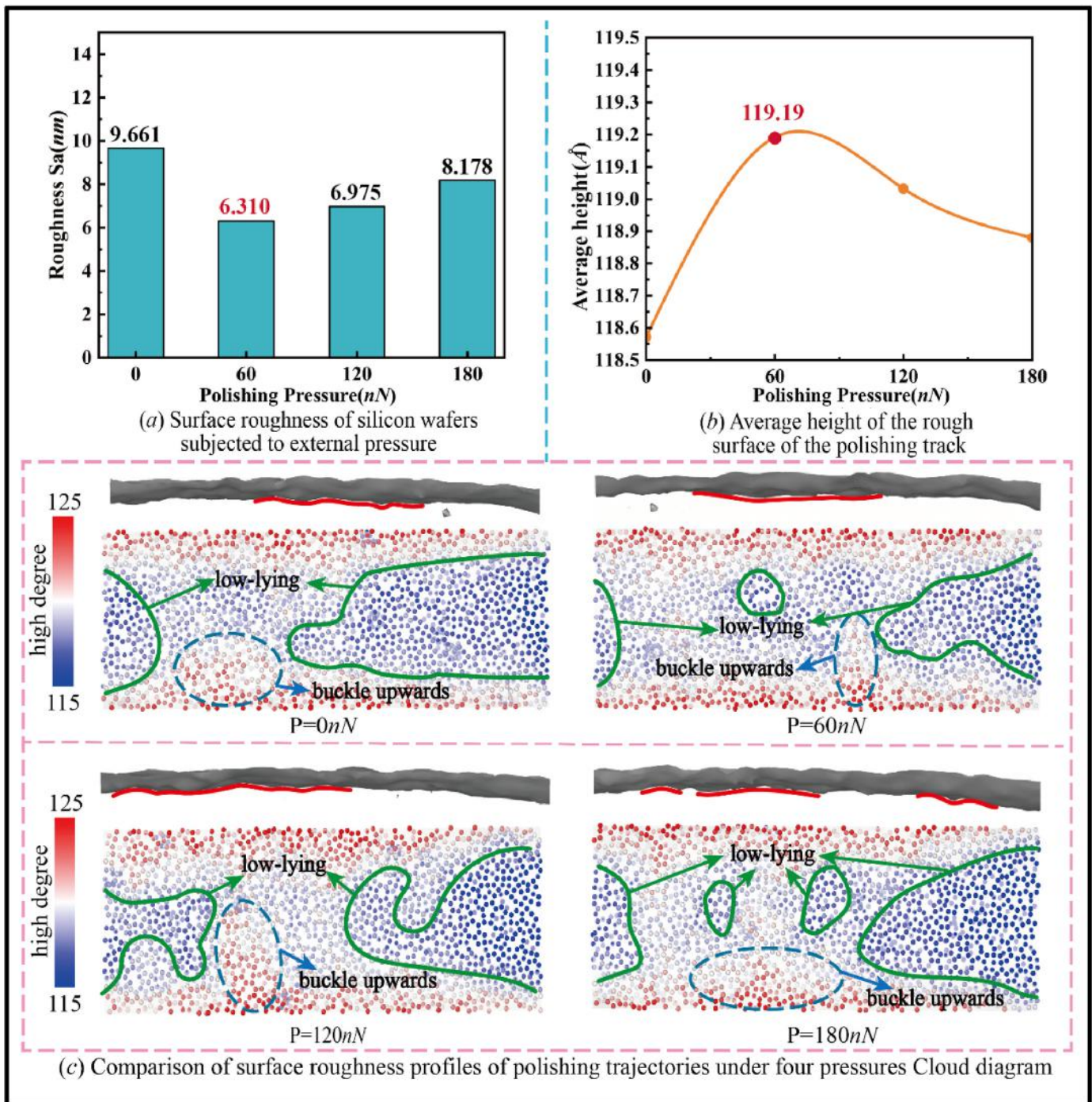


Fig. 5. Effect of external pressure on surface roughness and surface topography of silicon wafers. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

type dislocations vanish. Under 180 nN external stress, the number of hexagonal diamond structure atoms in the left red box increases with polishing distance, and Other-type dislocations disappear. Overall, under 60 nN external stress, as polishing distance increases, the sub-surface damage layer thickness decreases, and crystal structure phase transitions lead to dislocation formation and changes. Internal damage in the material gradually decreases, suggesting that this stress has a minor impact on material performance, beneficial for optimizing the polishing process.

4.3. Analysis of the change of friction under external pressure

Friction is a force that resists the relative motion between two contacting surfaces. It generates internal stress within the material through interface interactions, leading to deformation (strain). In molecular dynamics simulations, friction not only influences the stress distribution at the interface but also affects the internal stress-strain state of the material by transmitting stress. Fig. 9 illustrates the relationship between the normal friction force (F_z) and the tangential friction force (F_x) along the x-axis as a function of friction distance under different normal load conditions.

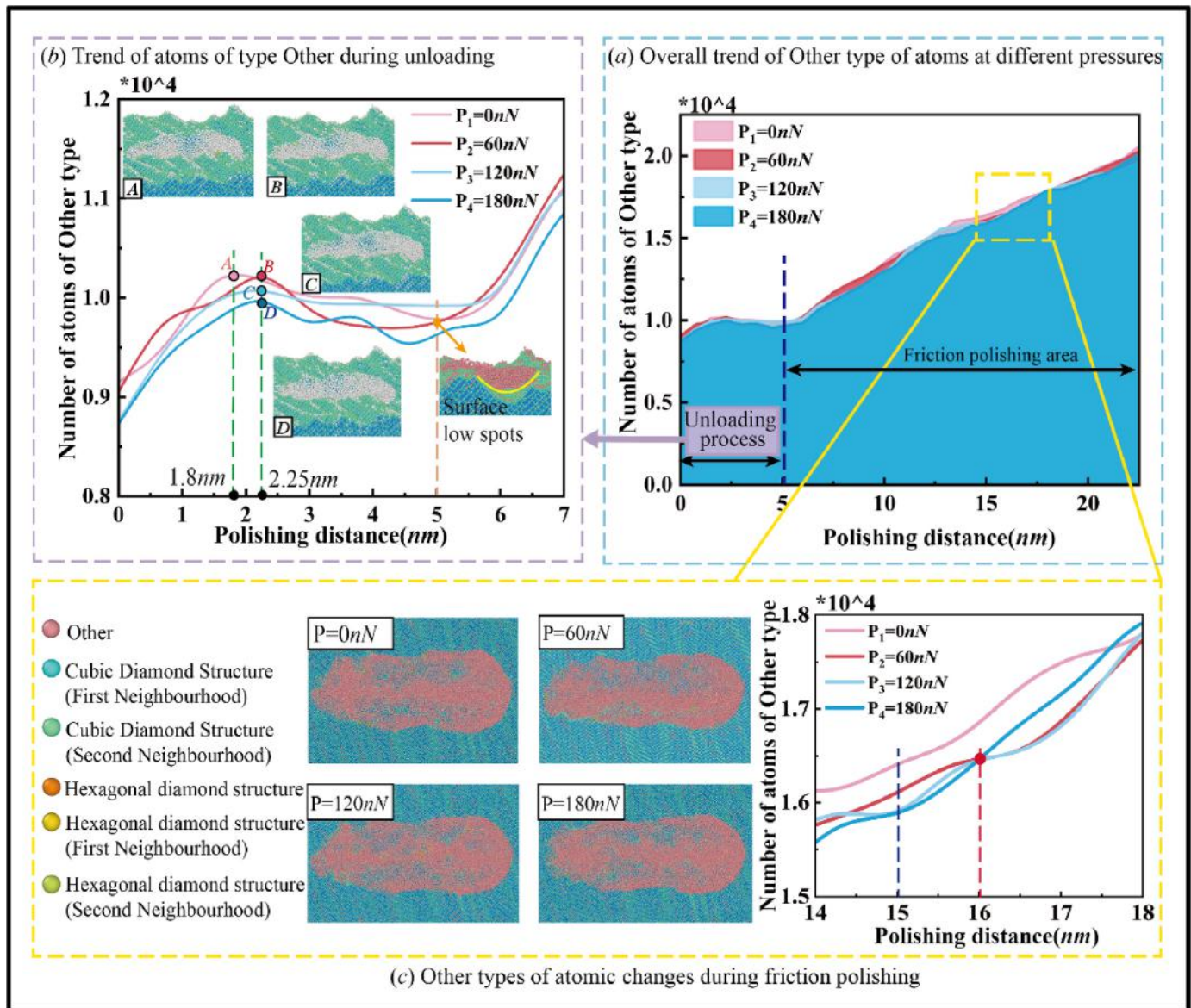


Fig. 6. Changes in the number of amorphized atoms under different pressures during polishing.

Fig. 9(a) exhibits the curve of normal friction F_z with friction distance under different external pressure conditions, while Fig. 9(b) shows the trend of the corresponding tangential friction F_x . From a molecular dynamics point of view, during friction simulations along the x-axis direction, the applied normal force affects the arrangement of atoms or molecules and the microstructure of the contact interface. As the normal pressure increases, the distance between atoms at the contact interface decreases, and the interaction between atoms intensifies, leading to an increase in normal friction. At the same time, higher normal pressure also increases the actual contact area between the interfaces, thereby affecting the performance of tangential friction. Fig. 9(a) shows that under different pressure conditions, as the friction distance increases, the normal friction force first decreases and then stabilizes. This may be related to the initial running-in process of the material surface morphology. Over a small friction distance, the normal friction force decreases rapidly due to modifications in surface roughness and adjustments in the initial contact area, and then stabilizes after a certain distance. Fig. 9(b) shows the variation trend of tangential friction force with friction distance under the same conditions. It can be observed that the tangential friction increases rapidly in the initial stage and then

gradually reaches equilibrium as the friction distance increases. This trend indicates that tangential friction is mainly influenced by interfacial shear deformation and dislocation slip within the material. As friction proceeds, plastic deformation and microstructural adjustment of the surface occur, leading to a gradual stabilization of the tangential friction. Dai et al. [28] have shown that shear stress plays a crucial role during the polishing process and significantly affects both the surface and subsurface quality of the workpiece. The normal friction, F_z , increases as the applied pressure increases, which is attributed to the fact that higher pressure leads to a decrease in the interatomic spacing between the contacting interfaces and an increase in the interatomic interaction force, as well as an increase in the contact area. Higher pressures also increase the tangential friction, which is due to the fact that the increase in normal pressure enhances the atomic contact between the interfaces, leading to an increase in shear stress and thus a rise in tangential friction. This is basically similar to the findings of the study by Dai et al. The initial decrease and subsequent stabilization of normal friction, as well as the initial increase and subsequent equilibrium of tangential friction, reflect the adjustment and stabilization of the microstructure of the material surface during friction.

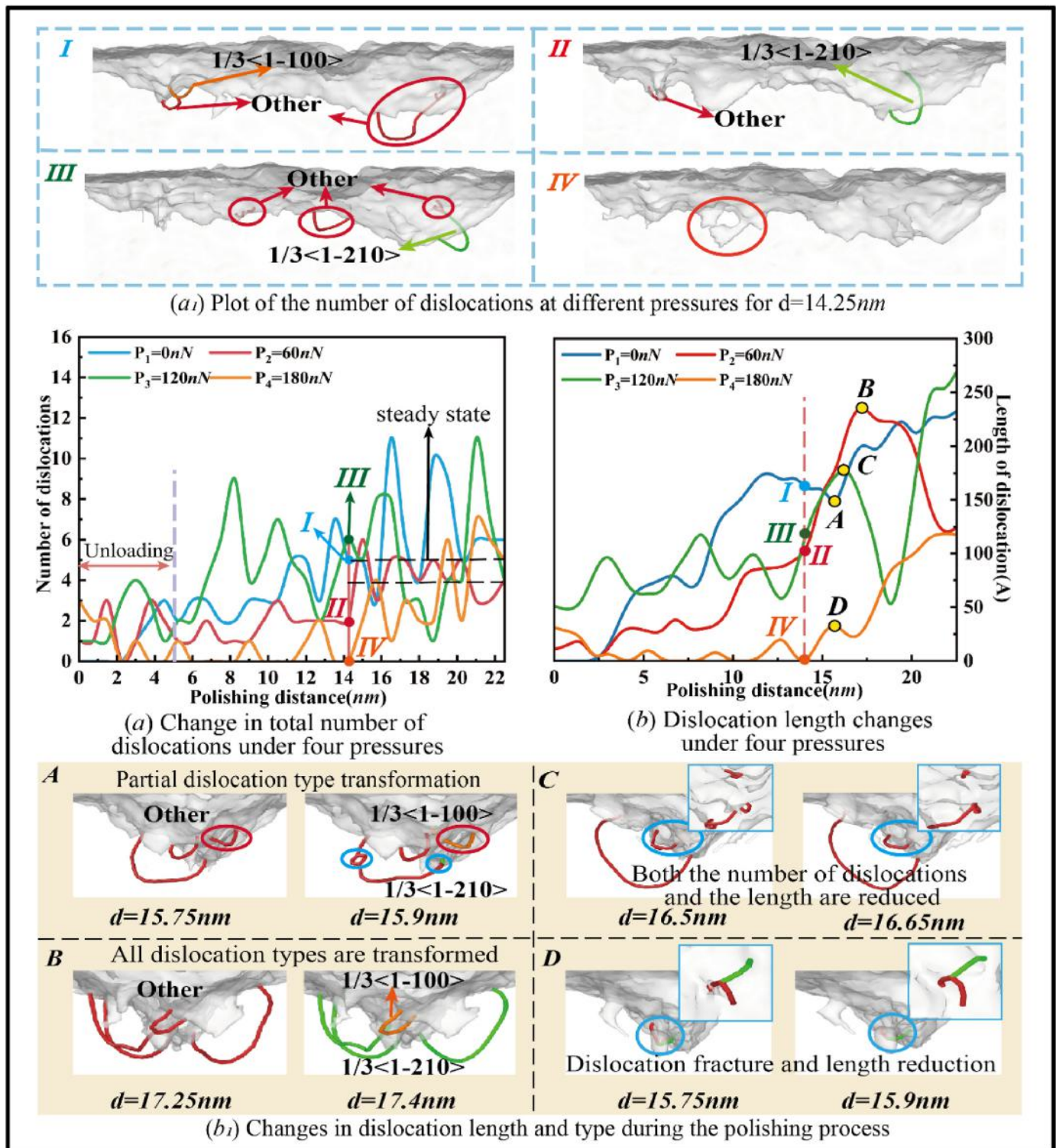


Fig. 7. Changes in the number and length of dislocations and dislocation evolution under different pressures.

Stress refers to the force generated inside a material under the action of an external force, while strain is the deformation of a material under the action of stress. Under the action of friction, the friction force on the contact surface will cause shear stress, which will cause local strain on the surface of the material and inside it.

The series of images in Fig. 10 show the evolution of stress and strain of a silicon wafer in a molecular dynamics simulation under different external pressures ($P = 0\text{ nN}$, 60 nN , 120 nN , 180 nN).

The top view on the left displays the distribution of shear strain, with colors ranging from blue to red indicating low to high strain levels. The distribution of strain concentration areas changes significantly with increasing applied pressure, suggesting that at higher normal forces, the regions of strain concentration within the material tend to expand and deepen. The image on the right provides the corresponding side view, showing that as the normal force increases, the position and shape of shear deformation change, leading to a greater number of dislocation

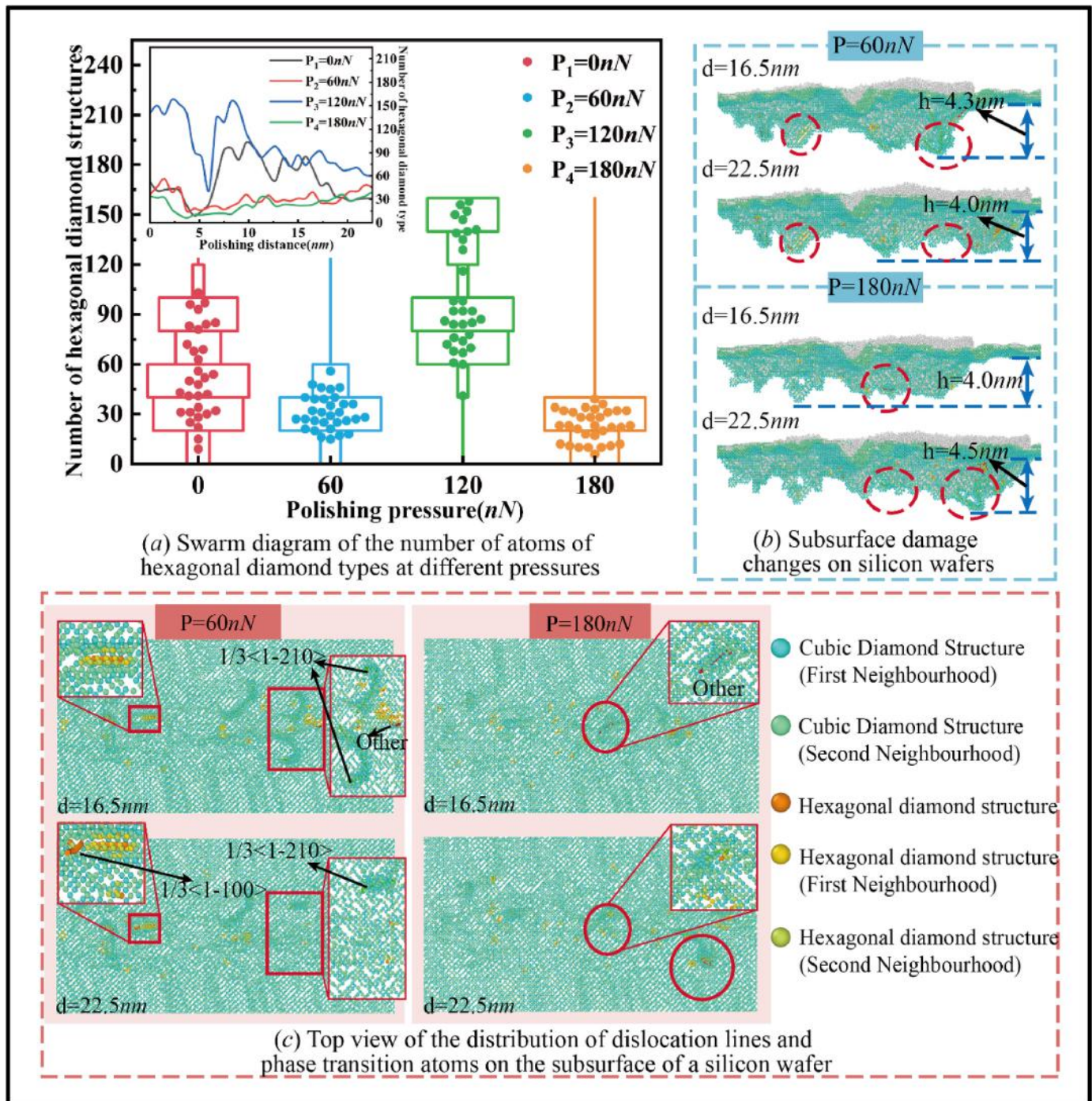


Fig. 8. Evolution of crystal structure under applied external pressure conditions.

slip bands. The shape and distribution of these slip bands exhibit significant evolution with increasing normal force. For example, at $P = 0\text{ nN}$, dislocation slip bands appear only in the surface layer. However, at $P = 180\text{ nN}$, dislocation slip bands penetrate into the material's interior, forming more complex shapes. This phenomenon can be explained by the stress concentration effect. As the normal force increases, the strain energy in the stress concentration areas within the material rises, leading to more dislocation slip and changes in the internal structure. These results indicate that variations in normal force significantly affect the stress-strain response of the material in molecular dynamics simulations, thereby impacting the material's microstructure.

4.4. Effect of gradient pressure on mechanical properties of silicon wafers

The radial distribution function (RDF) and atomic bonding characteristics play a critical role in determining material properties. The position and height of RDF peaks indicate the average interatomic distances and the degree of local structural order. Moreover, atomic bond strength and bond length directly influence material hardness and elastic modulus. Therefore, analyzing the RDF and atomic bonding behavior offers valuable insights into the effects of varying pressures on the performance of silicon wafers. As shown in Fig. 11, the radial distribution function and atomic bond changes during polishing.

Fig. 11 depicts the variation of radial distribution function (RDF) and

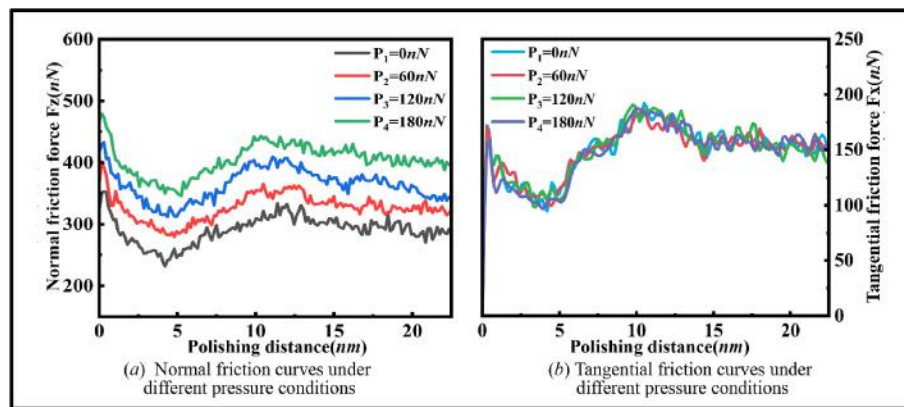


Fig. 9. Changes in friction under different pressure conditions.

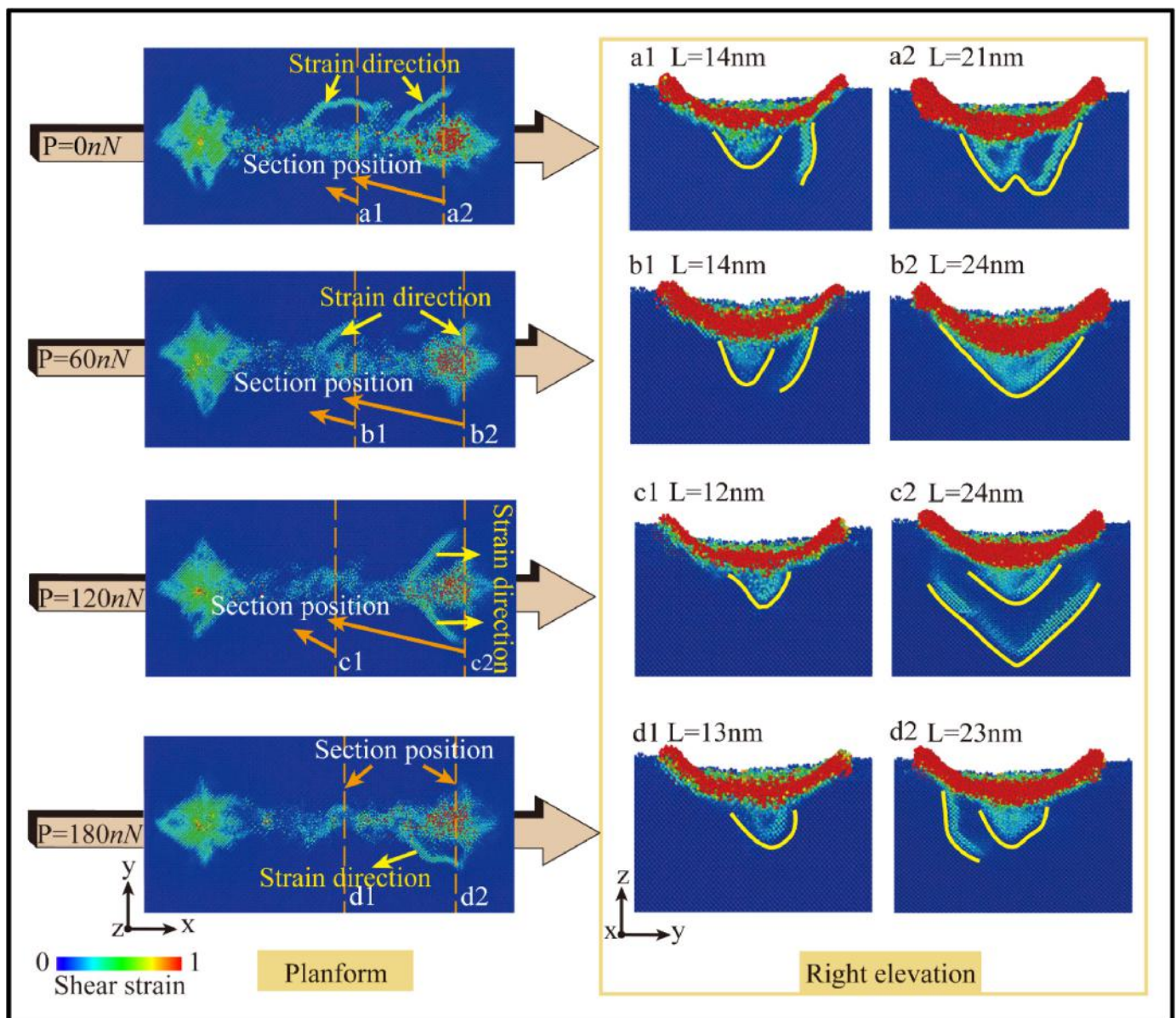


Fig. 10. Evolution of shear strain under different pressures.

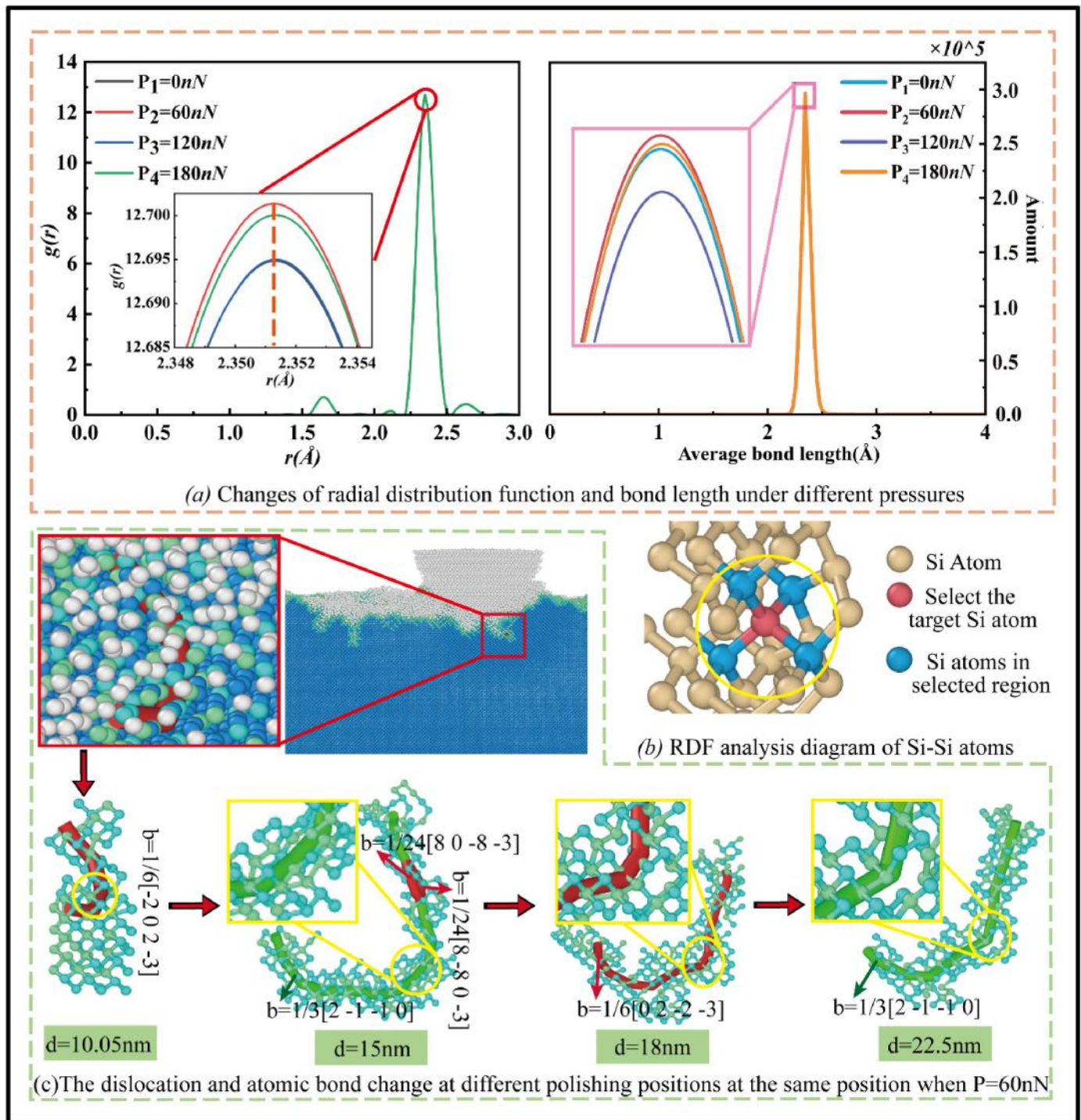


Fig. 11. Radial distribution function and atomic bond changes during polishing.

atomic bond lengths obtained from molecular dynamics simulations of the system at different pressures. First, in Fig. 11 (a), the trends of radial distribution function $g(r)$ and average bond length under different pressure conditions ($P_1 = 0\text{ nN}$, $P_2 = 60\text{ nN}$, $P_3 = 120\text{ nN}$, and $P_4 = 180\text{ nN}$) are demonstrated. Overall, the peaks of $g(r)$ are all at a truncation radius of $2.351\text{ \AA}$ and the average bond length of the silicon atoms is also $2.35\text{ \AA}$. The average bond length of the silicon atoms is also $2.35\text{ \AA}$. Tian et al. [29] studied the formation mechanism of subsurface damage in single-crystal silicon during nano-grinding and concluded that the perfect bond length of single-crystal silicon is 0.235 nm , which is consistent with the results of this study. As the pressure increases, the peak of $g(r)$

shows an increase and then a decrease, indicating that the atomic spacing changes with the pressure, which leads to a change in the local structure. The peak value of $g(r)$ is highest at a pressure of 60 nN , indicating that the crystal structure of the silicon wafer is in the diamond structure at this pressure, and fewer atoms undergo structural changes, so the lower the damage caused to the silicon wafer. Fig. 11 (b) further demonstrates a schematic of the RDF analysis of the Si-Si atoms, with a zoomed-in detail view of the arrangement of Si atoms in a particular region, highlighting the changes in the interactions between these atoms under different pressures. Fig. 11 (c) shows the dislocation changes and bond length evolution of atoms in different initial positions during the

stretching process when a pressure of 60 nN is applied. At a smaller friction distance, the Burgers vector of the dislocation line is $b = 1/6[-2\ 0\ 2-3]$. At this time, the local Si-Si bond shows a slight change, and the atomic arrangement is still relatively complete. The dislocation has not yet slipped on a large scale, so the local plastic deformation is relatively slight and the change in atomic spacing is not obvious. When the friction distance increases to 15 nm, the dislocation vector changes to $b = 1/6[0\ 2\ -2\ -3]$, and the dislocation begins to extend significantly between the surrounding atomic layers, showing the slip path of the dislocation line in the lattice. At the same time, the local atomic bond length further increased, indicating that at this friction distance, a significant reorganization of the atomic arrangement occurred inside the material. As the friction distance increases further, the dislocation vector becomes $b = 1/3[2\ -1\ -1\ 0]$, the dislocation continues to extend to more atomic layers, and the dislocation line further extends along the lattice direction. At this time, the deformation of atomic bonds is more severe, and the increase in bond length reflects the further development of stress concentration areas inside the material, and the interaction force between atoms is significantly enhanced. At the maximum friction distance of 22.5 nm, the dislocation vector becomes $b = 1/6[-2\ 0\ 2-3]$, and the dislocation has penetrated multiple atomic layers, showing significant slip and deformation. At this point, the atomic bond lengths increase significantly and violent plastic deformation occurs within the material, indicating that the material structure has reached its limit of change under external forces. At a pressure of 60 nN, the radial distribution function $g(r)$ and the atomic bond lengths of the silicon wafers show a relative stability of the crystal structure, and the slip and expansion of dislocations during friction lead to reorganization of the atomic arrangement and plastic deformation, but overall, the crystal structure of the silicon wafers under a pressure of 60 nN remains in a relatively stable state, with minimal damage to the material.

5. Conclusion

- (1) Using the diamond structure identification method, combined with the surface roughness morphology cloud map, friction force change curve and surface roughness angle analysis, with the increase of external stress, the surface roughness of the silicon wafer shows a nonlinear change trend, and the surface scratch morphology shows a "concave" shape evolution law. When 60 nN external stress is applied, the minimum roughness is 6.310 nm, and the degree of structural damage is the lowest. At this time, the surface scratch degree and subsurface damage rate of the silicon wafer are both low. There is literature by Guo et al. [30] to help verify the above experimental results.
- (2) By comparing the subsurface crystal structure type change curves under different external stress polishing, combined with the radial distribution function curve and shear strain cloud map, the strain expansion trend in the strain concentration area and the evolution mechanism of the subsurface "V"-shaped dislocation ring are analyzed. As the external stress increases, the shear strain expands and accumulates along the $\langle 110 \rangle$ and $\langle 1-10 \rangle$ crystal directions. The subsurface dislocation slip bands slip and increase along the strain expansion direction, gradually forming a "V"-shaped dislocation ring, thereby causing stress damage on the subsurface of the silicon wafer.

The subsurface external stress damage mechanism of nano-polished silicon wafers is revealed, providing key theoretical support and technical guidance for optimizing nano-scale processing technology.

CRediT authorship contribution statement

Jianbo Le: Writing – original draft, Methodology, Investigation.
Juan Liu: Writing – original draft, Formal analysis, Data curation. **Jian Liu:** Writing – original draft, Validation, Software. **Guiling Liu:**

Visualization, Project administration, Methodology. **Guoxing Tang:** Software, Resources, Conceptualization. **Nanxing Wu:** Writing – review & editing, Writing – original draft, Funding acquisition.

Data availability statement

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This study is sponsored by the projects found by the Opening Project of National Engineering Research Center for Domestic & Building Ceramics under Grants No. GXZX2305, the National Natural Science Foundation of China under Grants No. 51964022, the Key Project of Natural Science Foundation of Jiangxi Province under Grants No. 20212 A C B 204012 to which the authors are very grateful.

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