

**Nanoscale Mechanisms of Single-Asperity Contact,
Frictional Wear, and Particle Wear against Asperity
Walls in α -Quartz: A Molecular Dynamics Study**

Li Sheng

**Nanoscale Mechanisms of Single-Asperity Contact,
Frictional Wear, and Particle Wear against Asperity
Walls in α -Quartz: A Molecular Dynamics Study**

Doctoral Dissertation

by

Sheng Li

Department of Civil and Earth Resources Engineering, Graduate School
of Engineering, Kyoto University

This dissertation is submitted for the degree of

Doctor of Philosophy

© 2025

KYOTO UNIVERSITY

JAPAN

ACKNOWLEDGMENTS

令和7年、三十にして立つ。京大桂キャンパスにて、人生の歩みを進めました。

First and foremost, I extend my heartfelt gratitude to Prof. Eiichi Fukuyama for leading me to move from an engineering background to the fascinating world of seismology, a path I am determined to continue exploring in the future. Then, his unwavering guidance, sharp insights, and constant refinement of my research direction and attitude have profoundly shaped the way I approach scientific questions. One phrase he often repeated, *"Interpretation is important,"* has become a cornerstone of my research philosophy. I am also grateful to him for encouraging me to attend various international and domestic conferences—experiences that not only broaden my academic horizons but also allow me to meet like-minded peers. Those exchanges and friendships become the warm and healing parts of my life abroad, and I will cherish them always.

I would also like to sincerely thank Assistant Professor Yoshimitsu Nana for her continuous encouragement and support in both academics and daily life over the past three years. My heartfelt appreciation extends to Kyosuke Noda, Yasufumi Suehisa, Koyo Matsuda, and Kotaro Kusada, and the wonderful memories we shared in San Francisco and Washington D.C. are truly unforgettable. I am also grateful to lab mates Guohao Ma, Koki Morimoto, Ayane Kitagawa, and Naoya Ikuta for all the great moments we shared in the lab.

I am equally thankful to Associated Professor Fan Zhu, Dr. Zirui Lu, Dr. Jikai Sun and Dr. Tiannan Hu from Kyoto University, for their support in life. I appreciate the valuable academic exchanges with Jiayi Ye (ETH), Danyang Jiang (ETH), Dr. Xiaotian Ding (SUSTech), Dr. Ran Xu (TJU), Dr. Yang Chen (SYSU), Dr. Suifeng Wang (WHU), Jicheng Liu (XJTU), Zeyuan Wang (XJTU) and Yuhao Wu (XJTU). I am also grateful to Prof. Ling Xu (XJTU) and Associated Professor Tengyuan Zhao (XJTU) for their guidance and support in my academic journey.

Lastly, and most importantly, I wish to express my deepest gratitude to my parents, whose unconditional support and quiet strength have sustained me every step of the way. To my beloved fiancée, Dr. Mengya Tao, thank you for your constant companionship, your care, and your unwavering belief in me over the past seven years. Perhaps it was your quiet wish at Kiyomizu-dera a decade ago that led me to Kyoto University. Whatever it was, I am grateful that it brought me here, and I hope we can walk together and side by side, for all the years to come.

Computations were done using the supercomputer system at National Research Institute for Earth Science and Disaster Resilience. This work was supported by JST SPRING grant JPMJSP2110 and JSPS grant JP24KJ1375, JP23K22592, and JP22H01321.

ABSTRACT

This thesis aims to provide in-depth insights into the single-asperity contact mechanisms, as well as the single-asperity and single-particle friction wear mechanisms of rock materials at the nanoscale. To achieve the target, three-dimensional nonequilibrium molecular dynamics (MD) method was employed, using crystalline α -quartz, a common crustal mineral, as the representative material. Firstly, for clarifying the nanoscale contact mechanisms, the normal contact damage of a pair of α -quartz asperities was investigated under different asperity sizes and contact configurations (centrosymmetric contact and asymmetric contact). Moreover, the nanoscale simulation results in the centrosymmetric contact case were compared with macroscopic elastic and elastoplastic contact models in terms of the normal contact force versus interference distance to assess the multiscale applicability. Based on the simulation results, empirical contact models for the nanoscale single-asperity contact in centrosymmetric cases were also proposed. Then, for clarifying the single-asperity friction wear mechanisms, the wear damage and wear volume of a pair of α -quartz asperities were investigated under different normal forces and shear loading velocities at the plastic wear case. Then, the failure mode transition from plasticity to fracture of asperities was examined under varying normal forces, asperity sizes and contact configurations as well as two boundary conditions involving constant normal load and constant normal stiffness-like conditions. Additionally, the evolution of wear volume at the asperity fracture case was analyzed and the evolution of shear force was also compared in both plastic and fracture cases. Notably, a formula was introduced for predicting the wear volume under both plastic and fracture cases. Finally, for clarifying the single-particle friction wear mechanisms, the failure mode and wear volume of a single particle against asperity walls were investigated under the influence of the normal force, particle size, asperity interval, as well as particle location. Besides, the influence of particle wear failure mode on the shear force and friction coefficient was investigated. Based on the simulation results, the prediction of particle wear volume was also discussed.

TABLE OF CONTENTS

ACKNOWLEDGMENTS	I
ABSTRACT	II
TABLE OF CONTENTS	III
LIST OF FIGURES	VI
CHAPTER I	VI
CHAPTER II	VI
CHAPTER III	VI
CHAPTER IV	VII
CHAPTER V	VIII
CHAPTER VI	IX
CHAPTER VII	X
LIST OF TABELS	XI
CHAPTER III	XI
CHAPTER VI	XI
CHAPTER I: INTRODUCTION	1
1.1 RESEARCH BACKGROUND	2
1.2 LITERATURE REVIEW	3
1.2.1 Asperity contact theory	3
1.2.2 Frictional wear of asperity	7
1.2.3 Frictional wear of particles	9
1.3 LIMITATIONS OF PREVIOUS RESEARCH	11
1.3.1 Single-asperity contact	11
1.3.2 Single-asperity friction wear	11
1.3.3 Frictional wear of a single particle	12
1.4 RESEARCH OBJECTIVES AND CONTENT	12
CHAPTER II: MOLECULAR DYNAMICS METHOD	16
2.1 GOVERNING FUNCTION	17
2.2 POTENTIAL FUNCTION	17
2.2.1 α -Quartz	17
2.2.2 Vashishta potential	18
2.2.3 Verification	19
2.3 BOUNDARY CONDITION	20
2.4 CANONICAL ENSEMBLE (NVT)	21
2.5 VELOCITY VERLET ALGORITHM	24
CHAPTER III: CONTACT BEHAVIOR OF ASPERITIES	25
3.1 INTRODUCTION	26
3.2 NUMERICAL MODEL	26
3.3 SIMULATION PROCEDURE	28
3.4 NORMAL CONTACT FORCE	28
3.4.1 Centrosymmetric contact	30
3.4.2 Asymmetric contact	33

3.5 CONTACT DAMAGE	34
3.5.1 Centrosymmetric contact	34
3.5.2 Offset contact	37
3.6 DISCUSSION	40
3.7 CONCLUSION	42
APPENDICES	43
APPENDIX 3.A. EMPIRICAL CONTACT MODELS FROM MD SIMULATIONS.....	43
CHAPTER IV: PLASTIC WEAR MECHANISM OF ASPERITIES	47
4.1 INTRODUCTION	48
4.2 NUMERICAL MODEL	48
4.3 SIMULATION PROCEDURE	49
4.4 POTENTIAL FUNCTION VERIFICATION	50
4.5 DYNAMIC WEAR MECHANISM	51
4.6 COMPARISON WITH THE ARCHARD LAW	58
4.7 WEAR VOLUME PREDICTION	62
4.8 DISCUSSION	65
4.9 CONCLUSION	69
APPENDICES	70
APPENDIX 4.A: TANGENTIAL FORCE AND AVERAGED FORCE RATIO UNDER DIFFERENT ASPERITY SIZES AND HORIZONTAL LOCATIONS.	70
CHAPTER V: ASPERITY FAILURE MODE TRANSITION	73
5.1 INTRODUCTION	74
5.2 NUMERICAL MODEL	74
5.3 SIMULATION PROCEDURE	76
5.4 ASPERITY DAMAGE	76
5.4.1 CS-like condition.....	76
5.4.2 CL condition	81
5.5 FAILURE MODE TRANSITION PREDICTION	88
5.6 WEAR VOLUME PREDICTION	90
5.7 DISCUSSION	91
5.7.1 Comparison with prior nanoscale observation.....	91
5.7.2 Failure mode transition mechanism.....	92
5.7.3 Formation mechanism of vertical damage bands	94
5.7.4 Grooving and non-grooving mechanism.....	96
5.7.5 Friction evolution under different failure modes	98
5.8 CONCLUSION	99
CHAPTER VI: PARTICLE WEAR AND ITS ROLE IN FRICTION	101
6.1 INTRODUCTION	102
6.2 NUMERICAL MODEL	102
6.3 SIMULATION PROCEDURE	104
6.4 WEAR DAMAGE AND WEAR VOLUME OF PARTICLES.....	104
6.4.1 Computation results for Model 1	104

6.4.2 Computation results for Model 2	107
6.4.3 Computation results for Model 3	109
6.4.4 Computation results for Model 4	111
6.5 FRICTION COEFFICIENT	113
6.6 WEAR VOLUME PREDICTION	115
6.7 DISCUSSION	115
6.8 CONCLUSION	121
CHAPTER VII: DISCUSSION	123
7.1 ASPERITY CONTACT	124
7.2 ASPERITY FRICTION WEAR	125
7.3 PARTICLE FRICTION WEAR	127
7.4 COMPLEX GEOLOGICAL SETTINGS.....	128
CHAPTER VIII: CONCLUSION	130
REFERENCES.....	133

LIST OF FIGURES

Chapter I

Figure 1. 1. A brief illustration of the fault contact and friction process	3
Figure 1. 2. (a) Hertz elastic contact model of two spheres. (b) An explanation of the interference distance.	5
Figure 1. 3. A schematic overview of the main content in the thesis.....	15

Chapter II

Figure 2. 1. The schematic diagram of α -quartz crystal structure	18
Figure 2. 2. The schematic diagram of Periodic Boundary Conditions (PBC).....	21

Chapter III

Figure 3. 1. A schematic illustration of crystal structure of α -quartz and the contact configuration of asperities.....	27
Figure 3. 2. Stress-strain curve from uniaxial compression test in MD simulation	30
Figure 3. 3. The normal contact force F_n between MD simulations and four contact models (Hertz, CEB, ZMC, and KE) as a function of interference distance ω under different asperity radii.....	32
Figure 3. 4. The normal contact force under varying offset distances.....	33
Figure 3. 5. Four typical snapshots of von Mises shear strain.....	36
Figure 3. 6. The final breakage configurations of asperities at five different asperity radii.	37
Figure 3. 7. Four typical snapshots of damage evolution (von Mises shear strain) of asperities at an offset distance $\delta = R$ and asperity radius $R = 20a$	39
Figure 3. 8. The final breakage configurations for $R = 8a$ with varying offset distances	40
Figure 3. 9. The temperature of the system as a function of the normalized interference distance under varying asperity radii in centrosymmetric contact of asperities	41

Figure 3. 10. The normalized contact force and interference distance under varying asperity radii in centrosymmetric contact of asperities.....	42
---	----

Chapter IV

Figure 4. 1. A schematic illustration of the simulated material and model.....	49
Figure 4. 2. The evolution of tangential force and averaged force ratio.....	51
Figure 4. 3. The snapshots of wear processes under different normal forces at the loading velocities of 10 m/s and 40 m/s.....	53
Figure 4. 4. The snapshots of von Mises local shear strain at the loading velocity ranging from 10 to 40 m/s under different normal forces (1 nN, 2.57 nN, 5.13 nN, 8.98 nN, 11.55 nN)	55
Figure 4. 5. The snapshots of wear processes under different normal forces (3.85 nN ~17.96 nN) at the loading velocity of 10 m/s.	56
Figure 4. 6. The typical wear attrition mechanisms under (a) the low ($F_n = 2.57$ nN) and (b) the high normal force ($F_n = 19.25$ nN) at the loading velocity of 10 m/s and loading distance of 6 nm and 8 nm	57
Figure 4. 7. The wear volume and the specific wear rate under different F_n and V	60
Figure 4. 8. The total wear volume under different F_n and V	61
Figure 4. 9. The total wear volume under different loading velocities (10 m/s ~ 45 m/s) at the normal force (a) 1 nN, (b) 2.57 nN, (c) 5.13 nN, (d) 8.98 nN, and (e) 11.55 nN ($L \approx 8.125$ nm).....	62
Figure 4. 10. The tangential force, wear volume and tangential shear work with loading distance at 2.57 nN under the loading velocities of (a) 10 m/s, (b) 20 m/s, (c) 30 m/s, and (d) 40 m/s.	63
Figure 4. 11. The tangential force, wear volume and tangential shear work with loading distance at 11.55 nN under the loading velocities of (a) 10 m/s, (b) 20 m/s, (c) 30 m/s, and (d) 40 m/s.	64
Figure 4. 12. The wear volume and height as a function of shear work in simulations and experiments	64
Figure 4. 13. Contact length with loading distance 3 nm under different normal forces from 2.57 nN to 11.55 nN (front view).....	66

Figure 4. 14. Amorphous zone (red atoms) with loading distance 3 nm under different normal forces from 2.57 nN to 11.55 nN at $V = 10$ m/s (front view).....	66
Figure 4. 15. The typical change of vertical displacement under (a) the low (2.57 nN) and (b) the high normal forces (11.55 nN) respectively at the loading velocity from 10 m/s to 45 m/s.....	67
Figure 4. 16. Contact length with loading distance about 3 nm under different loading velocities V from 10 m/s to 45 m/s ($F_n = 2.57$ nN)	68

Chapter V

Figure 5. 1. (a) The crystal structure of α -quartz and (b) The contact configurations of asperities and boundary conditions.....	75
Figure 5. 2. Two typical cases involving plastic and fracture failure modes for the case of Case II ($\Delta H = R/2$) with $R = 12a$ (A-D) and $R = 15a$ (E-H).....	77
Figure 5. 3. Snapshots of asperity wear failure for the case of $\Delta H = R/2$ with R ranging from $3a$ to $16a$ ($a \sim l$) under CS-like condition, except for $R = 12a$ and $R = 15a$	78
Figure 5. 4. Typical cases involving plastic and fracture failure modes for Case I ($\Delta H = R$) with $R = 3a$ (A-B) and $R = 12a$ (C-F)	80
Figure 5. 5. Snapshots of asperity wear failure for the case of $\Delta H = R$ under CS-like condition, with R ranging from $4a$ to $11a$ ($a \sim h$)	81
Figure 5. 6. Representative cases of plastic and fracture failure modes at $R = 8a$ under $F_n = 20$ nN (AB) and 80 nN (CD), and plastic wear with initial internal damage at $R = 12a$ under $F_n = 120$ nN (EF) and 150 nN (GH)	83
Figure 5. 7. Snapshots of asperity wear failure for the case of $R = 8a$ under CL condition, subjected to normal forces ranging from 20 nN to 110 nN ($a \sim p$), except for 20 nN and 80 nN.....	85
Figure 5. 8. Snapshots of asperity wear failure for the case of $R = 12a$ under CL condition, subjected to normal forces ranging from 100 nN to 170 nN ($a \sim l$), except for 120 nN and 150 nN	86
Figure 5. 9. Snapshots of asperity wear failure for the case of $R = 4a$ under CL condition, subjected to normal forces ranging from 10 nN to 60 nN ($a \sim l$).....	87
Figure 5. 10. The conditions under which asperity plastic wear and fracture occur under CS-like condition (constant normal stiffness-like condition)	88

Figure 5. 11. The conditions under which asperity smoothing wear and fracture occur under CL condition	90
Figure 5. 12. The linear relationship between the total wear volume and tangential shear work for typical asperity fracture cases	91
Figure 5. 13. The normal force F_n (nN) as a function of loading distance L (nm) under the case of $R = 12a$ and $R = 16a$	95
Figure 5. 14. The contact profiles and damage band from two cases under Case II of CS-like condition	96
Figure 5. 15. Schematic illustration of asperity fracture modes	98
Figure 5. 16. The typical contact length measured at $R = 5a$ (Case I) and $R = 12a$ (Case II) under CS-like condition	98
Figure 5. 17. The tangential shear force (F_t) as a function of loading distance (L) under various asperity radius and contact configurations under CS-like condition for the case of (a) $\Delta H = R/2$ (Case I) and (b) $\Delta H = R$ (Case II)	99

Chapter VI

Figure 6. 1. Materials and simulation model.	103
Figure 6. 2. The typical wear processes of α -quartz particles in Model 1 under various normal forces (40 nN, 50 nN, and 60 nN, 70 nN) at the loading distance of about 75nm.	106
Figure 6. 3. The wear volume and specific wear rate versus loading distance for Model 1.....	106
Figure 6. 4. The typical wear processes of α -quartz particles in Model 2 under various normal forces (40 nN, 50 nN, 60 nN, and 70 nN) at the loading distance of about 75nm.	108
Figure 6. 5. The wear volume and specific wear rate versus loading distance for Model 2.....	108
Figure 6. 6. The typical wear processes of α -quartz particles under various normal forces (40 nN, 50 nN, 60 nN, and 70 nN) in Model 3 at the loading distance of about 75nm.	110
Figure 6. 7. The wear volume and specific wear rate versus loading distance for Model 3.....	110

Figure 6. 8. The typical wear processes of α -quartz particles under various normal forces (42.5 nN, 45 nN, 47.5 nN, and 50 nN) in Model 4 at the loading distance of about 75 nm.	112
Figure 6. 9. The wear volume and specific wear rate versus loading distance for Model 4.....	112
Figure 6. 10. The tangential shear force as a function of loading distance at the case of (a) Model 1; (c) Model 2; (e) Model 3. The averaged tangential shear force as a function of the normal force at the case of (b) Model 1; (d) Model 2; (f) Model 3.	114
Figure 6. 11. The wear volume and tangential shear work as a function of loading distance at typical wear cases for (a) Model 1, (b) Model 2, (c) Model 1 and (d) Model 4.....	115
Figure 6. 12. The contact length under different normal forces in Model 2.....	116
Figure 6. 13. The Von Mises shear strain of the typical cases of particle fracture for (a) $F_n = 65\text{nN}$ and (b) 70 nN of Model 1 and (c) $F_n = 60\text{nN}$ and (d) 70 nN for Model 3.	117
Figure 6. 14. The typical wear surface morphology and critical loading distance of nanoscale α -quartz particles under (a) Model 1 for $F_n = 70\text{ nN}$; (b) Model 3 for 60 nN; (c) Model 3 for 65 nN; (d) Model 3 for 70 nN	118
Figure 6. 15. The typical fragment motion after fracture under the normal force of 70 nN for two typical cases. (a) Case 1 is observed in Model 1 and (b) Case 2 is observed in Model 3	120
Figure 6. 16. The simulation box height as a function of loading distance at the case of Model 1 between $F_n = 35\text{ nN}$ and 70 nN.	121

Chapter VII

Figure 7. 1. The non-spherical asperities and fractal surface.....	125
Figure 7. 2. Multiple gouge particles with different sizes between rocks.	128
Figure 7. 3. Typical geological materials, along with gas and fluid molecules.	129

LIST OF TABELS

Chapter III

Table 3. 1. Mechanical parameters in the Hertz, CEB, ZMC and KE models.....	29
---	----

Chapter VI

Table 6. 1. The model description and simulation parameters.....	104
Table 6. 2. The critical sliding distance (L_c) from Model 1 to Model 4 under different normal forces (F_n).	113
Table 6. 3. The average w_s in stable and sub-stable wear modes from Model 1 to Model 4.....	113
Table 6. 4. The average μ_a in the linear increase stage from Model 1 to Mode 3	114

CHAPTER I

Introduction

1.1 Research Background

Crustal earthquakes, among the most devastating natural disasters globally, have caused immense casualties and economic losses throughout history (Pitarka et al., 1998; Fukuyama et al., 2007; Koketsu and Miyake, 2008; Jia et al., 2023). Currently, it is widely accepted that these events originate from frictional instabilities along faults (Brace and Byerlee, 1966; Scholz, 1998). Therefore, clarifying the mechanisms of fault friction has become a cornerstone to investigate earthquake source physics.

However, uncovering fault friction mechanisms requires close attention to asperity-scale processes on fault surfaces instead of focusing solely on macroscopic slip behavior such as friction curves (Marone, 1998). In particular, it demands a deep understanding of at least three key aspects: asperity contact behavior, asperity wear behavior, and the wear behavior of gouge particles with asperities. This lies in the fact that fault surfaces are generally rough, with the nominal contact area composed of multiple and multiscale asperities (Figure 1.1a). In the initial stage prior to fault slip (Figure 1.1b), asperities can compress each other to form contact points when tectonic forces act on the fault surfaces. At this stage, the interaction between asperities can result in normal contact-induced deformation including plastic yielding or fracture (Stesky & Hannan, 1989), which directly affects the static friction of the fault as resistance to initial sliding is transmitted from these contact points. Therefore, this underscores the importance of investigating the first key aspect.

Furthermore, as fault slip initiates upon the overcoming of shear resistance, asperities experience frictional collisions that induce wear through plastic deformation, fracture, and material removal (Figure 1.1c) (De Paola, 2013). The wear damage can dynamically alter fault strength by degrading asperities, thus playing a crucial role in dynamic friction properties of faults. In addition, asperity wear can generate gouge particles (Hirose et al., 2012), which actively participate in frictional process and undergo progressive wear (Figure 1.1d). The wear can alter the geometry of particles and promote breakage, significantly affecting force transmission along the fault and

contributing to the dynamic evolution of fault friction. Here, these dynamic wear processes of asperities and particles that occur during friction further underscore the importance of investigating the asperity wear and the wear behavior of gouge particles with asperities.

Therefore, this thesis seeks to deepen the understanding of the three aforementioned aspects concerning asperity contact behavior, asperity wear, and gouge particle wear, which could significantly contribute to the interpretation of both static and dynamic fault friction mechanisms in the geotribology community. In the next section, a literature review regarding the three aspects will be presented.

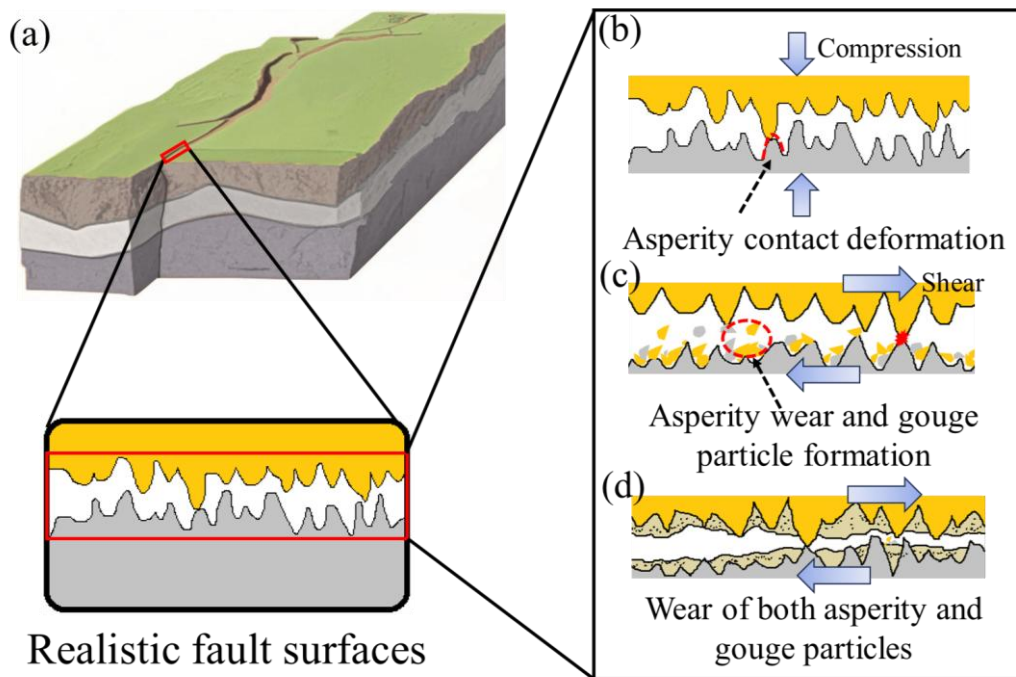


Figure 1. 1. A brief illustration of the fault contact and friction process.

1.2 Literature Review

1.2.1 *Asperity contact theory*

Over the past decades, a number of investigations have been performed to elucidate the contact deformation of rock asperities through numerical simulations (Yan & Wang, 2023), laboratory experiments (Beeler & Hickman, 2001; Tang et al., 2016) and theoretical modeling (Brown & Scholz, 1986; Tang et al., 2017; Zhao et al., 2020).

While the phenomena such as elastic and plastic deformation have been observed, significant focus has been placed on developing the asperity contact model, given its fundamental importance in understanding the deformation mechanism of rock asperities. However, rock surfaces include numerous asperities and the deformation of neighboring asperities commonly can influence each other, making it very difficult to get theoretical solutions. Therefore, the modeling process typically assumes that the deformation is independent and starts with modeling the contact deformation of a single-asperity contact. Here, a brief overview of four fundamental contact models that are typically used to model the single-asperity contact behavior will be described as below. Specifically, the key aspect in the models, namely the relation between the normal contact force and the interference distance, will be primarily detailed and compared.

The first contact model has been proposed by Hertz in 1882 (Johnson, 1985) and belongs to the elastic contact model. Based on purely elastic theory, the Hertz model describes an exponential relation between the normal contact force F and the interference distance ω when two semi-spherical asperities are in contact (Figure 1.2), which can be expressed as:

$$F_{\text{HZ}} = \frac{4}{3} E^* R^{\frac{1}{2}} \omega^{\frac{3}{2}} \quad (1.1)$$

where E^* and R^* represent the equivalent modulus and the equivalent radius of asperities, respectively. Specifically, the two parameters can be further expanded as $\frac{1}{E^*} = \frac{1-\nu_1^2}{E_1} + \frac{1-\nu_2^2}{E_2}$ and $\frac{1}{R^*} = \frac{1}{R_1} + \frac{1}{R_2}$ respectively, where E_1 and E_2 , ν_1 and ν_2 , R_1 and R_2 are the elastic modulus, Poisson's ratio and the radius of two asperities, respectively. Here, these contributions have laid the groundwork for modeling the deformation of single-asperity contact for over a century. Furthermore, it has also informed the contact modeling of nonspherical contact (Zhao et al., 2018) and roughness contact (Greenwood & Williamson, 1966). Commonly, when two asperities come into contact with a sufficiently small ω , the Hertz contact model can well predict

the evolution of the normal contact force, as the contact typically is within the elastic regime for most materials (Adams & Nosonovsky, 2000). However, if the interference distance increases to a relatively large value, the normal contact force will significantly deviate from the elastic model, accompanied by the onset of plastic deformation as demonstrated in many contact experiments (Handzel-Powierza et al, 1992; Pugliese et al, 2008). Consequently, incorporating plastic deformation becomes essential in modeling the contact behavior.

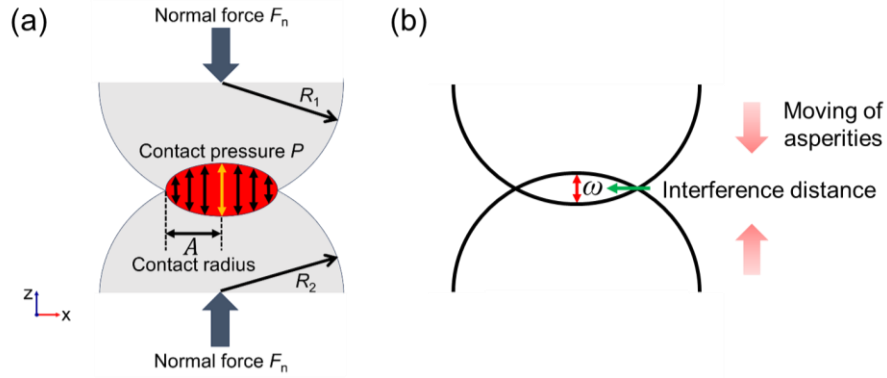


Figure 1. 2. (a) Hertz elastic contact model of two spheres. R_1 and R_2 represent the radii of the upper and lower sphere respectively. A is the radius of contact surface and P represents the contact pressure. F_n shows the normal force. (b) An explanation of the interference distance.

For the improvement of this defect, the CEB model proposed by Chang et al. (1987) incorporates a fully plastic contact stage derived by volume conservation. It assumes that when the interference distance ω exceeds a critical distance ω_c , two asperities enter the fully plastic stage, which is expressed as:

$$F_{\text{CEB}} = \pi R^* \omega \left(2 - \frac{\omega_c}{\omega} \right) KH \quad \omega \geq \omega_c \quad (1.2)$$

where K is the maximum contact pressure factor and H is the hardness of the softer material. Here, the normal contact force during the elastic stage still follows the Hertz model. The critical interference distance ω_c for the inception of fully plastic stage can be expressed as $R^* \left(\frac{\pi KH}{2E^*} \right)^2$.

Generally, in contrast to the Hertz model, the CEB model is more efficient to predict

the contact force, as it includes the potential damage of material that can occur during contact process. However, a notable point is that in the CEB model, there is a discontinuity or jump in the normal contact force at ω_c . Additionally, the model only considers two contact stages while neglecting the elastoplastic stage that bridges the fully elastic and fully plastic stages. These defects will undoubtedly lead to the inaccurate prediction of the normal contact force, as the stress evolution during the intermediate state differs significantly from the purely elastic or purely plastic stage. Therefore, the subsequent models, represented by the ZMC (Zhao et al., 2000) and KE (Kogut & Etsion, 2002), have made refinements for the shortcoming.

In the ZMC contact model, while the Hertz model is employed to model the fully elastic stage, the elastoplastic stage is formulated by contact mechanics and incorporates the results from the spherical indentation experiments by Francis (1976). Here, the normal contact force during the elastoplastic stage can be written as:

$$F_{ZMC} = H[1 - (1 - k) \frac{\ln \omega_2 - \ln \omega}{\ln \omega_2 - \ln \omega_1}] [1 - 2(\frac{\omega - \omega_1}{\omega_2 - \omega_1})^3 + 3(\frac{\omega - \omega_1}{\omega_2 - \omega_1})^2] \times \pi R^* \omega \quad \omega_1 \leq \omega < \omega_2 \quad (1.3)$$

where ω_1 and ω_2 represent the inceptions of elastoplastic and fully plastic stages, respectively. Specifically, ω_1 can be further denoted as $(\frac{3\pi kH}{4E^*})^2 R^*$ where k is the mean contact pressure factor and ω_2 can be estimated by the numerical results from Johnson (1985) as $54\omega_1$. Notably, in the ZMC model, when $\omega \geq \omega_2$, the contact of asperities enters the fully plastic stage but is modeled differently compared to the CEB model. Here, the plastic stage in the ZMC model follows the expression $2\pi R^* \omega H$, based on Abbott and Firestone (1933).

On the other hand, in the KE model, the elastoplastic deformation is also taken into consideration. However, in comparison with the single elastoplastic stage in the ZMC model, the KE model has further divided into the transitioning stage into two empirical expressions to more precisely capture the contact behavior within the intermediate stage. Based on the results of finite element simulation, the two elastoplastic stages are modeled as:

$$F_{KE} = \begin{cases} F_{ec} 1.03 \left(\frac{\omega}{\omega_c}\right)^{1.425} & \omega_c \leq \omega < 6\omega_c \\ F_{ec} 1.40 \left(\frac{\omega}{\omega_c}\right)^{1.263} & 6\omega_c \leq \omega < 110\omega_c \end{cases} \quad (1.4)$$

where F_{ec} is the critical normal contact force and is expressed as $\frac{2}{3}KH\pi R^*\omega_c$. Here, when $\omega_c \leq \omega < 6\omega_c$, the contact of asperities is under the first elastoplastic stage. When $6\omega_c \leq \omega < 110\omega_c$, the second elastoplastic stage is initiated. Notably, during the fully elastic ($\omega < \omega_c$) and fully plastic stages ($\omega \geq 110\omega_c$), the KE model adopts the expressions same as the ZMC model.

Overall, in comparison with the elastic contact model, the plastic model can effectively capture a broader range of contact deformations of asperities, which is relatively reasonable for describing the contact deformation characteristics of rock asperities.

1.2.2 Frictional wear of asperity

The frictional wear at asperity contact is referred to as two-body wear in tribology. Notably, in laboratory friction experiments, to simulate the stick-slip effect of fault slip, experimental fault surfaces are usually polished smooth. Therefore, the asperity scale involved in wear is typically on the micrometer and below, which is the primary focus of this thesis.

Based on the previous studies, focuses on the microscopic rock asperity wear have been centered on developing wear models for material loss (Wang & Scholz, 1994; Hirose et al., 2012; Boneh & Reches, 2018) and damage mechanism (Sagy & Brodsky, 2009; Dascher-Cousineau et al., 2018). For the former, the development of wear models can be categorized into two distinct groups. The first group comprises the models directly constructed from macroscopic rock friction experiments (Hirose et al., 2012). In contrast, the second group concentrates initially on the modeling of the wear behavior of a single asperity at a micrometer scale or below. Then, by integrating the distribution characteristics of asperities on the contact surfaces, the macroscopic wear volume is quantified (Archard, 1953; Wang & Scholz, 1994; Boneh & Reches, 2018). Here, it should be noted that the Archard law (Archard, 1953), which originates from the quantification of material loss in mechanical science, is one of the few but most

classical asperity-based wear models. In the law, the predicted wear volume, assuming plastic contact, is expressed as:

$$W = K_w \frac{F_n}{H} L \quad (1.5)$$

where W is the wear volume (m^3), H is the hardness of the softest material (N/m^2), L is the loading distance (m), F_n (N) and K_w are the normal force and the dimensionless wear coefficient, respectively. This equation predicts a proportional relation between the wear volume and the product of loading distance and the normal force, i.e., $W \propto F_n L$. In a specific material, the scaling factor $\frac{K_w}{H}$, called specific wear rate (w_s), is assumed as a constant (Kumar & Dhiman, 2013). Notably, based on previous friction experiments, the Archard law has been demonstrated to be effective at low loading velocities (Scholz, 1987; Hirose et al., 2012; Boneh & Reches, 2018). However, for the cases at high loading velocities, the models proposed by Hirose et al. (2012) and Boneh & Reches (2018) could be more suitable. Therefore, the wear volume of rocks exhibits a velocity dependence, which must be carefully considered when developing wear models.

On the other hand, for the microscopic asperity-asperity wear damage mechanism, there are generally two types of descriptions, including abrasive wear and adhesive wear. It should be noted that this concept originates from metal tribology, which has become an important reference for geotribology research. Specifically, abrasive wear occurs when softer materials are removed or displaced by cutting, plowing, or breaking induced by harder materials. Adhesive wear, on the other hand, arises from adhesion between contacting asperities, where micro-welding may occur, leading to adhesive material transfer from one surface to another. Here, based on previous findings, adhesive wear could be the primary wear mechanism for microscopic rock asperities during friction (Candela & Brodsky, 2016). Therefore, a review of the research findings on adhesive wear mechanism is merely detailed. Typically, Siman-Tov et al. (2013), in explaining the formation of nanoparticles on fault mirror surfaces, argued that the fault slip first induces the plastic deformation of grains on fault surfaces, forming twin boundaries. Then, the nanoparticles are generated by the brittle fracture of subgrains. Therefore, they suggested a plastic-brittle failure mechanism of nanoscale asperities. On the other hand, Candela & Brodsky (2016) suggested that at small scales, the brittle failure of asperities may be suppressed, favoring plastic deformation (smoothing wear).

Moreover, there is also another perspective, suggesting a transition between either plastic flow or fracture of asperities, which is governed by the adhesion force at the contact interface (Aghababaei et al., 2016). This, in turn, depends on the contact length. If the contact length is sufficiently large to generate an adhesion force strong enough to induce fracture, cracks initiate from the asperity root at an angle, producing gouge particles. Conversely, asperity deformation occurs through plastic flow.

Overall, the current opinions on the adhesive wear-induced failure of microscopic rock asperities are generally consistent with the typical perspectives described above, which can be summarized as three main aspects, including plastic flow, brittle fracture, and plastic-brittle failure. These insights construct an important framework for understanding the adhesive wear behavior of rock asperities.

1.2.3 Frictional wear of particles

Unlike the two-body wear described above, the gouge particles or gouge layer wear process on fault surfaces during friction is referred to as third-body wear in tribology. In previous studies, a series of physical experiments and numerical simulations have been conducted to investigate the wear behavior of gouge particles during friction. Based on the number of particles involved or the research targets, the studies can be categorized into gouge layer shearing and single-particle shearing. For the former, most research primarily focused on the friction behavior of mature faults, where the collective wear behavior of stacked particles was explored. In these studies, the influence of particle wear on the evolution of force chains and shear bands on the frictional strength has been widely discussed (Bedford & Faulkner, 2021; Casas et al., 2022; Rubino et al., 2022; Ikari & Conin, 2024). For the latter, research typically focused on the early stage of fault friction, when particles are generated by asperity-asperity collisions. Notably, in this stage, individual particles commonly serve as the primary points of force transmission (Zhao, 2013; Milanese et al., 2019). Therefore, investigating the wear mechanism of individual particles against fault asperities becomes crucial, and it may differ from gouge layer shearing where multiple particles interact collectively. Here, as this thesis focuses solely on the frictional wear of a single

particle, a review of the research on single-particle wear is detailed.

The frictional wear mechanism of a single gouge particle is similar to the two-body cases, which can also be classified into abrasive wear and adhesive wear (Fabbro et al., 2021; Arnaud et al., 2021; Svenningsson & Tatar, 2021). On the microscopic wear of rock particles, the latter also governs. However, to my knowledge, experimentally, the understanding of dynamic adhesive wear mechanism between gouge particles and asperities at microscopic scales remains limited, possibly due to the challenges of real-time observation of the dynamic wear process. Therefore, most insights come from numerical simulations, which could be more effective than physical experiments in revealing the dynamic wear mechanism of gouge particles. Currently, two kinds of methods have been primarily employed, including molecular dynamics (MD) and discrete element method (DEM). The former is primarily used for studying nanoscale particles, while the latter typically investigates particles with size ranging from micrometers to millimeters. Interestingly, outcomes differ significantly depending on the method and scale. Through DEM simulation, Zhao (2013) studied the wear behavior of a single gouge particle (radius 0.5 mm) between two smooth rock plates. The results revealed that with increasing shear distance, the gouge particle undergoes failure from minor adhesive wear to particle fragmentation. In comparison, Milanese et al. (2019) observed through MD simulations that the wear particle can exhibit a snowball effect that occurs when the critical junction size between the particle and asperities is achieved. Here, it should be noted that the contact length in the DEM simulation is far much larger than the critical length required in Milanese et al. (2019). Therefore, the particle size is a crucial factor influencing the wear characteristics of a single particle.

Overall, the single-particle wear failure can macroscopically manifest as fracture. However, as the particle size decreases, a volume increase phenomenon can still occur due to adhesive accumulation, highlighting the complicated size-dependent nature of the third-body wear mechanism.

1.3 Limitations of Previous Research

1.3.1 *Single-asperity contact*

From the literature review in Section 1.2.1, it is evident that the fundamental aspect of establishing a contact model lies in accurately describing the deformation mechanism of a single-asperity contact. However, significant uncertainties persist in applying both purely elastic and elastoplastic models to rock asperities, as several critical factors have been overlooked in the previous modeling efforts. Currently, contact models for rocks, as detailed above, typically assume asperity deformation within the confines of elastic and elastoplastic frameworks. Nonetheless, it is well established that rock materials, such as granite and sandstone, commonly exhibit fracture characteristics at the macroscopic scale (Zhou & Zhang, 2021). This introduces great concerns about whether fracture events also manifest at the microscopic asperity level, potentially challenging the foundational assumptions of current contact models. On the other hand, research on metal materials has demonstrated that both the asperity size and contact configuration can significantly influence the contact behavior of asperities (Xie et al., 2021). These factors, however, have not been investigated in the context of rock asperity contact but could have similarly important impacts on the deformation mechanism of rock asperities. Finally, current macroscopical contact models do not account for size effects and their multiscale applicability has also yet to be validated. Therefore, further investigation of these uncertainties is critical and necessary at the microscopic scale.

1.3.2 *Single-asperity friction wear*

Based on the review in Section 1.2.2, the research on the wear mechanism of microscopic asperities mainly involves establishing wear models and investigating wear damage mechanisms. However, both of the two aspects need to be further investigated. For the former, previous verifications of both empirical and asperity-based models were focusing on the evaluation of the wear volume from overall friction surfaces at a centimeter scale (Scholz, 1987; Wang & Scholz, 1994; Hirose et al., 2012; Boneh & Reches, 2018). Consequently, the discussion is limited regarding the

fundamental performance of wear models on individual micro-asperities, rendering the multiscale applicability of them unknown.

For the latter, the opinions remain divided. Both plastic deformation and plastic–brittle fracture have been considered as the failure mechanisms of small-scale asperities respectively. Moreover, these points are limited to post-analysis or empirical explanations based on worn surfaces. Therefore, there is still a lack of dynamic observation and evidence to confirm the failure modes of asperities. Notably, while the concept of critical junction size may help quantify the failure modes, its application has been primarily limited to metals and not yet conclusively extended to rock materials. Whether this idea can be used to quantify the asperity failure modes in rocks remains to be further investigated.

1.3.3 Frictional wear of a single particle

As discussed in Section 1.2.3, the wear behavior of a single particle differs significantly depending on the method and scale used in simulations. At the microscopic scale that this thesis focuses on, although Milanese et al. (2019) observed the snowball effect in a particle through molecular dynamics simulations, this phenomenon has not been investigated or verified in rock materials. Therefore, further analysis is needed.

1.4 Research Objectives and Content

In response to the limitations discussed in Section 1.3, this thesis primarily focuses on investigating the single-asperity contact mechanisms, the frictional wear mechanisms of single-asperity collision and the frictional wear mechanisms of a single particle at microscopic scale. Notably, in the friction cases, the evolution of friction force will also be discussed.

Here, conducting in-situ 3D observations of the dynamic contact and frictional wear process on microscopic asperities remains challenging (Sato et al., 2012, 2022). Hence, numerical simulations play a vital and practical role in explicitly comprehending these opaque processes. Inspired by numerical studies on the contact and friction processes of microscopic asperities (Xie et al., 2021; Wang et al., 2021b; Kajita et al., 2023), molecular dynamics (MD) emerges as a promising method to unveil the opaque contact

and wear processes of microscopic asperities. Therefore, all the research in this thesis is conducted using molecular dynamics method, which also allows for a comparative discussion with previous molecular dynamics results. Notably, considering the substantial computational resources required for studying cases at the micrometer scale, all cases are chosen to be at the nanoscale. Additionally, in molecular dynamics method, simulating the multi-component complexity of real rocks indeed demands substantial computational resources and the development of more complicated potential functions (Li and Fukuyama, 2025). For simplification, crystalline α -quartz is selected to construct the contact and friction systems. Notably, α -quartz is a common natural mineral and widely found in the Earth's crust, particularly in granite, sandstone, and many sedimentary deposits (Balasubramanian, 2017; Götze et al., 2021). Therefore, it is deemed that using α -quartz as a representative material can provide valuable insights into the nanoscale contact behavior and two-body as well as third-body frictional wear behavior of faults.

Overall, the structure of this thesis is as follows. Chapter I presents the research background, literature review and limitation of previous research related to the asperity contact and frictional wear mechanisms as well as particle wear mechanisms. Chapter II presents a basic introduction to the structure of α -quartz, the governing equations, the potential function, boundary conditions, the simulation ensemble and the solution of the kinematic equation of molecular dynamics method. Chapter III applies the simulation method to investigate the nanoscale normal contact behavior of a pair of α -quartz asperities prior to friction. Chapters IV and V investigate the two-body wear mechanisms of a pair of α -quartz asperities during friction. Chapter VI focuses on third-body wear mechanisms involving a single α -quartz particle interacting with asperity walls. Chapters VII and VIII provide the overall discussion and conclusion. Here, the main content from Chapters III to Chapters VI are summarized as follows:

- For the single-asperity contact, the contact-induced failure of α -quartz asperities is investigated under different asperity sizes and contact configurations

(centrosymmetric contact and asymmetric contact). Moreover, the nanoscale simulation results are compared with macroscopic elastic (Hertz) and elastoplastic contact models (CEB, ZMC, KE) in terms of the normal contact force versus interference distance to assess the multiscale applicability. Finally, empirical contact models are also established at the nanoscale.

- For the single-asperity friction wear, the damage mechanisms and wear volume of asperities are firstly investigated under different normal forces and loading velocities at the plastic wear case. Besides, the wear volume evolution is compared with the Archard law to discuss the multiscale disparity of wear model and a formula for predicting the wear volume of plastic wear is also introduced. Then, the failure mode transition from plasticity to fracture of asperities is examined under varying asperity sizes, normal forces and contact configurations as well as two boundary conditions involving constant normal load (CL) and constant normal stiffness (CS)-like conditions. Additionally, the evolution of wear volume and shear force under plastic and fracture cases is compared and discussed. Finally, the wear volume prediction of fractured asperities is also analyzed.
- For the frictional wear of a single particle, the failure mode and wear volume are investigated under different normal forces, particle sizes, asperity intervals, and contact configurations. Moreover, a formula is introduced to predict the particle wear volume. Finally, the influence of particle wear failure modes on the shear force and friction coefficient is investigated.

Figure 1.3 shows a schematic overview of the main content in this thesis.

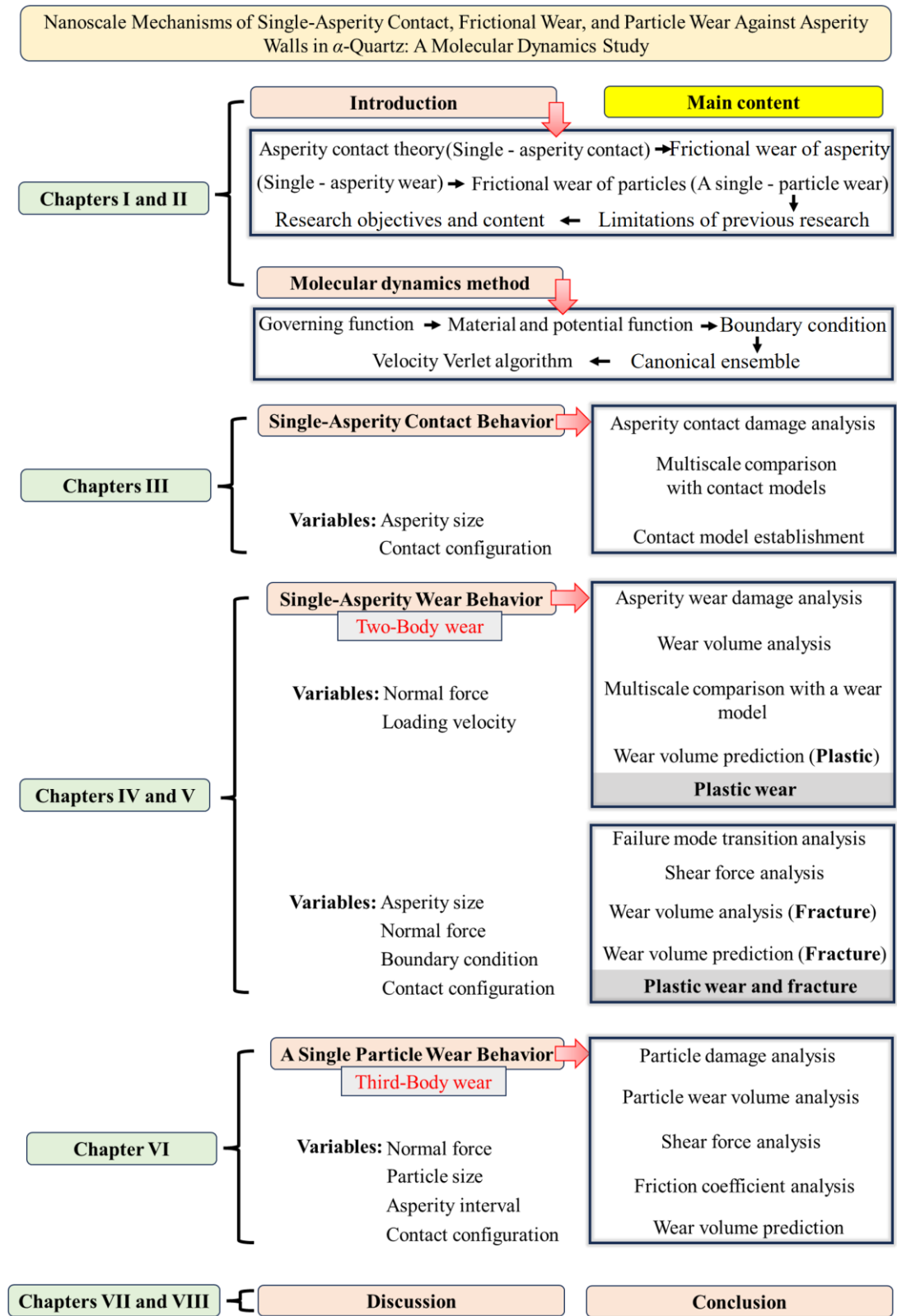


Figure 1. 3. A schematic overview of the main content in the thesis.

CHAPTER II

Molecular Dynamics Method

2.1 Governing Function

Molecular Dynamics (MD) method is a numerical technique used to investigate the physicochemical and mechanical properties of atomic and molecular systems under classical mechanics. Over the past decades, it has been widely applied in the fields of materials science, physical chemistry, life sciences, geosciences, computational fluid dynamics and so on, which serves as a powerful tool for understanding the microscopic mechanisms of atomic and molecular systems in materials.

Molecular dynamics simulations require the selection of an appropriate ensemble. In simulating the contact and friction processes, the microcanonical ensemble (NVE) is commonly used to simulate atomic motion. The system is isolated from changes in the number of particles (N), volume (V), and energy (E), corresponding to an adiabatic process with no heat exchange. A microcanonical molecular dynamics trajectory can be interpreted as a transfer of energy between potential and kinetic forms, with the total energy remaining constant. For a system with N atoms, the motion of each atom is typically described by Newton's second law:

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = \vec{F}_i \quad (2.1)$$

where m_i is the mass of atom, $\vec{r}_i$ the position of atom, and $\vec{F}_i$ the force acting on the atom. However, in MD simulation, the force $\vec{F}_i$ is calculated from the potential energy function, $\vec{F}_i = -\Delta_i U(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$. Therefore, it is clear that the precision of molecular dynamics simulations is directly related to the accuracy of the potential function, which governs the interatomic interactions.

In next section, the atomic structure of α -quartz, the potential function modeling α -quartz, and the validation of the potential function will be detailed.

2.2 Potential Function

2.2.1 α -Quartz

Figure 2.1 shows the schematic diagram of α -quartz crystal structure. As seen in

Figure 2.1, the lattice parameters of α -quartz are $a = b = 4.9019(1) \text{ \AA}$, and $c = 5.3988(1) \text{ \AA}$ measured at $T = 20 \text{ K}$ (Tucker et al., 2001), which belongs to the trigonal system. It is composed of silicon and oxygen atoms. Each silicon atom is covalently bonded to four oxygen atoms to form a silicon oxygen tetrahedron (SiO_4). The silicon oxygen tetrahedra are connected by shared oxygen atoms to form the three-dimensional trigonal lattice of α -quartz. Therefore, in developing the potential function for α -quartz, it is necessary to consider not only the evolution of potential energy caused by the distance variation between silicon and oxygen atoms, but also the evolution of potential energy resulting from bond angle changes. Here, the specific expression of the potential function used for modeling α -quartz will be detailed as follows.

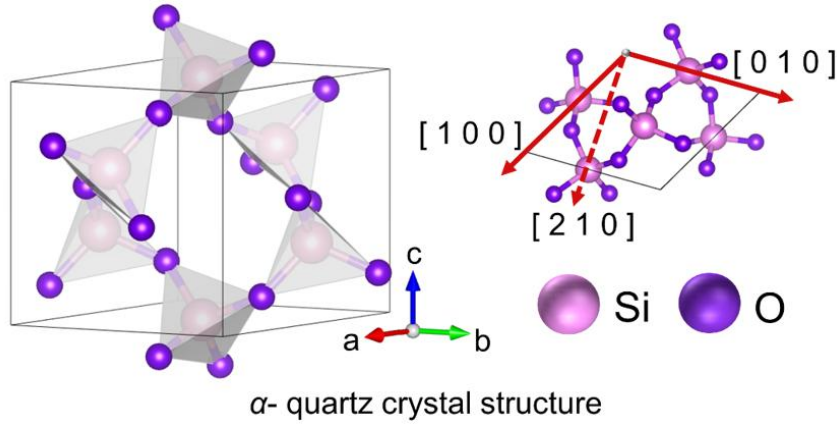


Figure 2. 1. The schematic diagram of α -quartz crystal structure

2.2.2 Vashishta potential

In this thesis, the 1997-version Vashishta potential is selected to model the interatomic forces of α -quartz (Vashishta et al., 1990; Broughton et al., 1997). In the function, the potential energy U of the atomic system consists of the two-body term $U_{ij}^{(2)}(r_{ij})$ and three-body term $U_{ijk}^{(3)}(r_{ij}, r_{ik}, \theta_{ijk})$ (Vashishta et al., 1990), where θ_{ijk} is the interatomic angle and r_{ij} and r_{ik} are the interatomic distances (the subscript is the atomic indices). Here, r_c and r_0 are the cutoff distances for $U_{ij}^{(2)}$ and $U_{ijk}^{(3)}$,

respectively, which are 5.5 Å and 2.6 Å in Vashishta potential. The two-body $U_{ij}^{(2)}$ is expanded as (Vashishta et al., 1990; Broughton et al., 1997; Vashishta et al., 2008; Branicio et al., 2009):

$$U_{ij}^{(2)}(r) = \frac{H_{ij}}{r^{\eta_{ij}}} + \frac{Z_i Z_j}{r} \exp\left(-\frac{r}{\lambda_{1,ij}}\right) - \frac{D_{ij}}{r^4} \exp\left(-\frac{r}{\lambda_{4,ij}}\right) - \frac{W_{ij}}{r^6} \quad (2.2)$$

where $\frac{H_{ij}}{r^{\eta_{ij}}}$ models the steric repulsion; $\frac{Z_i Z_j}{r}$ and $\frac{D_{ij}}{r^4}$ model the Coulomb and charge-dipole interactions, respectively. η_{ij} , $\lambda_{1,ij}$, $\lambda_{4,ij}$ denote the steric repulsive exponents, screening lengths for Coulomb and charge-dipole interactions, respectively. $\frac{W_{ij}}{r^6}$ is related to the van der Waals interaction. D_{ij} can be further expressed as $\frac{\alpha_i Z_j^2 + \alpha_j Z_i^2}{2}$, where α_i is the electronic polarizability of the i_{th} atom. Here, the conventional long-range Coulomb interaction is numerically challenging to handle due to its infinite range, especially in large-scale molecular dynamics simulations where the computational cost becomes significant. To improve computational efficiency and avoid complex convergence issues, this study adopts a suitably adjusted screened Coulomb potential, which effectively limits the interaction range.

Moreover, the three-body term $U_{ijk}^{(3)}$ can be expressed as (Branicio et al., 2009):

$$U_{ijk}^{(3)}(r_{ij}, r_{ik}, \theta_{ijk}) = B_{ijk} \frac{[\cos \theta_{ijk} - \cos \theta_{0ijk}]^2}{1 + C_{ijk} [\cos \theta_{ijk} - \cos \theta_{0ijk}]^2} \exp\left(\frac{\gamma_{ij}}{r_{ij} - r_{0,ij}}\right) \exp\left(\frac{\gamma_{ik}}{r_{ik} - r_{0,ik}}\right) \quad (2.3)$$

where the interaction strength B_{ijk} , interatomic angle θ_{ijk} (subtended at a vertex), covalent bond angle $\theta_{0,ijk}$, the saturation C_{ijk} are included. Additionally, γ_{ij} and γ_{ik} are exponent parameters. Here, the specific parameters of the Vashishta potential used in this thesis are deposited in the dataset available at DOI: 10.17632/yv95bhcnrx.1.

2.2.3 Verification

The Vashishta potential function has already been demonstrated to be reliable in modeling various physical and mechanical properties of α -quartz and amorphous SiO₂. Nakano et al. (1994) demonstrated that the Vashishta potential can effectively capture the intermediate-range order in amorphous SiO₂, as evidenced by its accurate

reproduction of the FSDP (First Sharp Diffraction Peak). Koudriachova et al. (2001) validated that the Vashishta potential is capable of generating reasonable initial structures for quartz surfaces. Zhang (2017) confirmed the accuracy of the Vashishta potential for simulating α -quartz structural parameters through first-principles calculations. Notably, the first-principles calculation is widely recognized as one of the most precise methods for probing atomic-scale physical parameters of materials (Van de Walle & Neugebauer, 2004; Ganose et al., 2021). Pham-Ba and Molinari (2021) further explored the ability of the Vashishta potential to model the wear and rupture of silica asperities by comparing simulation outcomes with experimental observations. Furthermore, Otsuka et al. (2024) validated the phase transition between crystalline and amorphous states of α -quartz under high-energy beam irradiation. Moreover, in Chapter IV, we have also validated the applicability of the Vashishta potential function to frictional systems. Therefore, the 1997-version Vashishta potential function should be reliable in modeling the contact and friction behavior of α -quartz.

Next, the common boundary conditions used in molecular dynamics simulation will be introduced.

2.3 Boundary Condition

In molecular dynamics (MD) simulations for contact and friction scenarios, the boundary conditions commonly include Periodic Boundary Condition (PBC), Free Boundary Condition (FBC), Fixed Boundary Condition (FBC), and Shrink-Wrapped Boundary Condition (SBC). For Periodic Boundary Condition, an infinite number of identical units are replicated around the simulation cell (Figure 2.2). Therefore, in simulations, the properties of the original simulation box need only to be recorded and propagated, effectively simulating the mechanical behavior of an infinitely large system.



Figure 2. 2. The schematic diagram of Periodic Boundary Condition (PBC)

The PBC is quite different from the Fixed Boundary Condition (FBC), which restricts the degrees of freedom of atoms, ensuring that the boundary atoms remain completely still. The latter is typically applied to the bottom of contact and friction systems. In comparison, the Shrink-Wrapped Boundary Condition (SBC) allows the boundary to dynamically adjust based on the displacement of atoms in the contact and friction systems. As the particle displacement changes, the boundary automatically scales. Therefore, it is typically applied in the z -direction, simulating the boundary changes during contact and frictional wear process.

Here, after the introduction of boundary conditions, the NVT ensemble will be introduced next.

2.4 Canonical Ensemble (NVT)

For molecular dynamics simulations related to contact and friction cases, the NVT ensemble (Canonical Ensemble) is typically applied in addition to the NVE ensemble. The primary goal of employing the ensemble is to regulate temperature, as friction can cause localized temperature increases, especially under high-velocity loading conditions. Without temperature control, the temperature in the system could rise uncontrollably, which consequently leads to unphysical temperature fluctuations.

Specifically, the NVT ensemble maintains constant values for the number of particles

(N), volume (V), and temperature (T). In this ensemble, the temperature is controlled by a heat reservoir (thermostat) to ensure that the system remains in statistical thermal equilibrium. Currently, the common types of NVT thermostats include the Velocity rescaling thermostat, Berendsen thermostat, Langevin thermostat, and Nose-Hoover thermostat. Among these, the Nose-Hoover thermostat is based on the Nose-Hoover dynamics equation and strictly ensures that the system adheres to the NVT ensemble. It achieves real statistical temperature distributions by coupling the system with a virtual heat bath variable, making it suitable for long-term stable simulations. Therefore, in this study, the Nose-Hoover thermostat is used as the temperature regulator for the contact and friction simulations. Here, a brief introduction to the Nosé-Hoover thermostat is provided as follows.

The Nosé-Hoover thermostat was initially developed by Shuichi Nosé (1984) and later improved by William G. Hoover (1985). The core idea of the Nosé-Hoover method is to introduce an additional degree of freedom into the Hamiltonian system, enabling the system temperature to remain at a prescribed constant value. Here, assuming a system with N atoms, where each atom has a mass of m_i , the system can be described using the classical Hamiltonian formulation:

$$H = \sum_{i=1}^N \frac{|\vec{p}_i|^2}{2m_i} + U(\vec{q}_1, \vec{q}_2, \dots, \vec{q}_N) \quad (2.4)$$

where H is the total energy of the system; $\vec{q}_i$ the generalized coordinates of the i -th atom; $\vec{p}_i$ the generalized momentum of the i -th atom; m_i the mass of the i -th atom; $U(\vec{q})$ the potential energy of the system; $\sum_{i=1}^N \frac{|\vec{p}_i|^2}{2m_i}$ the total kinetic energy of the system.

To achieve the thermostat control, Nosé (1984) added the time scaling variable s ($dt = sd\tau$, t is real time) and its conjugate momentum p_s to construct an extended Hamiltonian system:

$$H_{\text{Nosé}} = \sum_{i=1}^N \frac{|\vec{p}_i|^2}{2m_i s^2} + U(\vec{q}) + \frac{p_s^2}{2Q} + gk_B T \ln(s) \quad (2.5)$$

where Q is the parameter controlling the timescale of the thermostat; k_B the Boltzmann constant; T the target temperature; g the number of degrees of freedom. Here, in the $H_{\text{Nosé}}$ system, the $\vec{p}$ and $\vec{q}$ are virtual variables, which are related to the real variables and the scaling relation can be found in the reference (Nosé, 1984). Here, Nosé's method originally evolves in a fictitious time, which is numerically inconvenient. Hoover transformed it through mathematical manipulations into a set of differential equations in real time (the Nosé–Hoover equations), making it more suitable for numerical simulations.

Here, I only present the rate of thermal bath variable ξ , which is one of the most important parts in the Nosé–Hoover thermostat for controlling temperature. Here, ξ is defined as $\frac{p_s}{Q}$ (Hoover, 1985) and p_s represents the conjugate momentum in terms of real physical time. Therefore, we can get the rate of ξ by considering $\frac{d\xi}{dt} = \frac{1}{Q} \cdot \frac{dp_s}{dt}$. However, if we want to obtain $\dot{\xi}$ in real physical time, we need to take the derivative of p_s in the extended Hamiltonian system in Eq. (2.5) with respect to the virtual time firstly, yielding Eq. (2.6).

$$\frac{dp_s}{d\tau} = \sum_{i=1}^N \left(\frac{|\vec{p}_i|^2}{m_i s^3} \right) - \frac{g k_B T}{s} \quad (2.6)$$

Then, using the time scaling relation $dt = s d\tau$, Eq. (2.6) is mapped into real physical time as follows:

$$\frac{dp_s}{dt} = \sum_{i=1}^N \left(\frac{|\vec{p}_i|^2}{m_i s^2} \right) - g k_B T \quad (2.7)$$

Since the differentiation is performed within the framework of $H_{\text{Nosé}}$, the momentum $\vec{p}$ appearing in Eq. (2.7) is the virtual momentum. As shown in Nosé (1984), the virtual momentum and the real momentum differ by a factor of s . Substituting the transformed real momentum into Eq. (2.7), we obtain:

$$\frac{dp_s}{dt} = \left(\sum_{i=1}^N \left(\frac{|\vec{p}_i|^2}{m_i} \right) - g k_B T \right) \quad (2.8)$$

Therefore, we can obtain the rate of thermal bath variable ξ under real time in Eq. (2.9).

$$\frac{d\xi}{dt} = \frac{1}{Q} \cdot \frac{dp_s}{dt} = \frac{dp_s}{dt} = \frac{\left(\sum_{i=1}^N \left(\frac{|\vec{p}_i|^2}{m_i} \right) - g k_B T \right)}{Q} \quad (2.9)$$

Here, one can find more about the concept and derivation process of the Nose-Hoover thermostat in the given reference (Hoover, 1985).

In next section, the algorithm solving the equations of atomic motion will be introduced.

2.5 Velocity Verlet Algorithm

In this thesis, the Velocity Verlet algorithm is adopted to solve the atomic equations of motion. Here, considering a single atom, one needs to predict the atomic trajectory $\mathbf{r}(t+dt)$ first based on the information at current time t , where dt is the time step between iterations. If assuming a small dt , the atomic trajectory $\mathbf{r}(t+dt)$ can be predicted by using a forward Taylor expansion:

$$\mathbf{r}(t + dt) = \mathbf{r}(t) + \dot{\mathbf{r}}(t)dt + \ddot{\mathbf{r}}(t)\frac{dt^2}{2!} \quad (2.10)$$

Therefore, if we know the velocity and acceleration at the initial moment, the position at the next time step can be predicted. Then, based on the new position $\mathbf{r}(t+dt)$, the new acceleration and velocity can be computed as:

$$\mathbf{a}(t + dt) = \frac{1}{m}\mathbf{F}(\mathbf{r}(t + dt)) \quad (2.11)$$

$$\int_t^{t+dt} \frac{d\mathbf{v}(s)}{ds} ds = \mathbf{v}(t + dt) - \mathbf{v}(t) \quad (2.12)$$

It is worth noting that the velocity update can be further expressed as:

$$\mathbf{v}(t + dt) = \mathbf{v}(t) + \frac{1}{2}[\mathbf{a}(t) + \mathbf{a}(t + dt)] \cdot dt \quad (2.13)$$

Based on Eqs. (2.10) – (2.13) and Eqs. (2.1) – (2.3), the particle position at the next time step can be further predicted. Here, one can refer to the work of Martys and Mountain (1999) for further details on solving the equations of motion.

CHAPTER III

Contact Behavior of Asperities

3.1 Introduction

In this chapter, the text and figures are taken from Li and Fukuyama (2025). I have analyzed the influence of asperity size and offset distance between asperity centers on the contact deformation of α -quartz asperities. I have also compared the simulation results with four macroscopical contact models (Hertz, CEB, ZMC, and KE) in terms of the evolution of the normal contact force to examine the multiscale applicability.

The results, maybe for the first time, demonstrate that the single-asperity contact of nanoscale α -quartz undergoes fracture during the contact process, challenging the traditional elastic or elastoplastic assumption. Moreover, the occurrence of fracture is closely related to both the asperity size and offset distance between asperity centers. In addition, I reveal that the contact displacement at which α -quartz asperity yielding occurs, as predicted by the CEB, ZMC, and KE elastoplastic models, shows the difference in multiples from the simulation results, highlighting a major multiscale disparity. These findings have significant implications for advancing the accurate modeling of microscopic contact models of rock asperities, which are also crucial for improving the modeling of asperity contact deformation-related areas such as rock friction, wear, and the hydraulic properties of fractures.

3.2 Numerical Model

Figure 3.1 shows the schematic diagram of the crystal structure of α -quartz and contact configurations of asperities. As seen in Figure 3.1a, for the convenience of applying boundary conditions, an orthorhombic unit cell is selected by changing crystallographic axis a from $[1\ 0\ 0]$ to $[2\ 1\ 0]$ direction (a changes to $8.4903\ \text{\AA}$) to fill in the rectangular simulation box (Figure 3.1bc). As shown in Figure 3.1bc, the simulation box has dimensions of $L_x = 5na$, $L_y = 5nb$ and the thickness of each substratum is $1.25\ nc$, where n is defined through $R = na$ and R is the radius of semi-spherical asperity. The box was further divided into three layers, involving rigid, thermostat (Nosé–Hoover thermostat) and free deformable parts. Two semi-sphere asperities were placed on the substrate surfaces in the freely deformable layer and the temperature of thermostat layer was kept constant (Figure. 3.1bc). Furthermore, in the

rigid layer of the upper block, a constant loading velocity V_n was applied in the normal direction. In contrast, the rigid layer of the lower block was fixed. In the x - and y -directions, periodic boundary conditions were enforced respectively (Figure 3.1bc). Here, given that the friction process along faults continuously generates new surfaces, it is common for the asperity contacts to have dangling atoms under vacuum conditions if the effect of water molecules is not considered. Therefore, in all models of this thesis, dangling atoms are not treated with hydrogenation or hydroxylation.

Overall, the centrally symmetric contact was modeled for comparison with the four macroscopical contact models (Hertz, CEB, ZMC, KE) (Figure 3.1b) and the single-asperity contact with asperity center offset was also modeled (Figure 3.1c). Five different asperity radii ($R = 8a, 12a, 16a, 20a$, and $24a$, where $a = 8.4903 \text{ \AA}$) were considered to investigate the influence of asperity size on the contact behavior of single-asperity contact. The number of atoms in the system was from about 6.9×10^5 to 1.8×10^7 depending on the asperity radius. For the offset case, five different offset distances between asperity centers, $\delta = 0.2R, 0.4R, 0.6R, 0.8R$ and R , were modeled for every asperity radius (Figure 3.1c).

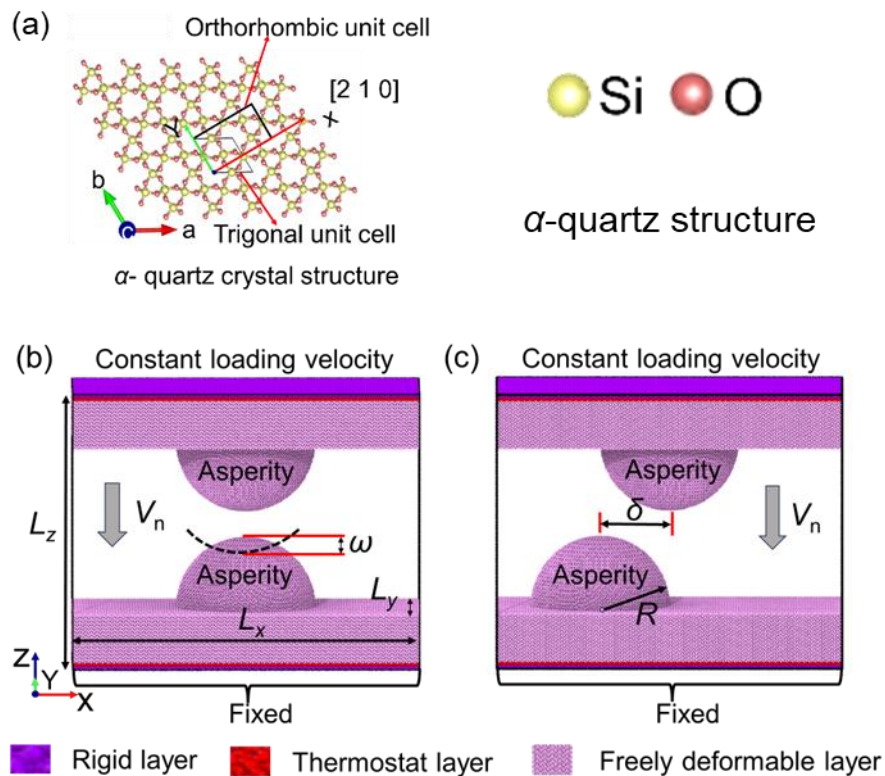


Figure 3. 1. A schematic illustration of the crystal structure of α -quartz and the contact configurations of asperities (Li and Fukuyama, 2025). (a) The crystal structure of α -

quartz (visualized by VESTA, Momma & Izumi, 2011). (b) The model with asperity top center symmetry. ω is the interference distance after contact. L_x , L_y and L_z stand for the dimensions of model space. V_n is the loading velocity in the normal direction. (c) The model with asperity top center offset. δ is the offset distance between asperity tops. R is the asperity radius.

3.3 Simulation Procedure

All simulations were carried out with the 3D Larger-scale Atomic / Molecular Massively Parallel Simulator (LAMMPS) in the thesis (Thompson et al., 2022). Overall, the simulation was performed by following stages. The conjugate gradient algorithm was first applied to minimize the energy of the initial system (Dickel et al., 2021). Next, the canonical ensemble (NVT) was applied with damping coefficient 0.25 (Tobias et al., 1993) to relax the atomistic system at temperature 300 K for 500 ps. This allows surface atoms to adjust their positions to reconstruct surface structures, stabilizing the surface energy. Here, the system was ensured to reach equilibrium by monitoring the evolution of total energy over the simulation time. Specifically, no significant drift or fluctuation in total energy was observed (Yang, 2014; Ma et al., 2023). After that, the canonical ensemble (NVT) in the freely deformable layer was transitioned to the micro-canonical ensemble (NVE) (Clavier et al., 2017) and the upper block was moved vertically to bring the asperities into contact. It should be noted that the constant loading velocity V_n was set at 10 m/s in simulations, which has been proved a proper velocity in MD simulation during single-asperity contact (Xie et al., 2021). Thus, the chosen velocity ensures both computational feasibility and the validity of comparing MD simulation results with macroscopic contact models. The timestep of the simulation was 0.0025 ps.

3.4 Normal Contact Force

In this section, the evolution of the normal contact force from MD simulations with the macroscopical contact models Hertz, CEB, ZMC, and KE for centrosymmetric contact was first compared in Section 3.4.1, where five different asperity radii cases were investigated ($8a$, $12a$, $16a$, $20a$, $24a$, where $a = 8.4903 \text{ \AA}$). Then, the effect of offset distance ($\delta = 0.2R$, $0.4R$, $0.6R$, $0.8R$, and R) on the normal contact force for each asperity radius was analyzed in Section 3.4.2. The parameters in the macroscopical

models, including elastic modulus E , Poisson ratio ν , hardness H , maximum contact pressure factor K and mean contact pressure factor k , are shown in Table 3.1. Notably, H was defined as $1.1s_y$ where s_y is the yield strength (Strozewski et al., 2021). Besides, due to the inherently brittle nature of α -quartz, it is difficult to observe a distinct yield point. Therefore, in this work, s_y is assumed as the peak strength shown in Figure 3.2. On the other hand, the parameter K in the KE model was defined as $K = 0.454 + 0.41\nu$ (Kogut & Etsion, 2002), where Poisson ratio ν is 0.17 (Ma et al., 2021). Additionally, elastic modulus and yield strength s_y were defined by stress-strain curve from uniaxial compression test in MD simulation (in this context, the elastic modulus specifically refers to the Young's modulus), as shown in Figure 3.2. Here, for the uniaxial compression, the system was initially subjected to energy minimization via the conjugate gradient (CG) method, which was followed by the relaxation process in the NVT ensemble at 300 K for 0.5 ns. After that, uniaxial compression was performed under the NPT ensemble and continued until the material exhibited complete failure.

Table 3. 1. Mechanical parameters in the Hertz, CEB, ZMC and KE models (Li and Fukuyama, 2025).

Elastic modulus, E (GPa)	Poisson's ratio, ν	Hardness, H (GPa)	Maximum contact pressure factor, K	Mean contact pressure factor, k
57.18	0.17	9.05	0.60	0.40

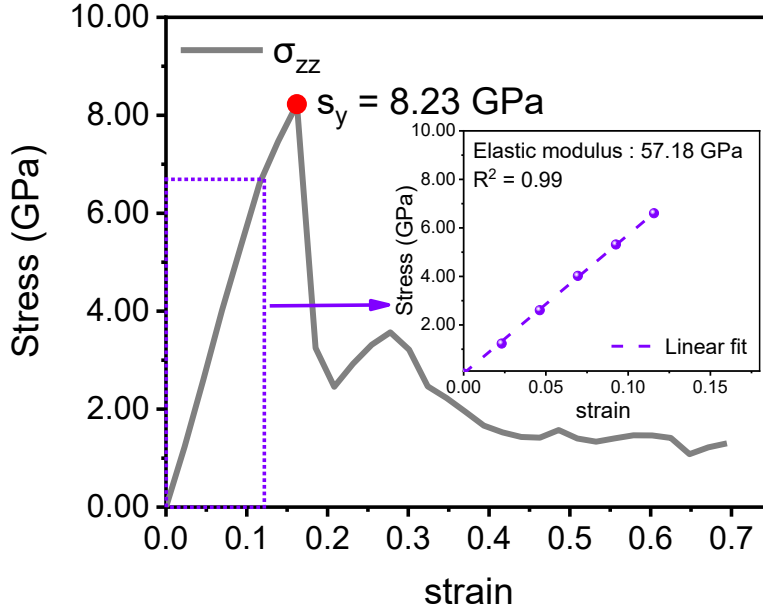


Figure 3. 2. Stress-strain curve from uniaxial compression test in MD simulation (Li and Fukuyama, 2025). Red point corresponds to the peak strength. The detailed data in the purple dotted square are shown in an inset plot.

3.4.1 Centrosymmetric contact

Figure 3.3 shows the normal contact force between MD simulations and four contact models (Hertz, CEB, ZMC, and KE) as a function of interference distance ω under varying asperity radii. The normal contact force was estimated by calculating the total force acting on the thermostat and rigid layer. As observed, the evolution of the normal contact force in nanoscale α -quartz asperities exhibits both elastic and inelastic behavior. The elastic contact phase generally follows the Hertz model at small ω across all asperity radii. However, the inelastic stage shows significant discrepancies compared to predictions from the macroscopical elastoplastic models. Here, one of the evident differences is in the magnitude of critical interference distance, ω_c . For example, at $R = 8a$, the normalized interference distance (ω_c/R) is predicted to be 0.084 by the CEB and ZMC models, and 0.064 by the KE model. In contrast, the simulation records it at approximately 0.37 (Table 3.A1) (Appendix 3.A), which is about 4 to 5 times higher than predictions from the contact models. Notably, similar findings have also been

reported in molecular dynamics simulations and experimental studies on metallic materials (Schreijäg et al., 2015; Xie et al., 2021), which may relate to the surface energy that matters to the mechanical properties of materials in the nanoscale.

On the other hand, the post-peak behavior observed in simulations differs significantly from that predicted by the elastoplastic models and reveals a strong size dependence. At $R = 8a$, unlike the abrupt changes predicted by the CEB, ZMC, and KE models, the normal contact force undergoes an extended stage resembling ideal plasticity after the peak force. As asperity size increases, the post-peak gradient (gradient after the first peak force) becomes steeper (red arrow in Figure 3.3f), indicating a transition from plasticity-dominated to brittle fracture-like contact behavior (Figure 3.3f). Here, although the normal contact force evolution after the peak force approaches the abrupt change at larger asperity sizes in simulations (Figure 3.3f), the complicated post-peak behavior, such as the bimodal evolution at $R = 16a$ and $R = 24a$, has been overlooked by existing contact models.

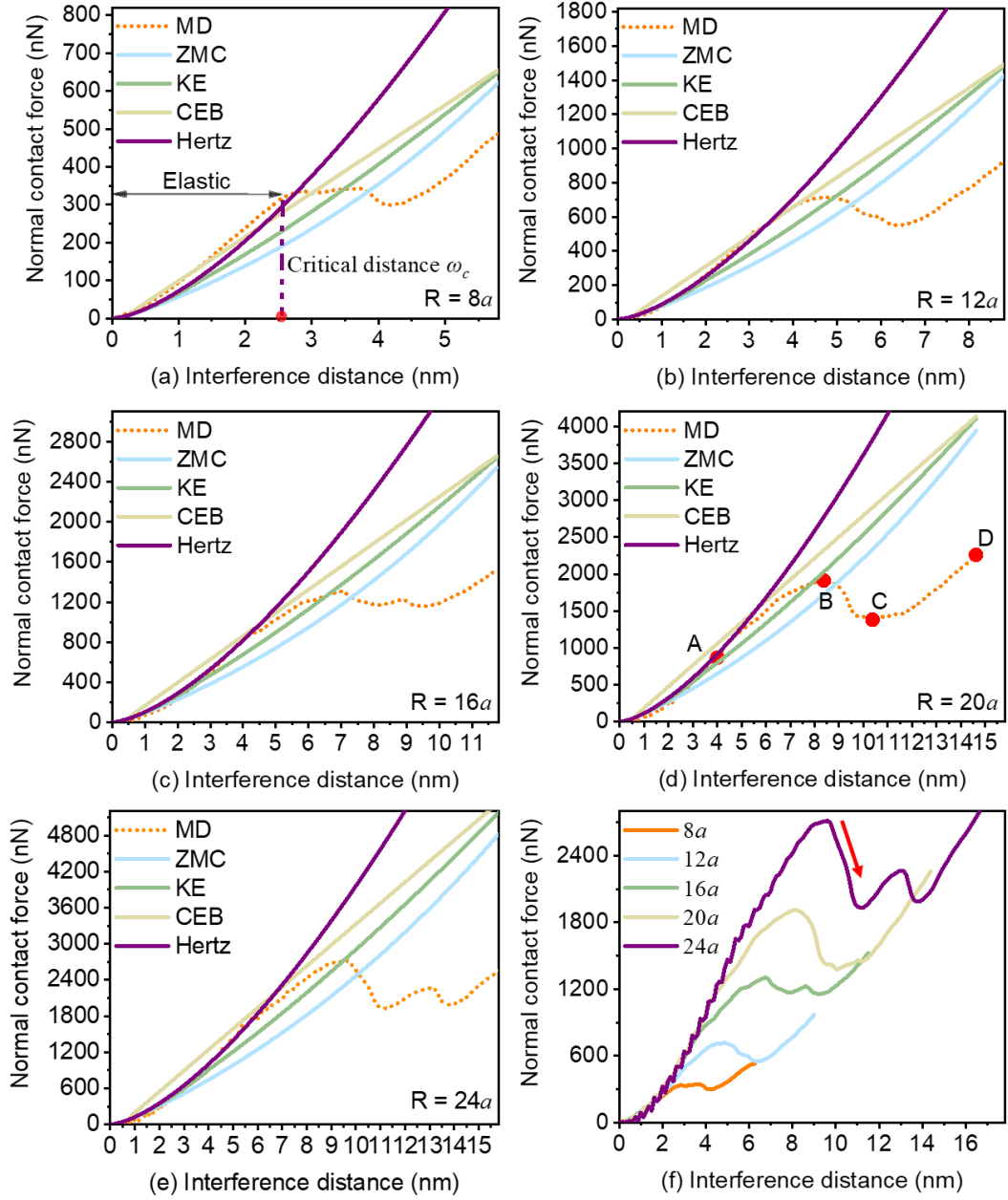


Figure 3. 3. The normal contact force F_n between MD simulations and four contact models (Hertz, CEB, ZMC, and KE) as a function of interference distance ω under different asperity radii (a) $R = 8a$, (b) $R = 12a$, (c) $R = 16a$, (d) $R = 20a$, and (e) $R = 24a$ (Li and Fukuyama, 2025). Figure 3.3f is the normal contact force versus the interference distance under all asperity radii in MD simulations. A, B, C and D in Figure 3.3d correspond to the elastic normal contact force, the maximum normal contact force, the residual normal contact force and the final normal contact force.

3.4.2 Asymmetric contact

In the offset contact, two typical cases at $R = 8a$ and $R = 20a$ are shown in Figure 3.4 to illustrate the evolution of the normal contact force, as the influence of offset distance is similar under other asperity radii. As can be seen, the evolution of the normal contact force also exhibits elastic and inelastic behavior for both asperity sizes under varying offset distances. However, the offset distance significantly impacts the evolution of the normal contact force. Specifically, in Figure 3.4a ($R = 8a$), a noticeable post-peak softening trend is observed at offset distances of $\delta = 0.2R$, $0.4R$, and $0.6R$. In contrast, increasing δ to $0.8R$ and R results in a hardening trend, accompanied by the disappearance of the peak force. This transition from softening to hardening trend is also apparent in larger α -quartz asperities, as shown in Figure 3.4b ($R = 20a$). However, at the same offset ratio δ/R (e.g., 0.8), the hardening trend is mixed with short softening stage at $R = 20a$, starkly contrasting with the complete hardening trend observed at $R = 8a$. Therefore, larger asperities typically need a greater offset ratio to achieve the full hardening trend, indicating a significant size dependence.

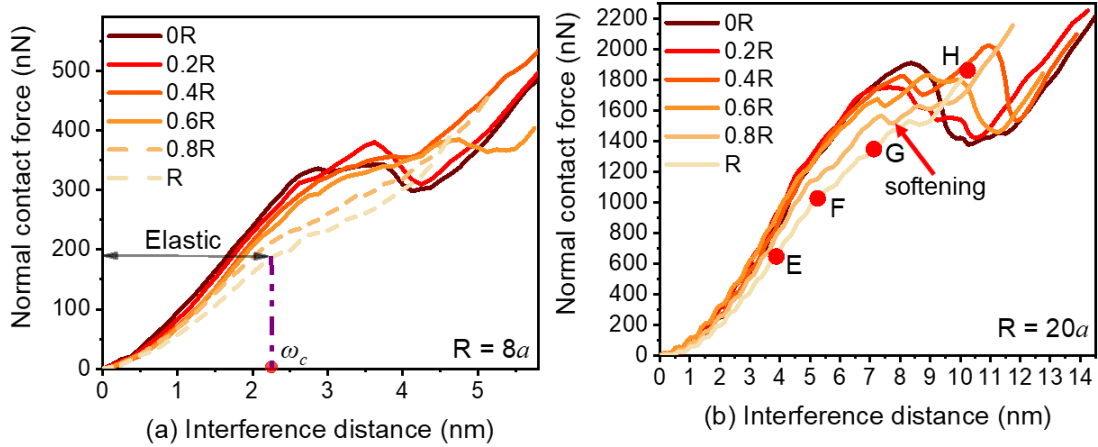


Figure 3. 4. The normal contact force under varying offset distances ($\delta = 0R, 0.2R, 0.4R, 0.6R, 0.8R$ and R) in the cases of (a) $R = 8a$ and (b) $R = 20a$ (Li and Fukuyama, 2025). E, F, G and H in Figure 3.4b correspond to the elastic normal contact force, the normal contact force entering inelastic contact stage, the inelastic normal contact force, and the final contact force, respectively.

3.5 Contact Damage

3.5.1 Centrosymmetric contact

Four snapshots of damage (von Mises shear strain) in α -quartz asperities at $R = 20a$ are typically shown in Figure 3.5, which correspond to the points A (elastic stage), B (the maximum normal contact force), C (the residual normal contact force) and D (final normal contact force) marked in Figure 3.3d. Additionally, the final breakage configurations for five different asperity radii ($R = 8a, 12a, 16a, 20a$ and $24a$) are further shown in Figure 3.6. The von Mises shear strain is visualized using OVITO software (Stukowski, 2010). It is calculated based on the Green-Lagrangian (GL) strain tensor $\boldsymbol{\eta} = \frac{1/2}{(\mathbf{E}^T \mathbf{E} - \mathbf{I})}$, where $\mathbf{E}$ is the atomic deformation gradient tensor and $\mathbf{I}$ is the unit tensor. Here, the deformation calculation relies on two sets of input particle configurations, where the reference (initial) configuration and the current (deformed) configuration are considered (Shimizu et al., 2007). Then, the von Mises shear strain is calculated by $\eta^{\text{mises}} = \sqrt{\eta_{yz}^2 + \eta_{xz}^2 + \eta_{xy}^2 + \frac{(\eta_{yy} - \eta_{zz})^2 + (\eta_{xx} - \eta_{zz})^2 + (\eta_{xx} - \eta_{yy})^2}{6}}$, where η_{ij} represents the component of the strain tensor.

As shown in Figure 3.5, with a small interference distance ω at Point A, the strain between atoms is relatively minor (dense area), where asperities are in an elastic contact phase. Then, as ω increases to Point B, the contact pressure rises and induces the gradual amorphization of atoms within the dense region, leading to the formation of Shear Transformation Zone (STZ) (above red dash line in Figure 3.5B) and finally forming a larger shear band. Here, as affected by the volumetric expansion from indentation, tensile crack propagation occurs within the asperity, which starts from the STZ. Meanwhile, meridian cracks have also been formed (right), potentially initiating the fragmentation of asperity. After that, when increasing ω to Point C, the tensile cracks at Point B continue to propagate and the direction of propagation deflects along the surface when approaching the substrate. This ultimately leads to the detachment of asperity from the substrate with the combination of tensile and shear stresses. Notably, at this stage, the meridian cracks also propagate and terminate at the surface, rendering the asperity fragmented as large particles (right). Consequently, when further increasing

ω to point D, the fragmented particles are sheared by a certain distance along the surface and a new contact phase is formed between residual parts.

Generally, the failure of α -quartz asperities at $R = 20a$ exhibits a brittle fracture-like characteristics, which is also observed at the asperity radii of $12a$, $16a$ and $24a$, as shown in Figure 3.6. However, as asperity size decreases to $R = 8a$, this fracture characteristic weakens, with most of the energy dissipated through plastic flow or amorphization. Therefore, a smaller proportion of fragmented particles at $R = 8a$ is observed (Figure 3.6). Notably, the transition from plasticity-dominated flow to fracture is also reflected in the post-peak behavior in Figure 3.3f, where steeper gradients indicate more evident fracture characteristics in α -quartz asperities.

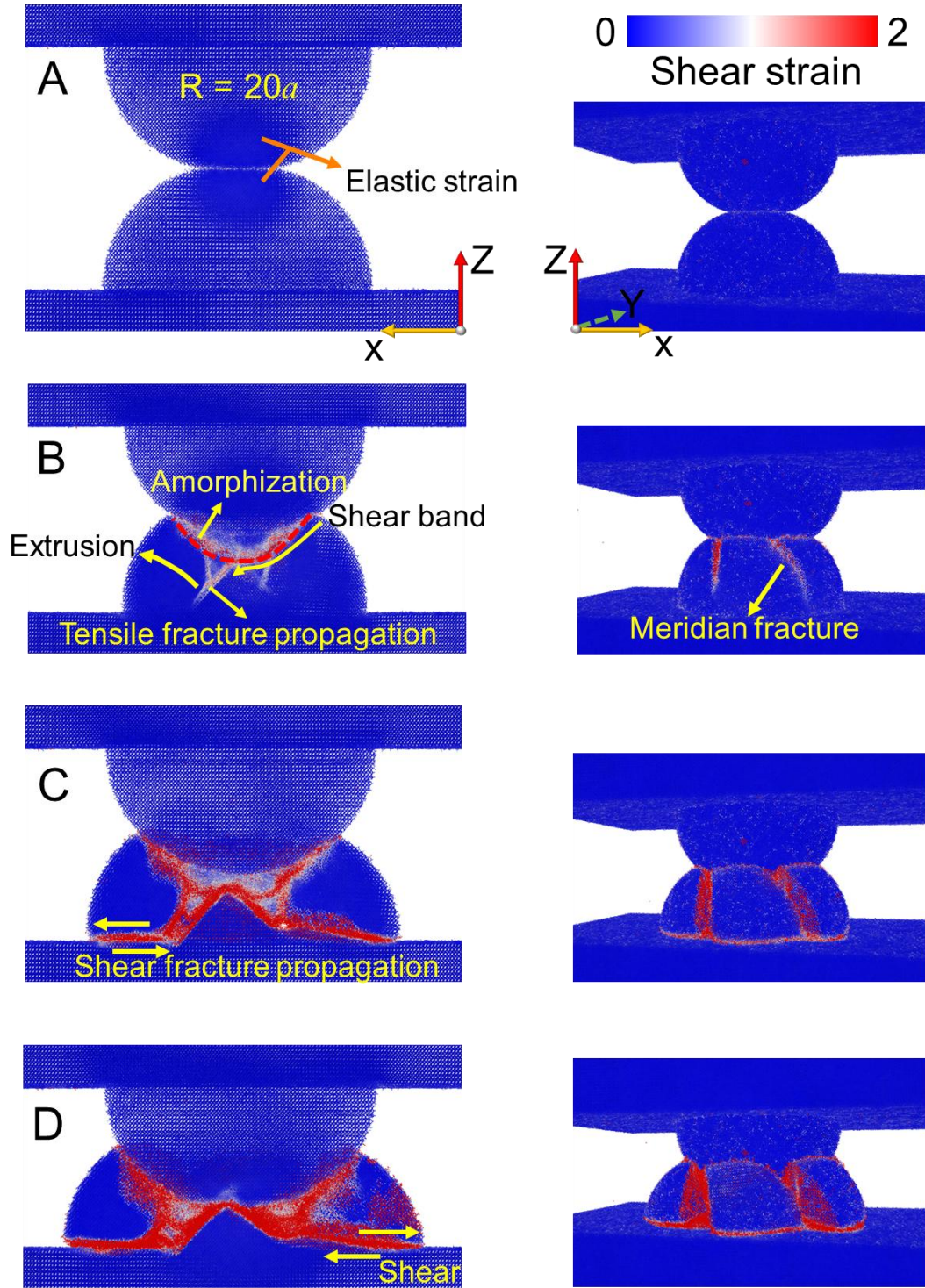


Figure 3. 5. Four typical snapshots of von Mises shear strain, which indicates the damage at $R = 20a$ (Li and Fukuyama, 2025). The left is the front view of asperity section and the right is oblique view. Figures A - D correspond snapshots at the timing of A - D shown in Figure 3.3d.

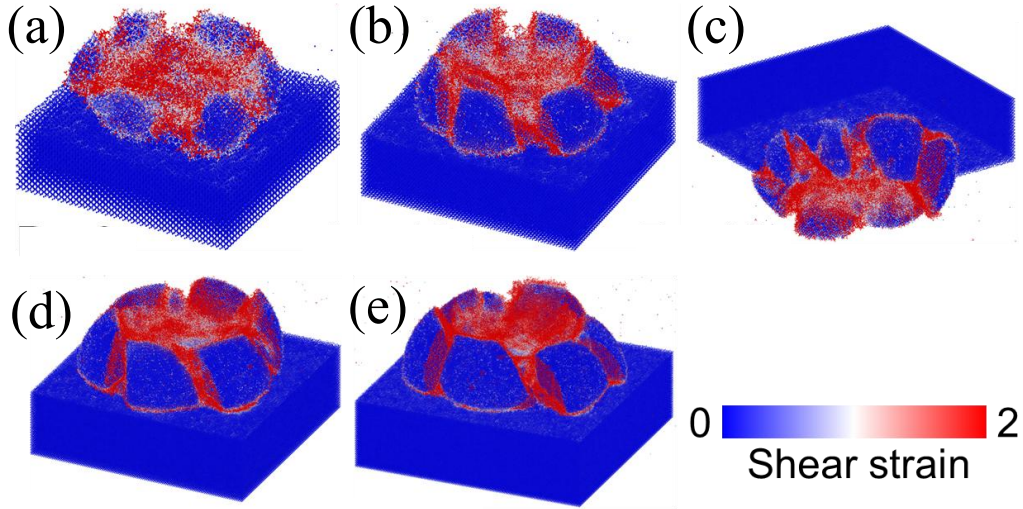


Figure 3. 6. The final breakage configurations of asperities at five different asperity radii for the case of (a) $R = 8a$, (b) $R = 12a$, (c) $R = 16a$, (d) $R = 20a$, and (e) $R = 24a$ (Li and Fukuyama, 2025). Only the breakage blocks are shown.

3.5.2 Offset contact

Figure 3.7 presents four typical snapshots of damage evolution (von Mises shear strain) in α -quartz asperities at the offset distance of $\delta = R$ and the asperity radius of $R = 20a$, corresponding to Points E, F, G, and H marked in Figure 3.4b. Additionally, since the influence of offset ratio on the failure type of α -quartz asperities is similar for $R > 8a$ (fracture occurs), the final breakage configurations at $R = 8a$ with varying offset ratios ($\delta/R = 0.2, 0.4, 0.6, 0.8$ and 1) are only shown in Figure 3.8.

As shown in Figure 3.7, the early stage of asymmetric contact (Point E) exhibits minimal strain between atoms, with the asperities remaining in an elastic contact state as indicated by the dense area. As the interference distance ω increases to Point F, the amorphization of α -quartz asperities begins at the contact surfaces due to the combined effects of compression and shear. This amorphous zone continues to grow as ω reaches Point G, where minor fracture appears and amorphous atoms are extruded toward the edges of the contact zone (right side). Finally, when ω increases to Point H, a thicker layer of amorphous atoms forms in the contact area, which is further extruded from both ends by plastic flow, leading to obvious pile-up between asperities. Here, the surface fracture is also observed at this stage.

Obviously, the above damage evolution demonstrates a plasticity-dominated deformation of asperities, in stark contrast to the brittle fracture-like failure observed in

centrosymmetric contact in Figure 3.5. This suggests that the offset distance δ significantly influences the failure type of α -quartz asperities, specifically the transition from plasticity to fracture. Larger δ will gradually promote the weakening of fracture characteristics in α -quartz asperities, leading to a transition towards plastic deformation. However, this transition is also influenced by asperity size. For example, when asperity radius decreases to $R = 8a$ (Figure 3.8), fracture occurs when δ is less than $0.6R$ and when $\delta = 0.8R$ and $\delta = R$, plastic flow governs the failure mode of α -quartz asperities. However, as shown in Figure 3.7, at $R = 20a$, fracture occurs even at $\delta = R$. Thus, the threshold (offset ratio) required for fully plastic flow of α -quartz asperities increases with asperity size. It can also be clearly seen in Figure 3.4. In Figure 3.4, the post-peak gradient of the curves still can be correlated with the transition from plasticity to fracture in α -quartz asperities influenced by the offset distance for each asperity radius. Steeper gradients (i.e., smaller δ) indicate more distinct fracture characteristics of α -quartz asperities. If the peak force disappears, it suggests a fully plastic flow.

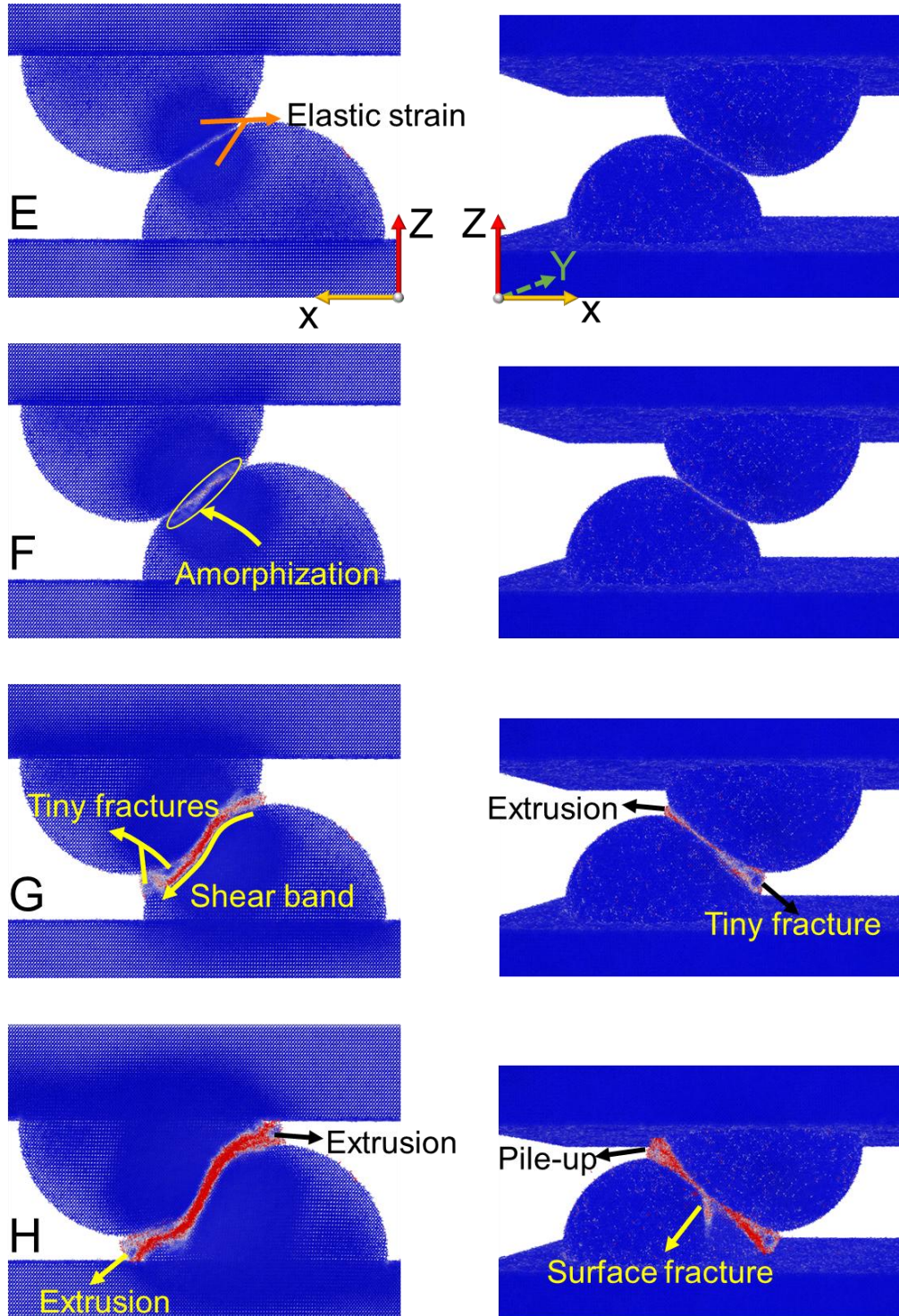


Figure 3. 7. Four typical snapshots of damage evolution (von Mises shear strain) of asperities at an offset distance $\delta = R$ and asperity radius $R = 20a$ (Li and Fukuyama, 2025). The left is the front view of asperity section and the right is oblique view. Figures E - H correspond to the snapshots at the timing of E - H shown in Figure 3.4b.

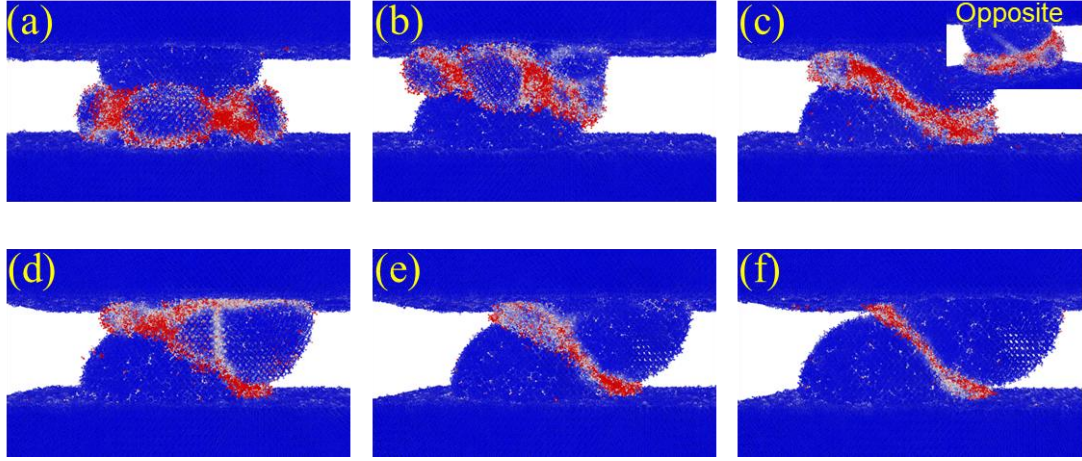


Figure 3. 8. The final breakage configurations for $R = 8a$ with varying offset distances for the case of (a) $\delta = 0$, (b) $\delta = 0.2R$, (c) $\delta = 0.4R$, (d) $\delta = 0.6R$, (e) $\delta = 0.8R$, and (f) $\delta = R$ (Li and Fukuyama, 2025). An opposite oblique view at $\delta = 0.4R$ is shown in the inset to show the occurrence of surface fracture.

3.6 Discussion

Molecular dynamics (MD) simulation is applied to investigate a series of contact behaviors of nanoscale α -quartz asperities under different asperity sizes and contact configurations. It is observed that fractures can occur in the nanoscale α -quartz asperities during the contact process. The specific failure mode of asperities, namely plastic flow or fracture, is influenced by both the asperity size and offset distance between asperity centers. However, it is worth noting that asymmetric fracture of α -quartz asperities consistently emerges, inconsistent with the traditional assumption of symmetrical destruction. It is confirmed that this phenomenon is not related to the box size, loading velocity, or loading boundary conditions. Notably, in the previous MD simulations of metal materials, a similar phenomenon was observed that asymmetric dislocations formed after the initial contact of two semi-spherical asperities (Xie et al., 2021). Moreover, Parab et al. (2017) also found an asymmetric deformation during the compression of two macroscopic glass spheres. These phenomena may be linked to surface energy or the non-uniform pressure distribution on the contact surface, which stems from the asymmetric crystal structure of the outer layers of α -quartz asperities.

Furthermore, the contact stiffness of nanoscale α -quartz asperities follows the Hertz model in the elastic contact stage. The macroscopically elastoplastic models fail to predict the non-elastic deformation of nanoscale α -quartz asperities in several key

aspects, such as the evolution of the normal contact force and critical interference distance. This discrepancy may arise because macroscopic models do not incorporate the surface and friction properties at the nanoscale, as well as the occurrence of fracture in asperities. Additionally, the simulation results also show that the temperature of the system increases with the normalized interference distance during contact process, as typically shown in centrosymmetric contact case (Figure 3.9). Here, the temperature T is calculated by $T = \frac{2\langle K \rangle}{(3N-f)k_B}$, where $\langle K \rangle$ is the total kinetic energy, N is the number of particles, $3N-f$ is the number of degrees of freedom, f is the number of degrees of freedom that are constrained and k_B is the Boltzmann constant. Such a change in temperature is also overlooked in macroscopic models but could have an important impact on the contact deformation in the nanoscale α -quartz asperities. Here, temperature rise is size-dependent and it could be a function of interference distance scaled by R .

Moreover, all these factors also likely contribute to the phenomena observed in Figure 3.10 and Tables 3.A1–3.A2, where the normalized critical interference distance and the evolution of the normalized contact force $F/F_{\max}$ versus the normalized interference distance ω/R fail to converge across different asperity sizes after peak force. Hence, developing contact models that integrate more physical factors in the nanoscale is essential and necessary in future studies.

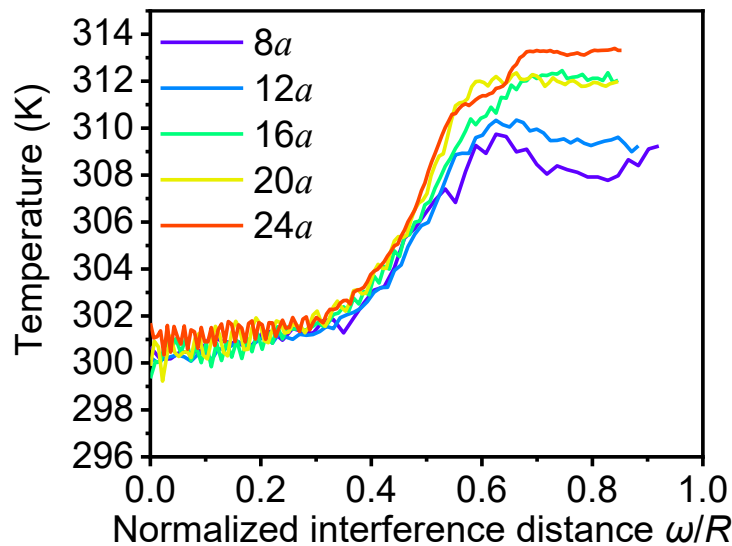


Figure 3. 9. The temperature of the system as a function of the normalized interference distance under varying asperity radii ($R = 8a$, $12a$, $16a$, $20a$ and $24a$) in centrosymmetric contact of asperities (Li and Fukuyama, 2025).

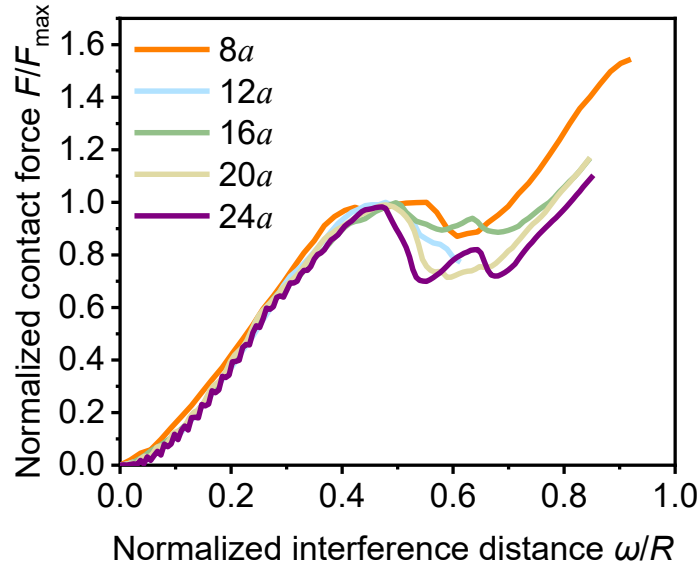


Figure 3. 10. The normalized contact force and normalized interference distance under varying asperity radii ($R = 8a, 12a, 16a, 20a$ and $24a$) in centrosymmetric contact of asperities (Li and Fukuyama, 2025).

3.7 Conclusion

The nanoscale contact behavior of single α -quartz asperity composed of millions of atoms is investigated by molecular dynamics simulations. The influence of asperity size and offset distance between asperity centers on contact-induced failure is investigated. Additionally, simulation results are also compared with macroscopic elastic (Hertz) and elastoplastic contact models (CEB, ZMC, KE) in terms of the normal contact force versus interference distance.

The results reveal that the nanoscale single-asperity contact of α -quartz undergoes both elastic and plastic deformation stages. However, fracture can occur during the contact process, where the traditional elastic and elastoplastic assumptions in the macroscopic models are not fully applicable to contact modeling of nanoscale α -quartz asperities. Moreover, the normalized interference distance for yielding in nanoscale α -quartz asperities is 4 to 5 times higher than the predictions from the macroscopic CEB, ZMC, and KE models. Therefore, a multiscale disparity exists between the macroscopical model predictions and the actual contact behavior at the nanoscale.

It is also found that the asperity size and offset distance play a crucial role in determining the contact failure mode of nanoscale α -quartz asperities. In the centrosymmetric contact, larger α -quartz asperities exhibit brittle fracture-like behavior, while smaller asperities primarily dissipate energy through plastic flow. This failure transition is also observed in the offset contact case, where larger offset distance typically leads to plastic deformation. The threshold of offset ratio for fully plastic flow increases with the nanoscale α -quartz asperity size. Notably, in both of the centrosymmetric and offset contact cases, fracture in α -quartz asperities leads to steeper post-peak gradients of the normal contact force versus interference distance, with fully plastic flow typically exhibiting a hardening process.

Based on the simulation results, the empirical contact models are proposed for nanoscale single α -quartz asperity contact in centrosymmetric cases.

APPENDICES

Appendix 3.A. Empirical contact models from MD simulations

Here, empirical fitting has been performed between the normal contact force and interference distance for the case of centrally symmetric contact based on the simulation data. Due to the complex evolution after the peak contact force, the non-elastic contact stage before the peak force (e.g., between points A and B in Figure 3.3d) and the final contact stage (e.g., after point C in Figure 3.3d) are only fitted. For the pre-peak contact behavior, the Logistic Curve is empirically employed to fit the data, which is described as:

$$F = \frac{L}{1 + e^{-k(\omega - \omega_0)}} \quad (3. A1)$$

where ω represents the interference distance; L , k , and ω_0 are the fitting parameters. Moreover, based on the fitting results shown in Figure 3. A1f, L can be further expressed as $8.95R^{1.9}$. The normalized ω_{cl} (ω_{cl}/R , the onset of elastoplastic behavior) and ω_p (ω_p/R , the arrival to the peak force) as well as the fitting parameters are presented in Table 3.A1. For the final stage of contact evolution, the power function is used for fitting,

which is expressed as:

$$F = \beta + \eta(\omega - \omega_r)^m \quad (3. A2)$$

where ω_r represents the interference distance corresponding to the residual normal contact force; β , η , and m are the fitting parameters. The fitting curves are shown in Figure 3.A2 and the normalized ω_r (ω_r/R) as well as the fitting parameters are shown in Table 3.A2.

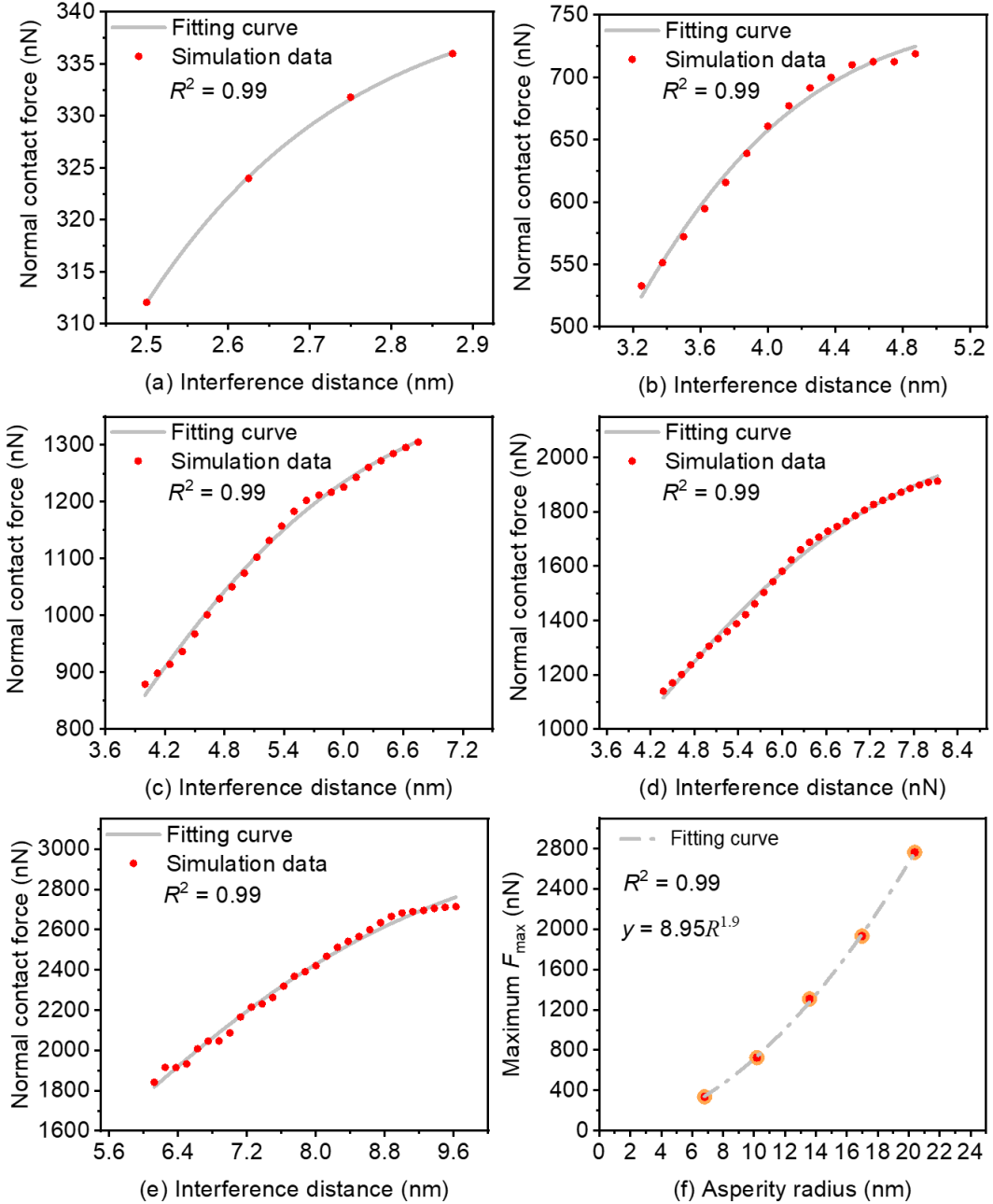


Figure 3.A1 The normal contact force as an empirical function of interference distance under different asperity radii (a) $R = 8a$; (b) $R = 12a$; (c) $R = 16a$; (d) $R = 20a$; (e) $R = 24a$. (f) The maximum normal contact force as an empirical function of asperity radii (Li and Fukuyama, 2025).

Table 3.A1. The normalized ω_{c1} and ω_p as well as the fitting parameters (Here, the unit of a is scaled up to nanometers) (Li and Fukuyama, 2025).

R	$0.8a$	$1.2a$	$1.6a$	$2a$	$2.4a$
ω_{c1}/R	0.37	0.32	0.29	0.26	0.30
ω_p/R	0.42	0.48	0.50	0.48	0.47
k	4.36	1.45	0.74	0.60	0.50
ω_0	1.97	2.69	3.42	4.19	5.43

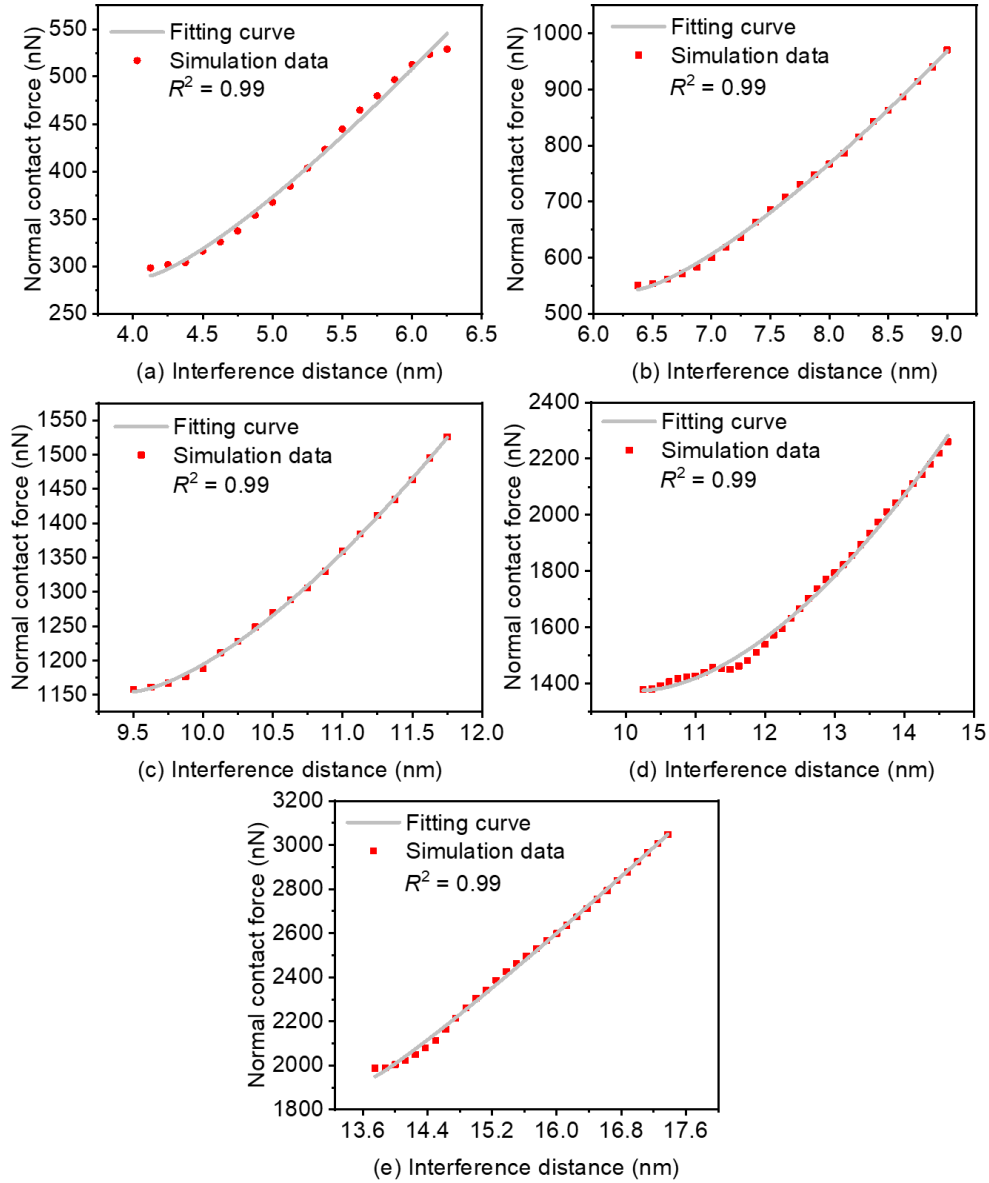


Figure 3.A2 The normal contact force as an empirical function of interference distance under different asperity radii (a) $R = 8a$; (b) $R = 12a$; (c) $R = 16a$; (d) $R = 20a$; (e) $R = 24a$ (Li and Fukuyama, 2025).

Table 3.A2. The normalized ω_r and the fitting parameters (Here, the unit of a is scaled up to nanometers) (Li and Fukuyama, 2025).

R	$0.8a$	$1.2a$	$1.6a$	$2a$	$2.4a$
ω_r/R	0.61	0.64	0.70	0.60	0.67
β	290.12	543.28	1154.66	1376.34	1950.35
η	98.21	117.48	110.99	71.01	266.82
m	1.27	1.33	1.49	1.72	1.10

CHAPTER IV

Plastic Wear Mechanism of Asperities

4.1 Introduction

In this chapter, a series of 3-D wear processes of two interlocked α -quartz asperities are explicitly reproduced. The dynamic wear damage under different normal forces and loading velocities is investigated. Besides, the simulation results are compared with the widely used Archard law (Archard 1953) to discuss its multiscale applicability in the wear volume prediction.

The results present a transition from an atom-by-atom wear attrition to layer removal as the normal force increases. Higher normal forces generally result in greater wear volumes and increased shear damage of α -quartz asperities, which can be attributed to the increased contact area and decreased energy barriers. Conversely, increasing the loading velocity generally decreases the wear damage and the wear volume of α -quartz asperities, which can be related to the decreased contact area and weaker force interactions between asperities caused by the increment of normal distance. Furthermore, the Archard law is limited to quantify the wear volume of nanoscale α -quartz asperity pairs, as it overlooks the velocity-dependent specific wear rate (w_s) and the transition from high w_s at initial running-in-like stage to a relatively low w_s at steady state-like stage. Instead, with a consideration of an instantaneous tangential force, the tangential shear work serves as a robust predictor as it generally scales with the wear volume. These results can provide great implications for the accurate modeling of multiscale wear phenomena and important explanation on the wear mechanism under high-speed rock friction experiments.

4.2 Numerical Model

Figure 4.1 shows a schematic description of the material and simulation model. The material parameters in Figure 4.1a are consistent with those in Chapter III and are therefore not repeated here and in the subsequent chapters. The simulation box ($L_x = 237.730 \text{ \AA}$, $L_y = 137.253 \text{ \AA}$ and $L_z = 172.796 \text{ \AA}$) includes about 2.7×10^5 atoms (Figure 4.1b). Two identical and semi-spherical asperities (diameter $d = 67.922 \text{ \AA}$) were located on the upper and lower surfaces respectively, with the centers being a radius apart. They

were initially non-contact and then pressed together by the normal force to be in contact. The system was divided into three parts, namely rigid, thermostat (Nose'–Hoover thermostat) and freely deformable layers, respectively. While the bottom of the lower block was fixed, a constant normal force F_n and a loading velocity V were applied respectively on the top layer of the upper block where it was allowed to move in the z -direction. Additionally, the pbz was applied along the x - and y -directions, respectively.

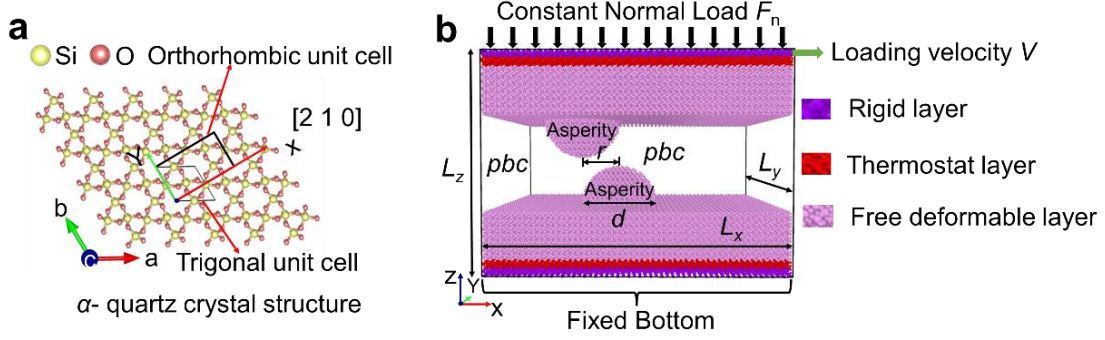


Figure 4. 1. A schematic illustration of the simulated material and model. (a) The crystal structure of α -quartz and (b) the simulation model. L_x , L_y and L_z stand for the dimension of model space. d is the diameter of asperity and r is the horizontal distance between the centers of two asperities ($r = d/2$).

4.3 Simulation Procedure

The simulation packages and timestep are the same as those used in Chapter III and are therefore not repeated here and in the subsequent chapters. The simulation procedures consist of four stages. The energy minimization was first performed to obtain the initial configuration. Then, the canonical ensemble (NVT) (damping coefficient 0.25) was applied to relax the atomistic system at temperature 300 K for 500 ps. After this stage, a constant normal force was applied on the top surface of the upper rigid layer to press asperities together and the relax procedure was repeated for 2500 ps to make the box stable in the z direction. Simultaneously, the freely deformable layer was transformed from the NVT to the micro-canonical ensemble (NVE) system. Finally, the friction process was initiated by applying a constant shear loading velocity.

Overall, two series of parameters are investigated. Group1 consists of 15 different F_n (1 nN $\sim$ 19.25 nN) under $V = 10$ m/s to explore the normal force-dependent wear mechanisms. Group2 consists of 15 different V (from 10 m/s to 45 m/s with an

increment of 2.5 m/s) under five different F_n (1 nN, 2.57 nN, 5.13 nN, 8.98 nN, 11.55 nN) to explore the velocity-dependent wear mechanisms. The normal force of 1 nN corresponds to the normal stress of about 3.06 MPa on the top surface of the box. The averaged force ratio ξ_a is investigated in Group1 by using the time-averaged tangential force (F_{ta}) with the normal force (F_n) based on the formula $F_{ta} = \xi_a F_n + c$, where c is the cohesion.

4.4 Potential Function Verification

Here, to further illustrate the performance of the Vashishta potential function on the tribology system, the evolution of tangential force (F_t) measured under different normal forces (1 nN ~ 19.25 nN) with a constant loading velocity of 10 m/s is shown in Figure 4.2a. Loading distance L denotes the displacement of the rigid layer ($V \times$ sliding time), which might not always be identical to local slip displacement on the asperity contact. F_t is obtained by summing the tangential force of atoms in the thermostat and rigid layer (Zheng et al., 2013). In general, as shown in Figure 4.2a, during the strengthening stage, the tangential force initially rises from zero and then to its peak value with loading distance (static friction force), which is followed by the weakening regime (dynamic friction force). As two asperities separate in the final stage, the tangential force diminishes approximately to zero. This pattern follows the evolution of friction force observed in the similar models from other simulations and methods (Mulvihill et al., 2011; Vadgama et al., 2015). Besides, the static friction force generally increases with the normal force, which is consistent with conclusions identified in laboratory experiments (Byerlee, 1978). Therefore, the 1997-version Vashishta potential can generally reproduce the characteristics of tribology system.

Moreover, an intriguing result is found that the averaged force ratio ξ_a is measured at 0.7 (Figure 4.2b), which is in good agreement with dry friction coefficient from the nanoscale friction tests of quartz-rich rocks under constant temperature (Chen et al., 2013). Here, supplementary calculations by changing the asperity radius ($R = d/2$) and horizontal separation distance (r) between asperity centers (see in Appendix 4.A) are also conducted. The results suggest that the averaged force ratio ξ_a is more sensitive to r than R . ξ_a is closer to the macroscopic friction coefficient in the case of interlocked

asperities. Besides, the tangential force and the weakening distance of friction curves are also obviously influenced by r .

However, it should be emphasized that these results provide only a quite simple understanding of the nanoscale friction properties with a pair of α -quartz asperities. Macroscopic rock surfaces involve the interactions of multiple and multiscale asperities as Amontons' Law incorporates (Candela et al., 2012; Beeler, 2023). Moreover, the friction results from single-asperity contact typically show some differences compared to macroscopic models (Mo et al., 2009; McClimon et al., 2020). Establishing the multiscale relation between the averaged force ratio ξ_a and macroscopic friction coefficient remains a significant challenge to be solved (Vakis et al, 2018; Abdelbary, 2020).

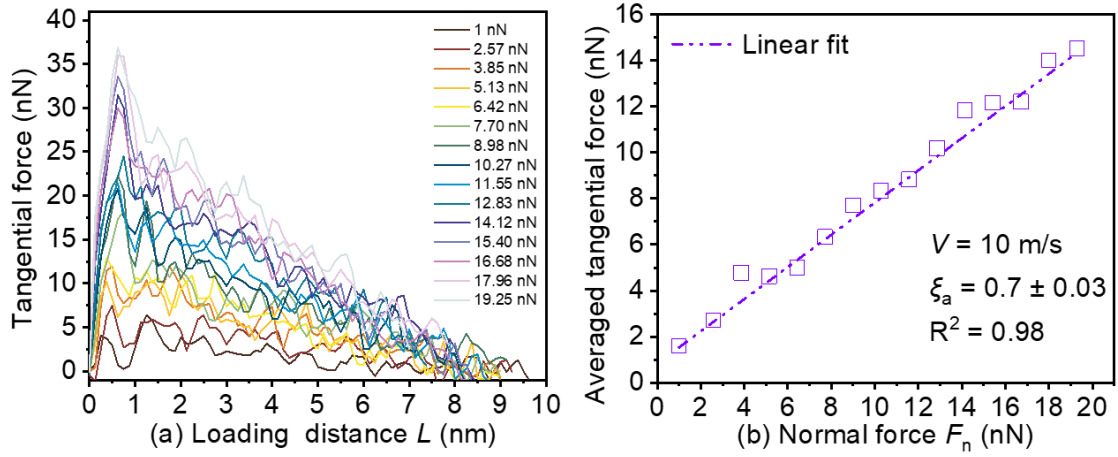


Figure 4. 2. The evolution of tangential force and averaged force ratio. (a) The evolution of tangential force with loading distance under different normal forces (1 nN $\sim$ 19.25 nN) at the loading velocity of 10 m/s. (b) The correlation plot of averaged tangential force (F_{ta}) with the normal force (F_n) at the loading velocity of 10 m/s. The gradient of the regression line becomes the averaged force ratio ξ_a . Note that the averaged tangential force F_{ta} is the average value of tangential force F_t (Figure 4.2a) under every normal force at the same loading distance ($L = 7$ nm).

4.5 Dynamic Wear Mechanism

Figure 4.3 shows the snapshots of wear processes of asperities under different normal forces (1 nN, 2.57 nN, 5.13 nN, 8.98 nN, 11.55 nN) at the loading velocities of 10 m/s and 40 m/s. Corresponding snapshots of von Mises local shear strain at the loading

velocities ranging from 10 m/s to 40 m/s are shown in Figure 4.4. Here, in Figure 4.5, the snapshots of wear processes under different normal forces (3.85 nN ~17.96 nN) at the loading velocity of 10 m/s are also shown.

It is observed that the increasing normal force can obviously exacerbate the wear of asperities, with a gradual increase in the shear damage zone identified in Figures 4.3-4.5. It starkly contrasts with the wear phenomena induced by the increasing loading velocity, where the wear damage of asperities generally shows declining trend. On the other hand, the wear attrition mechanisms on asperities are less influenced by the loading velocity but is primarily governed by the normal force. Here, the typical wear attrition mechanisms under the low (2.57 nN) and the high normal force (19.25 nN) at $V = 10$ m/s and $L = 6$ nm and $L = 8$ nm are shown in Figure 4.6.

Under the low normal force, worn atoms are primarily from the bonding and shear traction between interfacial atoms, with single atom or molecule attrition scattered on the shallow surfaces. This wear process resembles the atom-by-atom wear mechanism (Bhaskaran et al., 2010; Wang et al., 2021b). However, it contrasts remarkably with the wear observed under the high normal force condition, where a significant plastic flow by layered shear motion predominates and atoms on asperities are more prone to be detached as clusters. Meanwhile, the higher normal force results in the larger clumps of attrition on asperities (see also in Figure 4.5). Besides, there is a flow of worn debris between asperities under both normal force conditions, with the size of worn debris still dependent on the normal force.

Here, all dynamic wear damages of α -quartz asperities are mainly concentrated on the smoothing process, where the adhesive removal is dominant. This observation supports the idea that adhesive wear dominates in the wear processes of rock asperities at small scales (Candela & Brodsky, 2016).

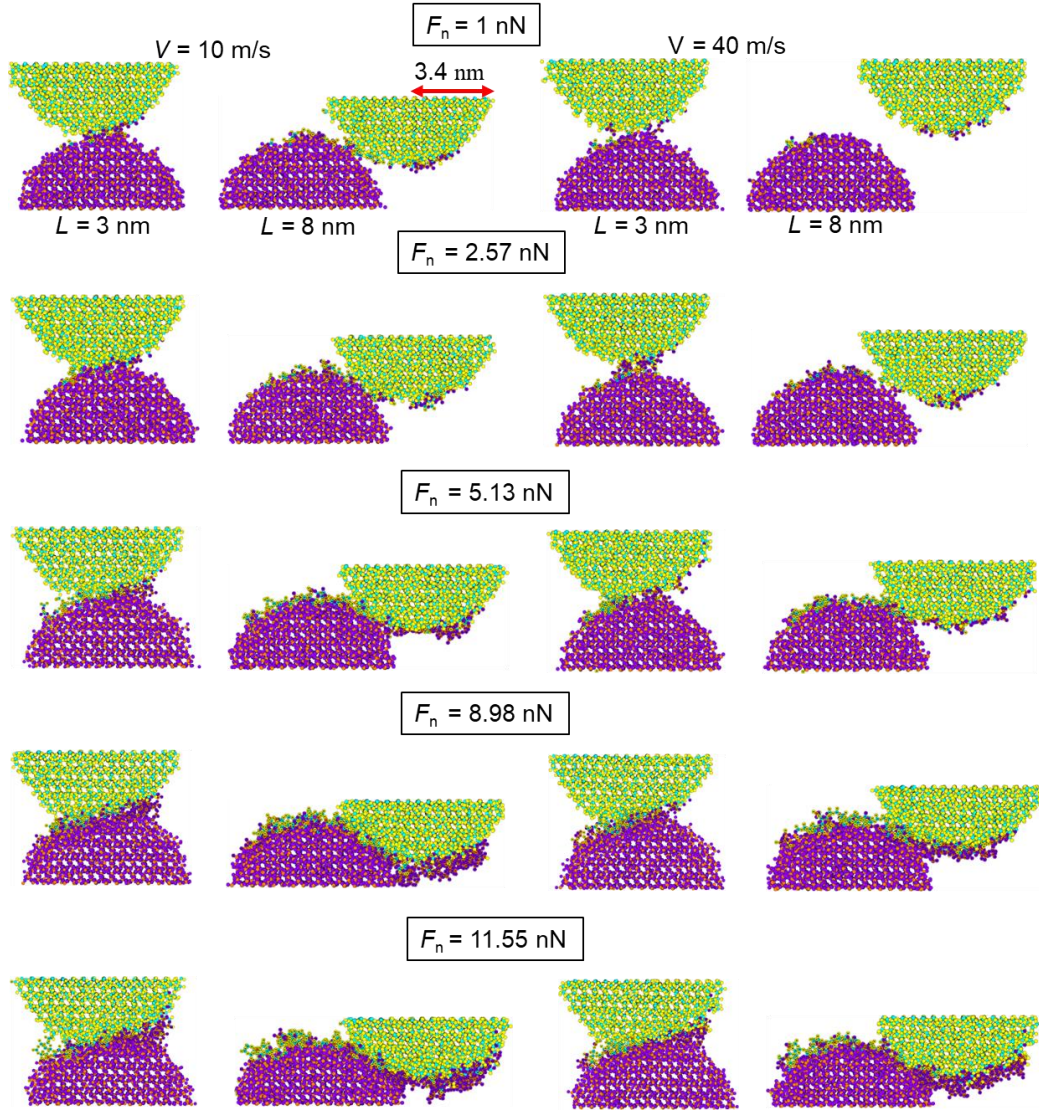
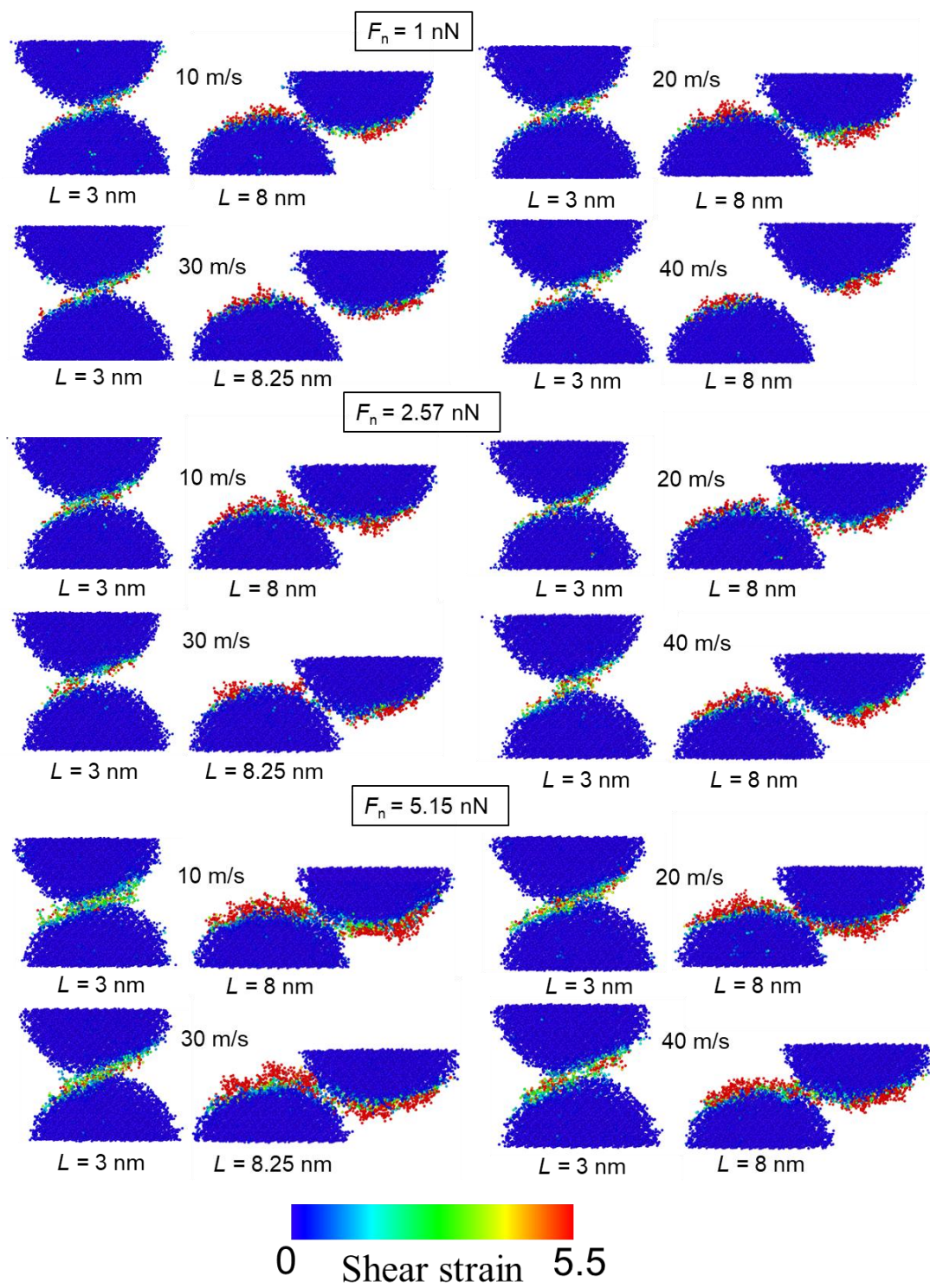


Figure 4. 3. The snapshots of wear processes under different normal forces (1 nN, 2.57 nN, 5.13 nN, 8.98 nN, and 11.55 nN) at the loading velocities of 10 m/s and 40 m/s. The worn atoms were defined if Euclidean distance between its locally original and real-time position on asperities is over cutoff distance ($5.5 \text{ \AA}$). Color scheme of each particle is same as in Figure 4.6.



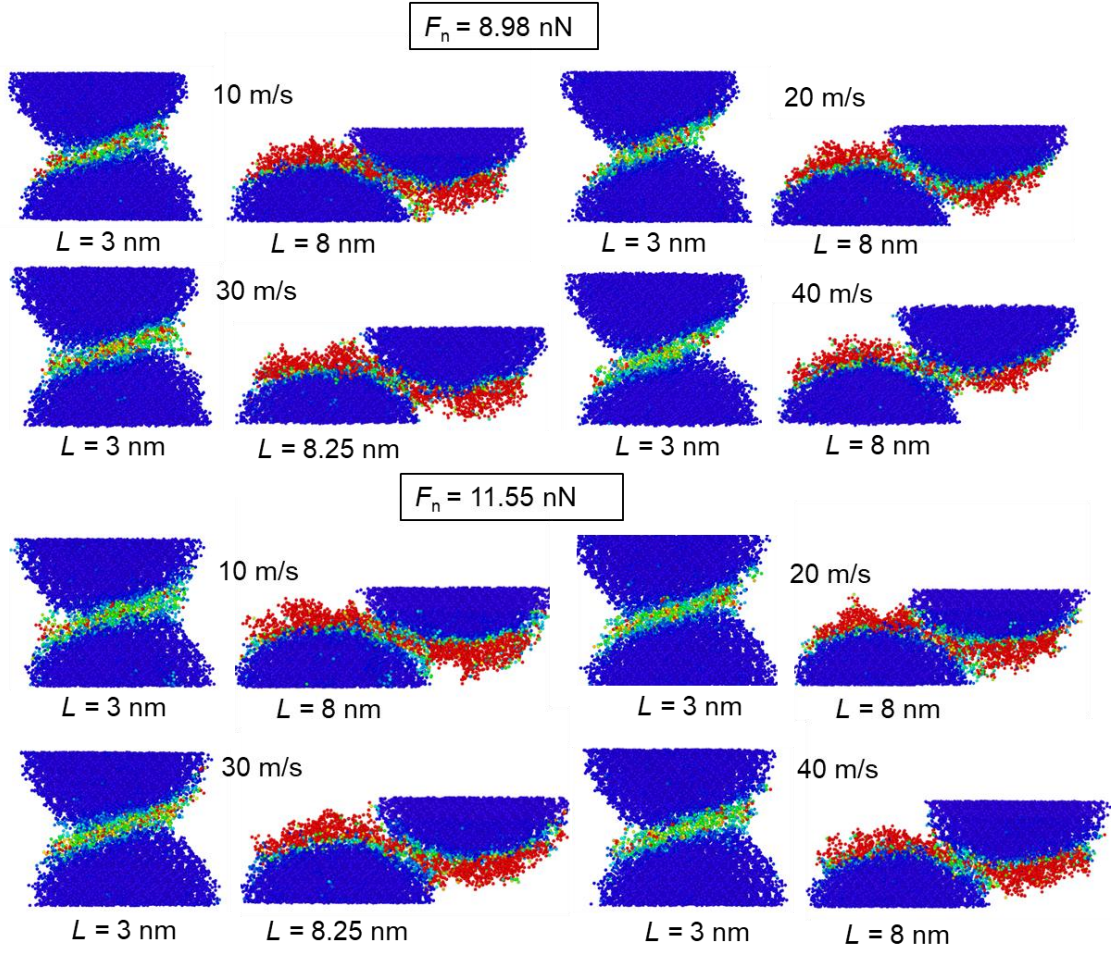


Figure 4. 4. The snapshots of von Mises local shear strain η^{mises} at the loading velocity ranging from 10 to 40 m/s under different normal forces (1 nN, 2.57 nN, 5.13 nN, 8.98 nN, 11.55 nN).

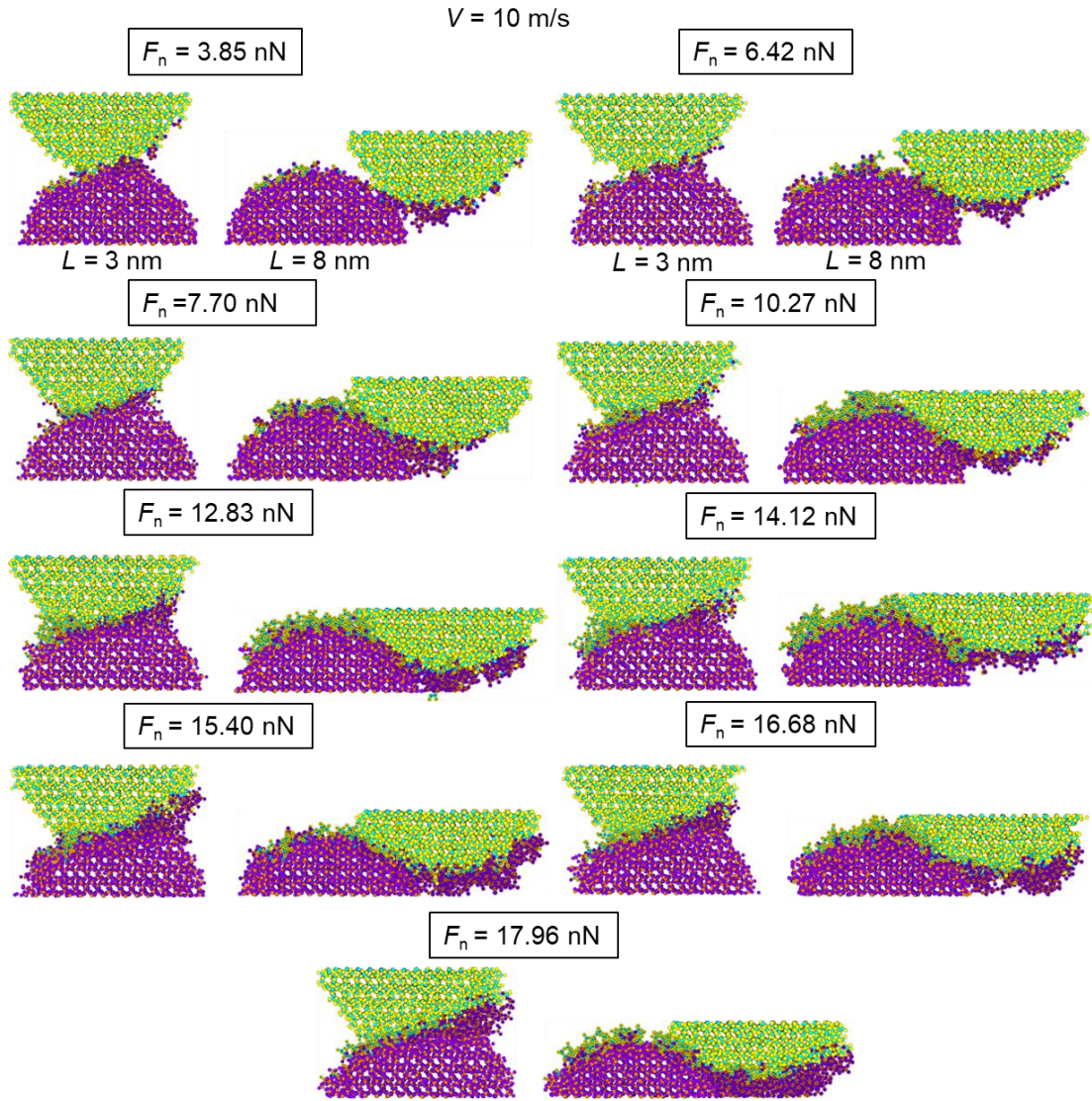


Figure 4. 5. The snapshots of wear processes under different normal forces (3.85 nN ~17.96 nN) at the loading velocity of 10 m/s.

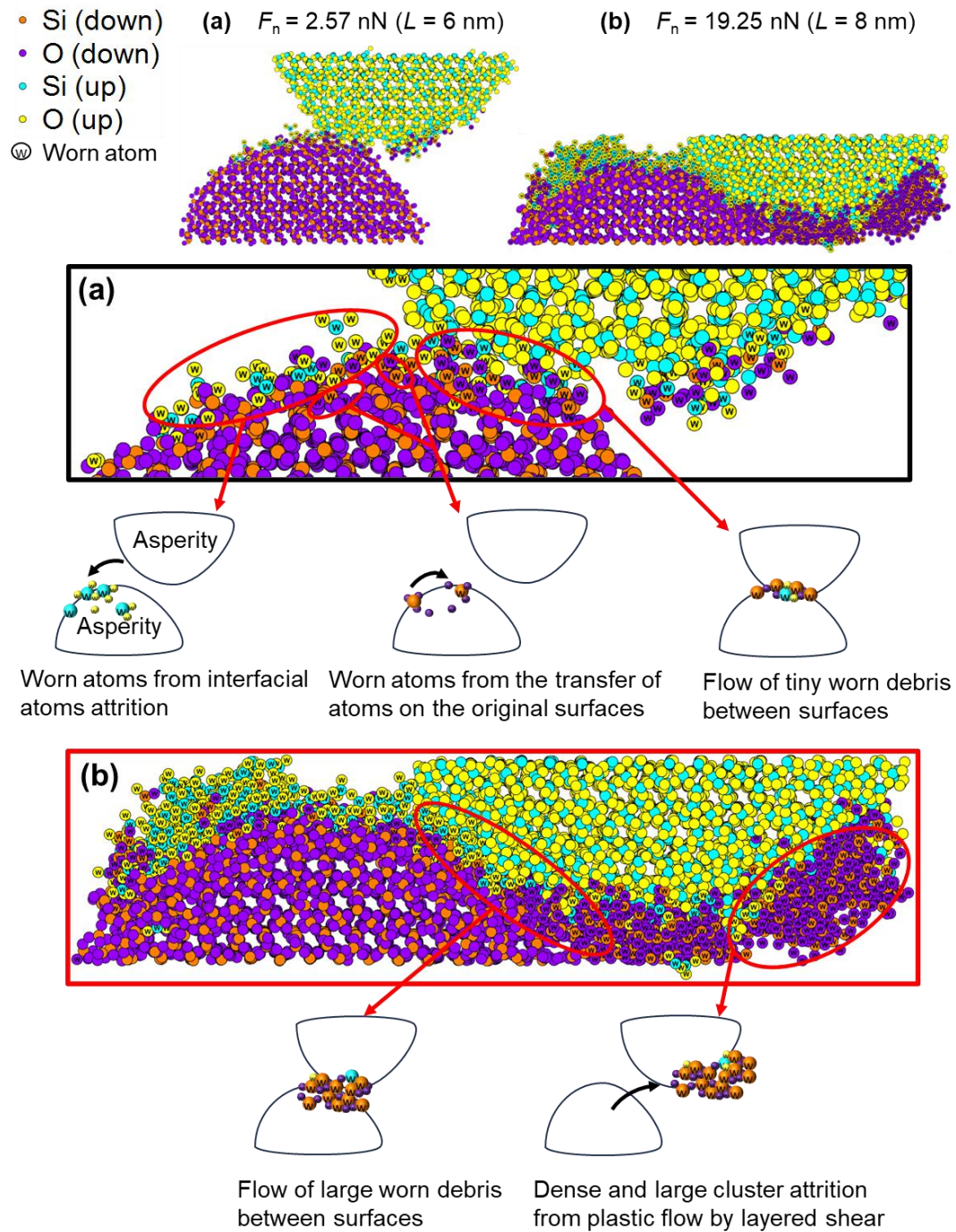


Figure 4. 6. The typical wear attrition mechanisms under (a) the low ($F_n = 2.57 \text{ nN}$) and (b) the high normal force ($F_n = 19.25 \text{ nN}$) at the loading velocity of 10 m/s and loading distance of 6 nm and 8 nm .

4.6 Comparison with the Archard Law

The specific expression of the Archard law can be seen in Section 1.2.2. Notably, Archard law typically predicts the macroscopic wear volume involving multiple asperity contacts. However, its origin lies in the modeling of the wear volume at the single-asperity contact (Archard, 1953). Therefore, investigating the performance of the Archard law, specifically the commonly assumed proportional relationship ($W \propto F_n L$), in the context of individual asperity contact is essential for a comprehensive understanding of its multi-scale applicability.

Figure 4.7 shows the wear volume versus L/R under different F_n and V (total loading distance is about 8.125 nm and $R = d/2 = 3.4$ nm) as well as corresponding specific wear rate (w_s). The specific wear rate is calculated by the formula $w_s = \frac{W}{F_n L}$ (see Eq. 1.5). It is observed that the wear volume generally presents a positive correlation with the normal force (Figure 4.7a), which aligns with the wear results identified in most macroscopic experiments (Wang & Scholz., 1994; Hirose et al., 2012; Boneh et al., 2013, 2014). Furthermore, both the running-in-like and steady state-like wear stages as exhibited macroscopically (Boneh et al., 2014) are also identified during the nanoscale wear processes (Figure 4.7g). Specifically, the high specific wear rate w_s is recorded during the initial stage of slipping (running-in-like stage), followed by a relatively low but steady w_s (steady state-like stage) (Figure 4.7g). This observation is inconsistent with the constant specific wear rate w_s over the entire loading distance requested by the Archard law. Here, the transition from the running-in-like stage to the steady-state-like one is about at $L/R = 0.59$. On the other hand, the wear volume generally decreases with the increasing loading velocity under all normal force conditions (Figure 4.7b-f). Particularly, the wear volume under the low normal forces (1nN and 2.57 nN) is obviously sensitive to the high loading velocities, with the value remaining nearly unchanged after sliding a short distance at 1 nN (shadow part). Such an obvious decreasing trend of wear volume indicates a strong velocity-dependent specific wear rate as also identified by Boneh et al. (2013) from rotary shear friction experiments (limestone and quartz-rich rocks), highlighting the limitation of the Archard law.

Moreover, the averaged w_s is calculated using the w_s data in steady-state-like region ($0.59 < L/R < 2.4$). The averaged w_s generally shows a weak dependence on F_n while the dependence on V is evident (Figure 4.7h). This indicates that in the steady-state-like

region, W almost presents a linear relationship with F_n under a fixed V . Therefore, when exploring the total wear volume (W_t) in Figure 4.8a, a linear relationship between W_t and F_n is well presented across all V . Here, W_t is defined as the W value at $L \approx 8.125$ nm. However, this linearity may break down under higher F_n in Figure 4.8b. Finally, in Figure 4.9, the velocity-decreasing trend of W_t also occurs due to the velocity-decreasing averaged w_s .

.

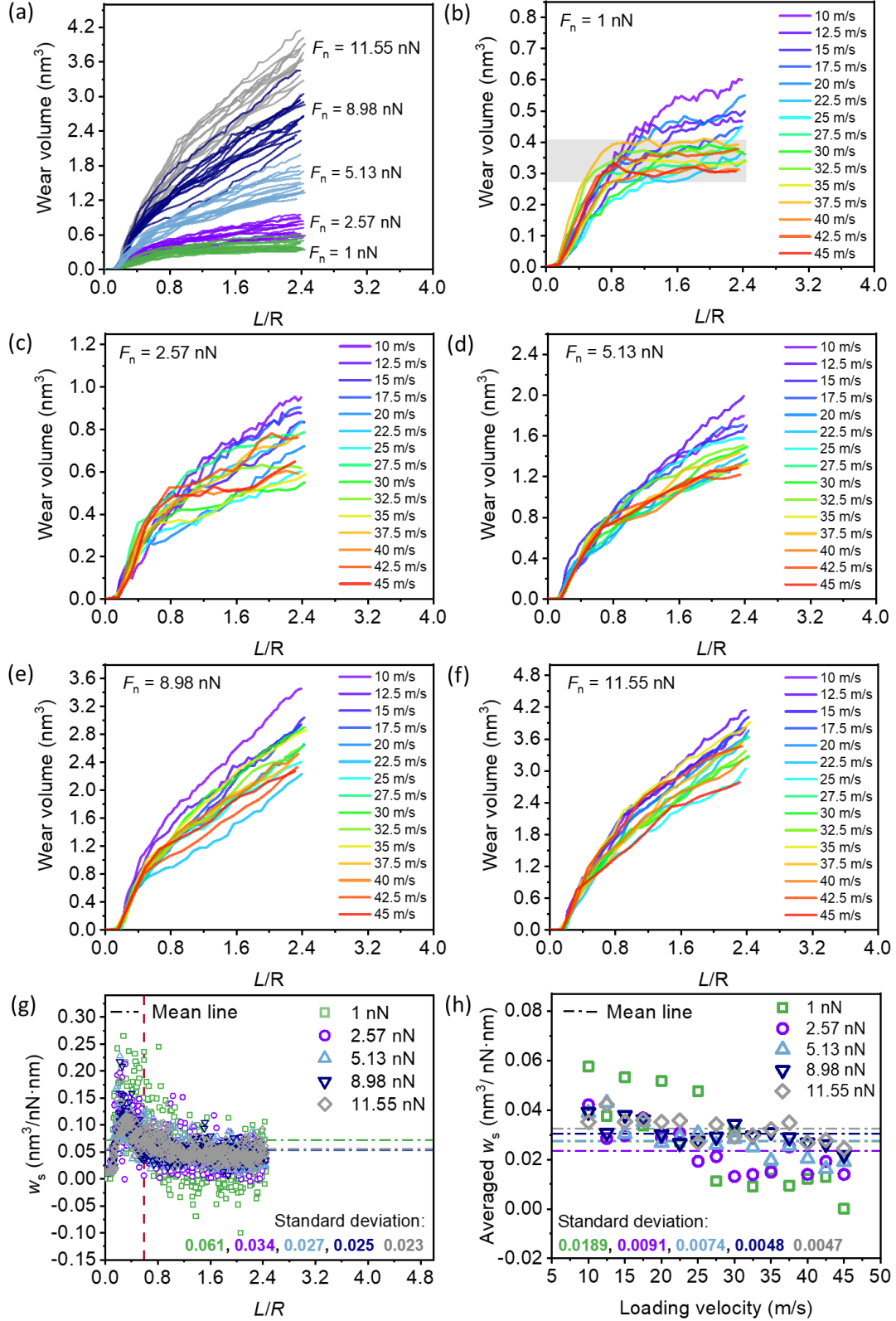


Figure 4. 7. (a) The wear volume W versus dimensionless loading distance L/R up to 2.4 ($L \approx 8.125$ nm) under different V (10 m/s $\sim$ 45 m/s) at $F_n = 1$ nN, 2.57 nN, 5.13 nN, 8.98 nN, and 11.55 nN. W versus L/R under different V at F_n (b) 1 nN, (c) 2.57 nN, (d) 5.13 nN, (e) 8.98 nN, and (f) 11.55 nN. (g) The specific wear rate w_s

versus L/R under different F_n (1 nN, 2.57 nN, 5.13 nN, 8.98 nN, and 11.55 nN) and V (10 m/s ~ 45 m/s). Vertical broken line indicates the transition between run-in-like and steady-state-like stages. (h) The averaged w_s in the steady-state-like region versus V (10 m/s ~ 45 m/s) under different F_n (1 nN, 2.57 nN, 5.13 nN, 8.98 nN, and 11.55 nN).

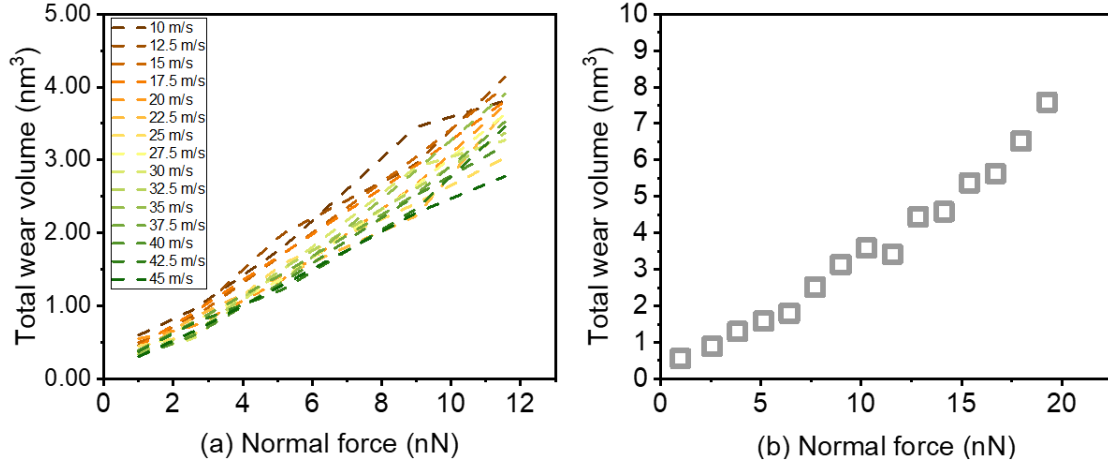


Figure 4. 8. The total wear volume under different normal forces and loading velocities. (a) The total wear volume under different normal forces (1 nN, 2.57 nN, 5.13 nN, 8.98 nN, 11.55 nN) and loading velocities (10 m/s ~ 45 m/s) ($L \approx 8.125$ nm); (b) The total wear volume under the normal force ranging from 1 nN to 19.25 nN at the loading velocity of 10 m/s. Note that, as the smallest weakening distance is 7 nm at 19.25 nN (when exceeding 7 nm, the wear debris on the upper asperity will interact with the low surface), the total wear volume in Figure 4.8b is obtained at $L = 7$ nm.

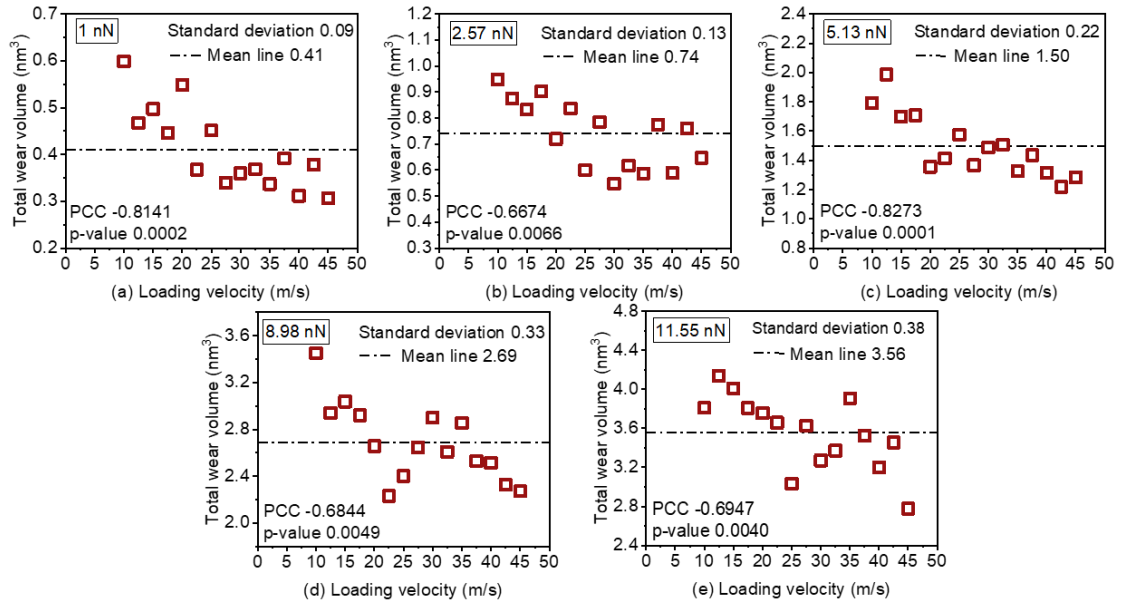


Figure 4. 9. The total wear volume under different loading velocities (10 m/s ~ 45 m/s) at the normal force (a) 1 nN, (b) 2.57 nN, (c) 5.13 nN, (d) 8.98 nN, and (e) 11.55 nN ($L \approx 8.125$ nm).

4.7 Wear Volume Prediction

As discussed above, the empirical Archard law is limited to predict the material loss of interlocked α -quartz asperities due to varying w_s under a given normal force. Here, based on Reye's (1860) perspective, coupled with the results from molecular dynamics and macroscopic studies (Badt et al., 2016; Aghababaei et al., 2017), under different normal forces and loading velocities, the wear volume of α -quartz asperities as a function of loading distance can be well predicted by considering the proportionality between the tangential shear work and the wear volume at the nanoscale (Figures 4.10-4.12a):

$$W = \frac{1}{q} \int F_t dL \quad (4.1)$$

where W represents the wear volume, F_t is a time-varying tangential force as stated by Ramalho (2010), L is the loading distance and q is the scaling factor. However, it should be noted that further analysis of rotary shear experiments on granite conducted by Mizoguchi & Fukuyama (2010) reveals that while the overall linear relationship between the friction work and the wear volume holds, scaling factor q varies under different experimental conditions (Figure 4.12b). Therefore, when upscaling Eq. (4.1)

in future studies, more investigations are necessary to evaluate the variation of q , where factors, such as the influence of gouge particles, thermal effects, and the different wear mechanisms of asperities during macroscopic friction process, are needed to be further considered.

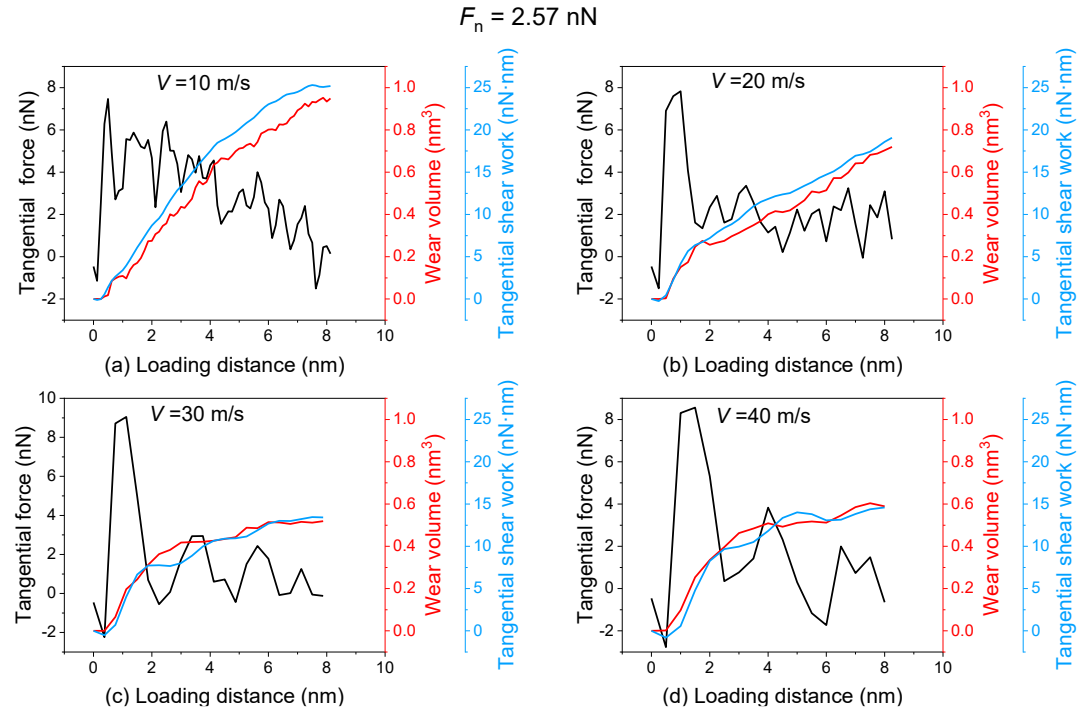


Figure 4. 10. The tangential force, wear volume and tangential shear work with loading distance at 2.57 nN under the loading velocities of (a) 10 m/s, (b) 20 m/s, (c) 30 m/s, and (d) 40 m/s.

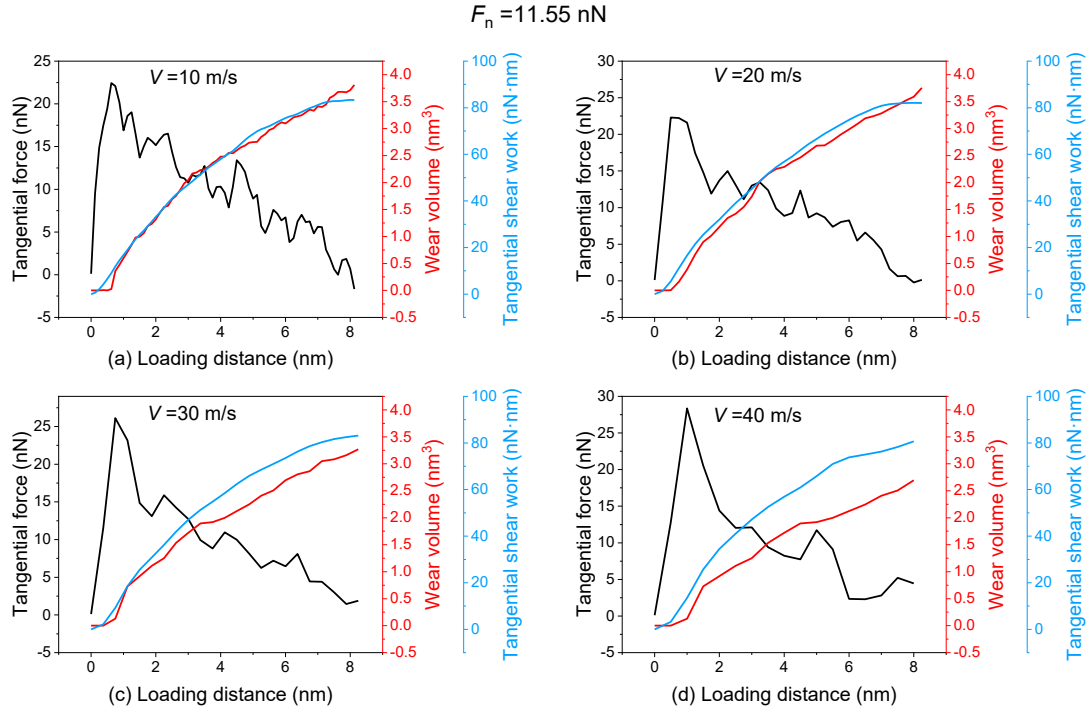


Figure 4. 11. The tangential force, wear volume and tangential shear work with loading distance at 11.55 nN under the loading velocities of (a) 10 m/s, (b) 20 m/s, (c) 30 m/s, and (d) 40 m/s.

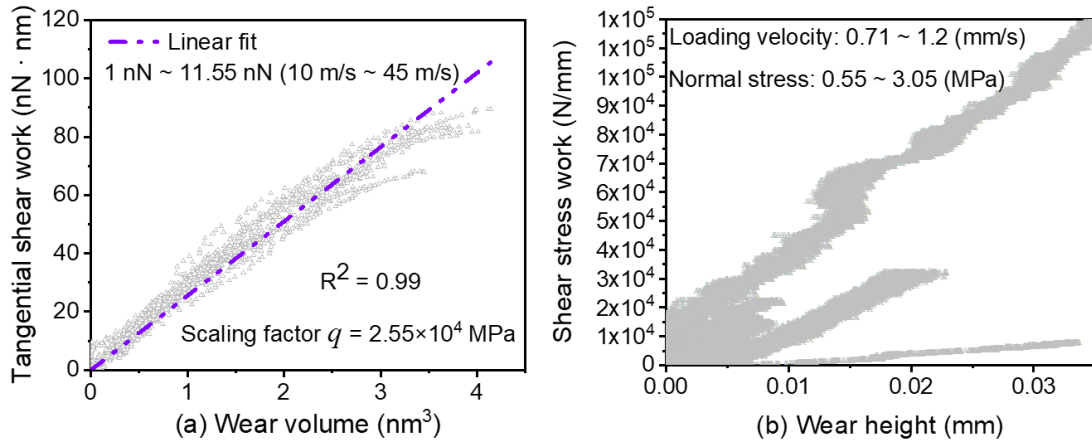


Figure 4. 12. The wear volume and height as a function of shear work in simulations and experiments. (a) The linear relation between the wear volume and tangential shear work under different normal forces (1 nN, 2.57 nN, 5.13 nN, 8.98 nN, 11.55 nN) and loading velocities (10 m/s ~ 45 m/s). (b) Shear stress work as a function of wear displacement using the data in Mizoguchi & Fukuyama (2010). The loading velocity

ranges from 0.71 mm/s to 1.2 mm/s and the normal pressure from 0.55 MPa to 3.05 MPa. Here, the wear displacement means the shortening displacement of rock samples during the friction experiments.

4.8 Discussion

It is observed that the wear volume and wear damage present the normal force and velocity-dependence. Under the increasing normal force, the wear volume and wear damage increase. In contrast, the wear volume and damage generally decrease with the increasing loading velocity under all the normal force conditions. Here, the former can be attributed to the increased contact length and decreased energy barriers, where contact length is used as an indicator of contact area here. Based on the Hertz contact model (Johnson, 1985), the contact radius between two spheres (A) holds a positive relation to the normal force (Figure 1.2). Hence, it is expected that an increase in the normal force will lead to a broader contact length during friction process. As typically demonstrated in Figure 4.13 for the case of $L = 3$ nm and $V = 10$ m/s, the contact length increases from 2.72 nm to 4.50 nm for normal force increase from 2.57 nN to 11.55 nN. Furthermore, this positive relation is still valid between the contact stress and the normal force in the Hertz model. Based on the thermal activation theory, the increasing stress can gradually reduce the activation energy that requires to initiate a reaction of atoms or molecules, which then are easier to overcome energy barriers and more susceptible to shearing (Lantz et al., 2009; Jacobs and Carpick, 2013; Spikes, 2018). Therefore, decreased energy barriers coupled with the increased contact length contributes to the normal force-dependent wear phenomenon (here an increase of amorphous zone in the case in Figure 4.13 is also shown in Figure 4.14).

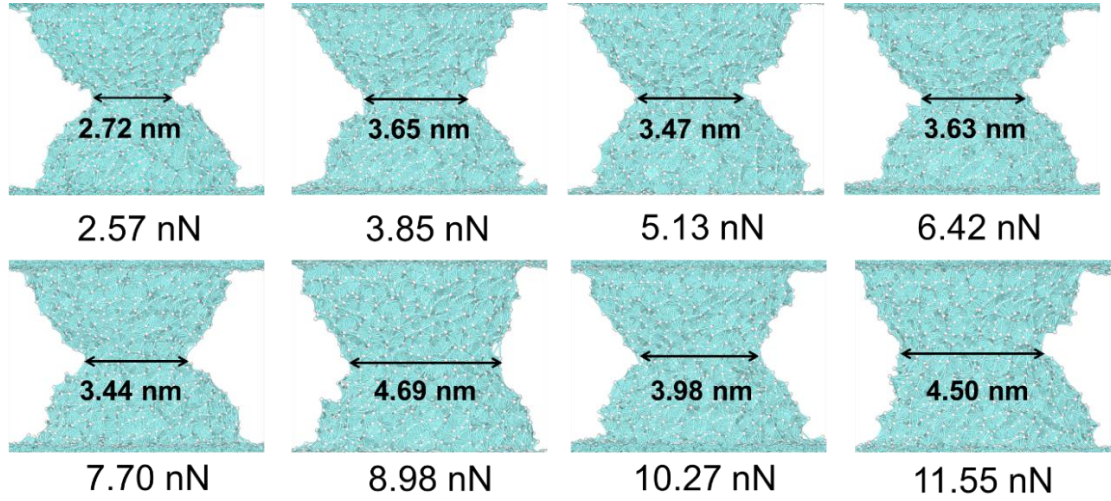


Figure 4. 13. Contact length with loading distance 3 nm under different normal forces from 2.57 nN to 11.55 nN (front view). Here, I take the case at $V = 10$ m/s as an example and use the contact length to imply contact area. Besides, the bonding distance is set as the same value as the cutoff radius 5.5 Å and the sporadic bonding cases are excluded from a measurement. However, it should be noted that as there is a flow of worn atoms on surfaces, the contact length (area) includes the indirect bonding with worn atoms between the upper and lower asperities. Therefore, the contact (length) area measured will not completely follow the Hertz contact model, but the overall trend is consistent.

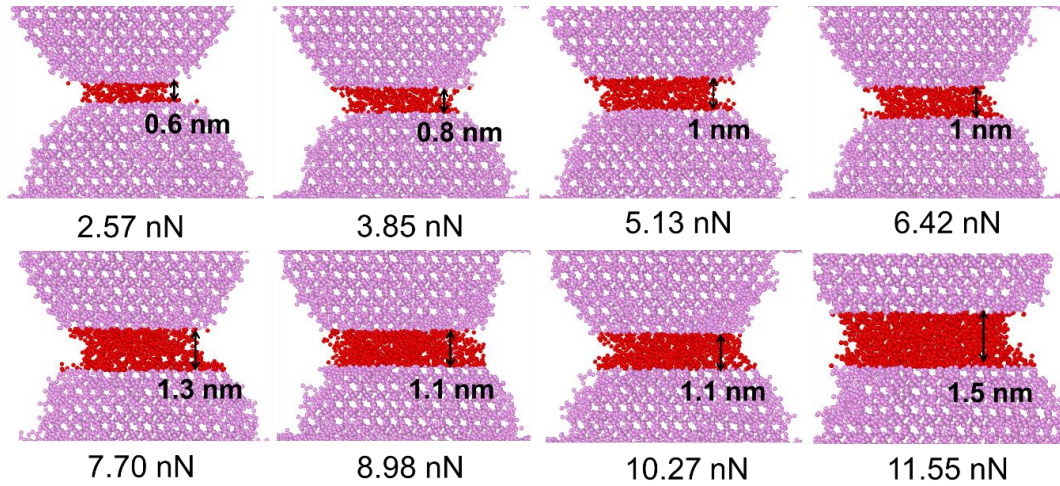


Figure 4. 14. Amorphous zone (red atoms) with loading distance 3 nm under different normal forces from 2.57 nN to 11.55 nN at $V = 10$ m/s (front view). Here, I just show the height of the amorphous zone, the length of which shows in Figure 4.13.

In contrast, the velocity-decreasing trend can be related to the decreased contact length and weaker force interactions between asperities caused by the increment of normal distance. Here, the typical change in the normal distance of simulation box under the low (2.57 nN) and the high normal force (11.55 nN) is shown in Figure 4.15, respectively at the loading velocity from 10 m/s to 45 m/s. It shows that the normal distance in both cases generally presents a velocity-increasing trend, with an increment of 4.5 Å (2.57 nN) and 2.7 Å (11.55 nN) estimated at $L = 3$ nm from 10 m/s to 45 m/s respectively. Such an increase in the normal distance can reduce the average contact length during the friction process. As shown in Figure 4.16, the contact length decreases from 2.72 nm to 1.09 nm as the velocity increases from 10 m/s to 45 m/s (with $L \approx 3$ nm at $F_n = 2.57$ nN as an example). Simultaneously, the increase in normal distance due to the higher loading velocity also signifies a rise in momentum in normal direction, resulting in weaker force interactions between asperities. Consequently, the decrease of the wear volume and damage of asperities is observed under increasing high loading velocities. Here, the normal distance should be related to the size, shape and the contact configuration of asperities. Besides, as the normal force can significantly limit the increase of normal distance (Figure 4.15b), it is expected that under much higher normal force, the influence of normal distance on the contact length can largely decrease or vanish. In this case, the effect of high loading velocity on the wear of asperities will be related to other important factors such as temperature.

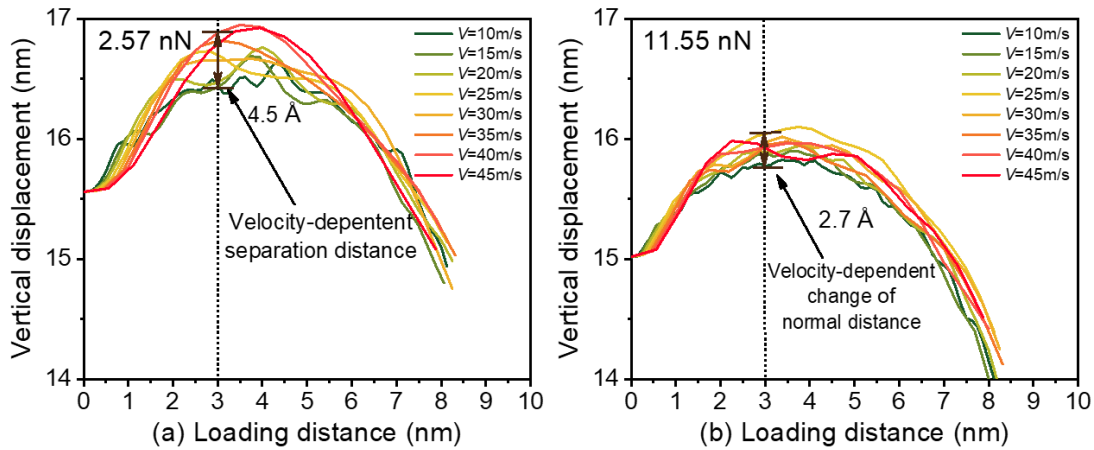


Figure 4. 15. The typical change of vertical displacement under (a) the low (2.57 nN) and (b) the high normal forces (11.55 nN) respectively at the loading velocity from 10 m/s to 45 m/s. The change of box height refers to the height of box at $V = 10$ m/s.

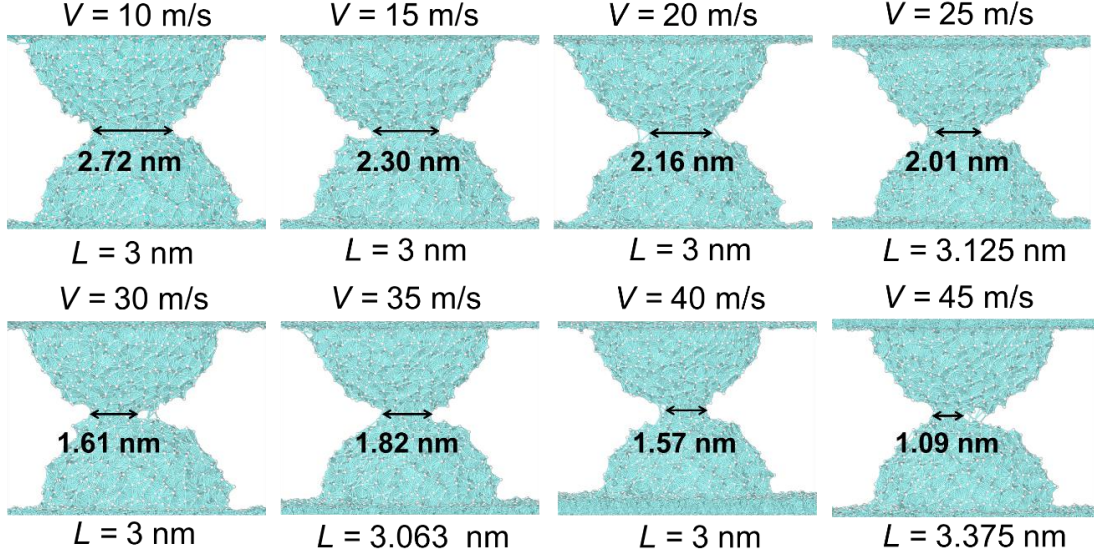


Figure 4. 16. Contact length with loading distance about 3 nm under different loading velocities V from 10 m/s to 45 m/s (front view). Here, I take the case at $F_n = 2.57$ nN as an example and use contact length to imply contact area. Besides, the bonding distance is set as the same value as the cutoff radius $5.5 \text{ \AA}$ and the sporadic bonding cases are excluded from a measurement. However, it should be noted that as there is a flow of worn atoms on surfaces, the contact (length) area includes the indirect bonding with worn atoms between the upper and lower asperities.

Moreover, similar to the empirical relation of Eq. (4.1), the well-known Archard's law also predicts a linear proportionality for adhesive wear (Archard, 1953). The law predicts a proportional relation $W \propto F_n L$ when assuming plastic contact. However, simulation results show a sublinear increase of W and a similar observation has also been reported (Bhamra et al., 2023), deviating from Archard's law. The limitations of Archard's law could stem from the time-varying contact area during friction caused by multiple factors such as loading velocities, interfacial properties, wear debris transfer and changes in asperity contact configuration. Eq. (4.1) incorporates these varying characteristics by integrating the time-varying F_t , which allows for a more accurate representation of the actual contact state and friction properties at the nanoscale. Here, it should be emphasized that Archard's law has achieved highly effective results macroscopically (Scholz, 1987; Wang & Scholz, 1994). The origin of these scale-dependent differences would require further investigation through multiscale simulations.

On the other hand, the effect of shear work on wear volume in adhesive wear can also be described by a predictive equation grounded in energy barrier changes. Firstly, the normal contact force promotes the bonding of surface atoms. At this stage, the number of surface atoms N_{ib} involved in one or more interfacial chemical bonds can be denoted as follows (Wang et al., 2021b):

$$N_{ib} = \frac{2}{A_{atom}} \exp\left(-\frac{\Delta U_{ib} - W_{\sigma}}{k_B T}\right) \exp\left[\frac{V_{atom}}{2Ek_B T} \left(\frac{F_n}{A_{rc}(F_n)}\right)^2\right] A_{rc}(F_n) \quad (4.2)$$

where A_{atom} is the surface area of per atom, ΔU_{ib} is the activation energy for interfacial bond formation, W_{σ} is the external work induced by normal stress, V_{atom} is the average atomic volume, $A_{rc}(F_n)$ is the real contact area as a function of F_n , k_B is the Boltzmann constant, T is the absolute temperature and E is the Young's modulus of the material. Furthermore, when sliding occurs, the number of worn atoms N_{wear} can be correlated with the external shear work W_{τ} (Wang et al., 2021b):

$$N_{wear} = \frac{2f_0 t}{A_{atom}} \exp\left(-\frac{\Delta U_{ib} + \Delta U_{wear} - W_{\tau}}{k_B T}\right) \times \exp\left[\frac{V_{atom}}{2Ek_B T} \left(\frac{F_n}{A_{rc}(F_n)}\right)^2\right] A_{rc}(F_n) \quad (4.3)$$

where N_{wear} is the number of worn atoms, ΔU_{wear} is the activation energy required to remove interfacial bonded atoms, f_0 is the attempt frequency and t is the sliding time.

In Eqs. (4.2) and (4.3), the contributions of normal and shear stresses to the associated energy barrier changes are clearly identified respectively. Moreover, in these equations, when the normal force exhibits either a linear or nonlinear relationship with the contact area, the wear volume evolves linearly or non-linearly (Wang et al., 2021b). This further explains why the results in this thesis exhibit nonlinear growth with loading distance, which relates to the dynamic change of contact area. Notably, when F_n becomes relatively high, the equations break down (Bhamra et al., 2023). Nevertheless, Eqs. (4.2) and (4.3) still provide crucial insights into developing a physics-based framework that links friction and wear in rocks, as both atomic force microscopy (AFM) experiments on silica-rich interfaces (Li et al., 2011) and simulation results have demonstrated that friction is governed by molecular interactions at the nanoscale, manifesting as an adhesive wear process.

4.9 Conclusion

This chapter provides insights into the plastic wear mechanisms using 3-D molecular dynamics (MD) simulations of interlocked α -quartz asperities at the nanoscale, focusing on the effects of the normal force and high loading velocity. A positive correlation between the shear damage zone or wear volume and the normal force has

been identified. Meanwhile, a negative correlation of the wear volume and asperity damage to the high loading velocity is also identified. Moreover, adhesive wear dominates the nanoscale wear process. The plastic wear mechanisms are primarily governed by the normal force. The low normal forces lead to wear through interfacial bonding and shear traction, while the high normal forces cause cluster detachment characterized by the layered shear motion. The higher normal force corresponds to the larger clumps of attrition on asperities. Finally, the wear volume generally shows a nonlinear positive correlation with the normal force and a nonlinear negative correlation with the high loading velocity. However, in all cases, the wear volume can be accurately predicted by the tangential shear work associated with the instantaneous tangential force, due to their proportional relationship.

APPENDICES

Appendix 4.A: Tangential force and averaged force ratio ξ_a under different asperity sizes and horizontal locations.

To explore the impact of asperity size and horizontal location of asperity centers on the tangential force and the averaged force ratio ξ_a , four additional models are modeled while keeping the simulation conditions identical to the original setup. Initially, in Figure 4.A1a-b, two models featuring variations in the horizontal relative distance of asperities are modeled. In the other models, one focuses on the change in asperity size (Figure 4.A1c), while the other incorporates adjustments in both the size and horizontal relative distance (Figure 4.A1d). Figure 4.A2 further shows the averaged force ratio ξ_a and corresponding loading curves of the four models. It is found that ξ_a is quite sensitive to the horizontal location of asperity centers than asperity size. In the cases of Figure 4.A1a and Figure 4.A1b, ξ_a is extreme low, with the value around 0.2 (Figure 4.A2a-b). Here, the negative ξ_a occurring in Figure 4.A2b lies in the dominated adhesion force between asperities in the nanoscale. In comparison, in Figure 4.A2c and Figure 4.A2d, ξ_a is around 0.53 and 0.87 respectively (0.7 observed in the original model), which indicates that ξ_a is obvious higher in the interlocked cases.

On the other hand, the tangential force and the weakening distance are also obviously influenced by the horizontal location of asperities. The tangential force (Figure 4.A2a-b) in the non-interlocked asperities (Figure 4.A1a-b) is overall lower than the interlocked asperities (Figure 4.A2c-d).

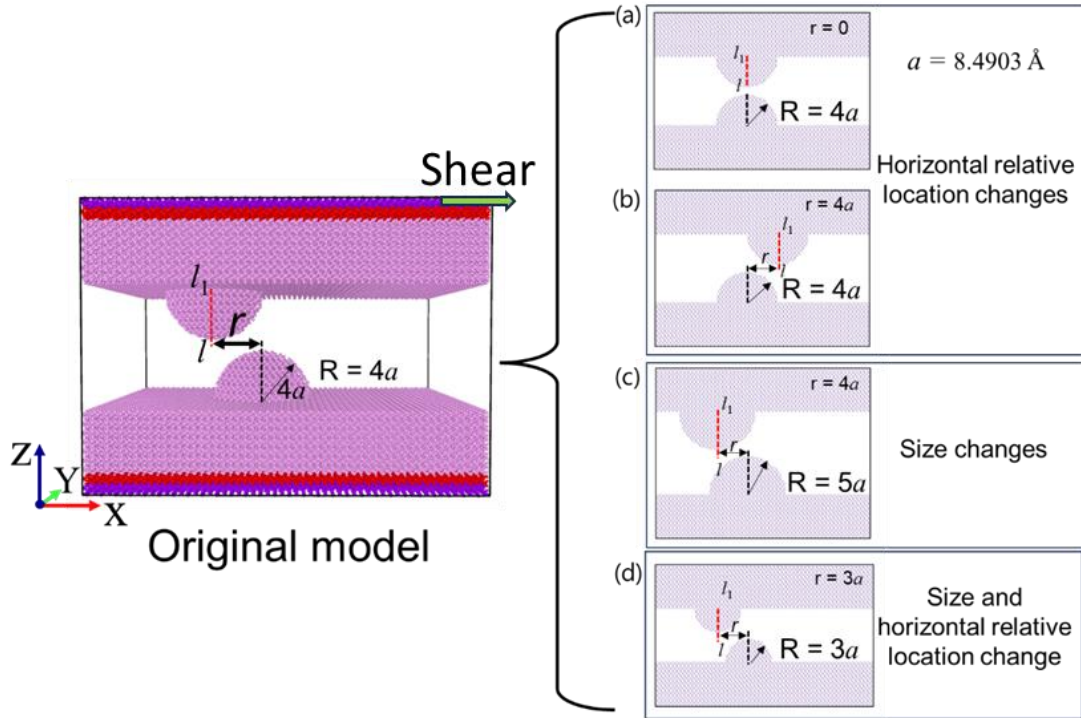


Figure 4.A1. Models with different asperity sizes and horizontal relative locations. (a) The offset of asperity centers is zero; (b) An opposite (X- direction) but the same offset distance ($4a$) between asperity centers compared with the original model; (c) The size change of asperities ($5a$); (d) both changes in the size ($3a$) and offset distance ($3a$) of asperities.

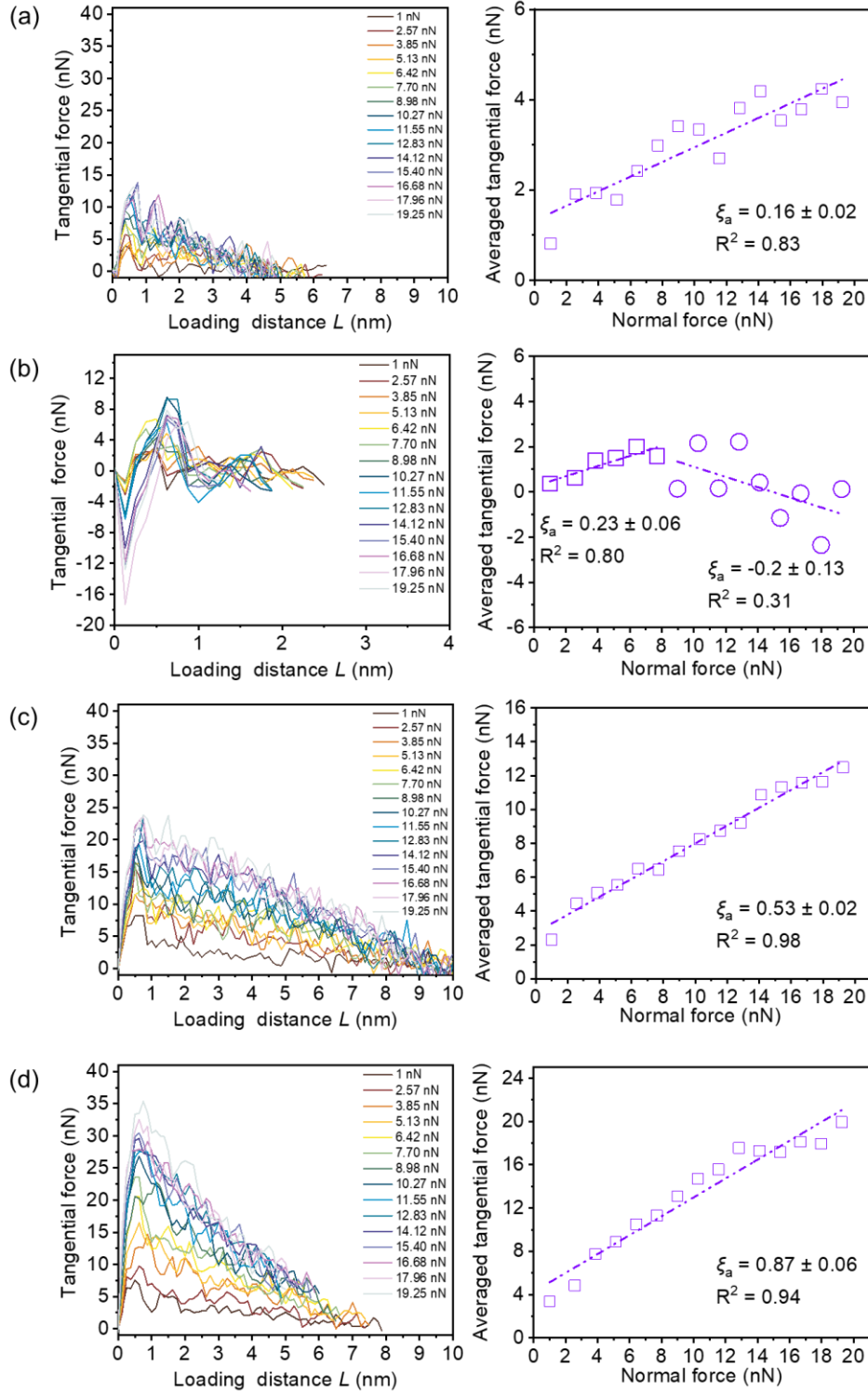


Figure 4.A2. The loading curves of tangential force with loading distance (left) and corresponding averaged force ratio ξ_a (right) of four models. (a) The offset of the centers of asperities is zero; (b) An opposite (X- direction) but the same offset distance (4a) between asperity centers compared with the original model; (c) The size change of asperities (5a); (d) both changes in the size (3a) and offset distance (3a) of asperities.

CHAPTER V

Asperity Failure Mode Transition

5.1 Introduction

This chapter aims to clarify the wear failure mode transition of nanoscale asperities under various loading conditions, asperity sizes, normal forces and contact configurations. The results indicate that both plastic deformation and fracture of α -quartz asperities can occur during frictional collision without creating surface grooves. Under constant normal stiffness-like condition, the failure transition can be mapped by the vertical overlapping distance normalized by R between the summits of two asperities, as a function of R . Under constant normal load condition, the failure transition can be reflected by the peak tangential force. Essentially, the failure mode transition is controlled by subsurface contact stress evolution through the dependence of R and contact configuration. Finally, the results also reveal that the total wear volume of fractured asperities scales linearly with the total tangential shear work. These findings provide deeper insights into the wear failure mechanisms of nanoscale rock asperities during friction, which also help shed light on microscopic fault friction mechanisms.

5.2 Numerical Model

Here, based on the model in chapter IV, two kinds of boundary conditions are applied to the rigid layer of top block, namely constant normal load (CL) and constant normal stiffness (CS)-like conditions, as shown in Figure 5.1. Here, the constant normal stiffness in (CS)-like condition refers to the bulk stiffness of the substrata. Furthermore, the simulation box has dimensions of $L_x = 5na$, $L_y = 5nb$ and the thickness of each substratum is $1.25 nc$, where n is defined through $R = na$ and R is the radius of semi-spherical asperity. In the initial setup, the height overlap (ΔH) between the asperity tops is set at R under CL condition (Case I in Figure 5.1b). Under CS-like condition, $\Delta H = R$ (Case I) and $\Delta H = R/2$ (Cases II) (Figure 5.1b) are set. Therefore, at the beginning, L_z becomes $2.5nc + R$ for CL condition and Case I in CS-like condition and $2.5nc + 1.5R$ for Case II in CS-like condition. At the beginning of the simulation, two asperities do

not contact nominally as the horizontal distance between two asperity summits is set at $1.8R$. Under CL condition, to capture the transition in failure modes, the normal load (F_n) range depending on R is considered: 10 nN $\sim$ 60 nN with an increment of 10 nN (60MPa $\sim$ 360MPa) for $R = 4a$ (1 nN corresponds to 6.0 MPa). 20 nN $\sim$ 110 nN with an increment of 10 nN (30 MPa $\sim$ 165 MPa) for $R = 8a$ (1 nN corresponds to 1.5 MPa), and 100 nN $\sim$ 170 nN (67 MPa $\sim$ 114 MPa) for $R = 12a$ with an increment of 10 nN (1 nN corresponds to 0.67 MPa). Under CS-like condition, the asperity radius from $R = 3a$ to $12a$ is considered for Case I and from $R = 3a$ to $16a$ for Case II. The normal load in the CS-like test varies dynamically as the loading distance (L) increases. Here, L is also defined as the horizontal displacement of the top rigid layer with respect to the fixed bottom rigid layer.

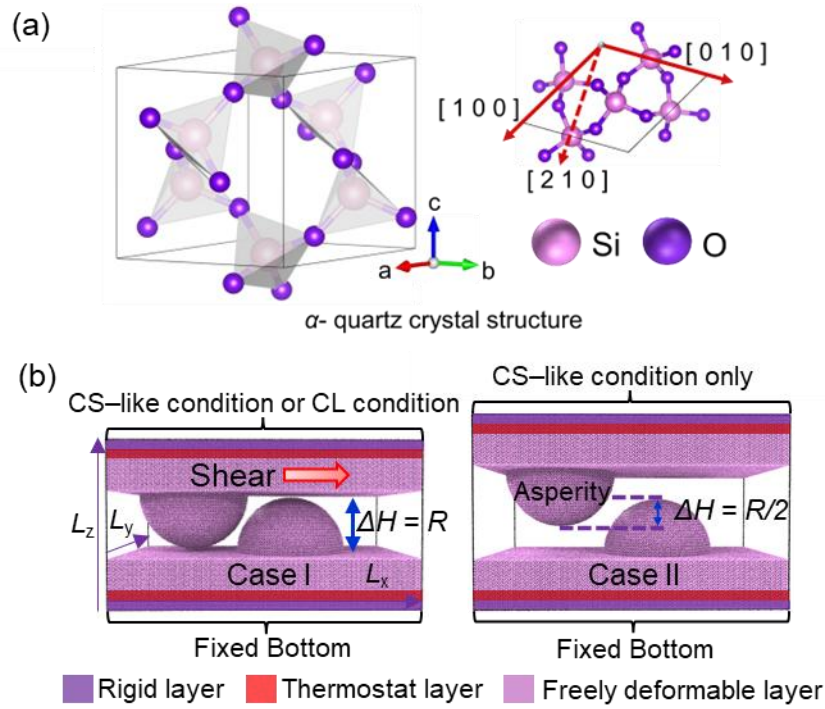


Figure 5. 1. (a) The crystal structure of α -quartz (visualized by VESTA, Momma & Izumi, 2011). The dashed line in the right (2D view) shows the rotation from $[100]$ to $[210]$ for selecting an orthorhombic unit cell. (b) The contact configurations of asperities and boundary conditions. ΔH represents the overlapping distance between asperity tops. In Case I, $\Delta H = R$. In Case II, $\Delta H = R/2$.

5.3 Simulation Procedure

Here, under CL condition, the simulation procedure is similar to that in Chapter IV. In contrast, under CS-like condition, the friction process begins immediately after the initial relaxation phase, with NVT switching to NVE while keeping other simulation procedures the same as that under CL condition. In all simulations, V was set to 20 m/s.

5.4 Asperity Damage

5.4.1 CS-like condition

For Case II ($\Delta H = R/2$) condition, the models from $R = 3a$ to $16a$ are computed. In Figure 5.2, two typical cases involving different failure modes for $R = 12a$ and $R = 15a$ are shown. Other cases are shown in Figure 5.3. When $R = 12a$, plastic flow occurs (Figure 5.2A-D). The asperity initially deforms elastically when colliding with each other, storing elastic strain energy (Figure 5.2A). As L increases, the amorphization on contact surfaces initiates, leading to the formation of an amorphous layer with finite thickness (Figure 5.2B). The thickness of the amorphous layer progressively increases with continuing shear loading, persisting until the asperities pass each other (Figure 5.2C-D). Here, localized damage area inside the asperity is not distinctly observed. However, when increasing the asperity size, a vertical damage layer develops within the asperity (Figure 5.2F), while the asperity collision initially follows the elastic deformation stage (Figure 5.2E) similar to the plastic case. In the fracture case, the damage layer acts as a weak defect inside asperities, contributing to the subsequent initiation of fracture of asperities as shear displacement increases (the dotted square region in Figure 5.2F and Figure 5.2G). Ultimately, the fracture planes gradually form, leading to the fragmentation of the asperity and the formation of wear particles. Here, the above trends can also be found in Figure 5.3.

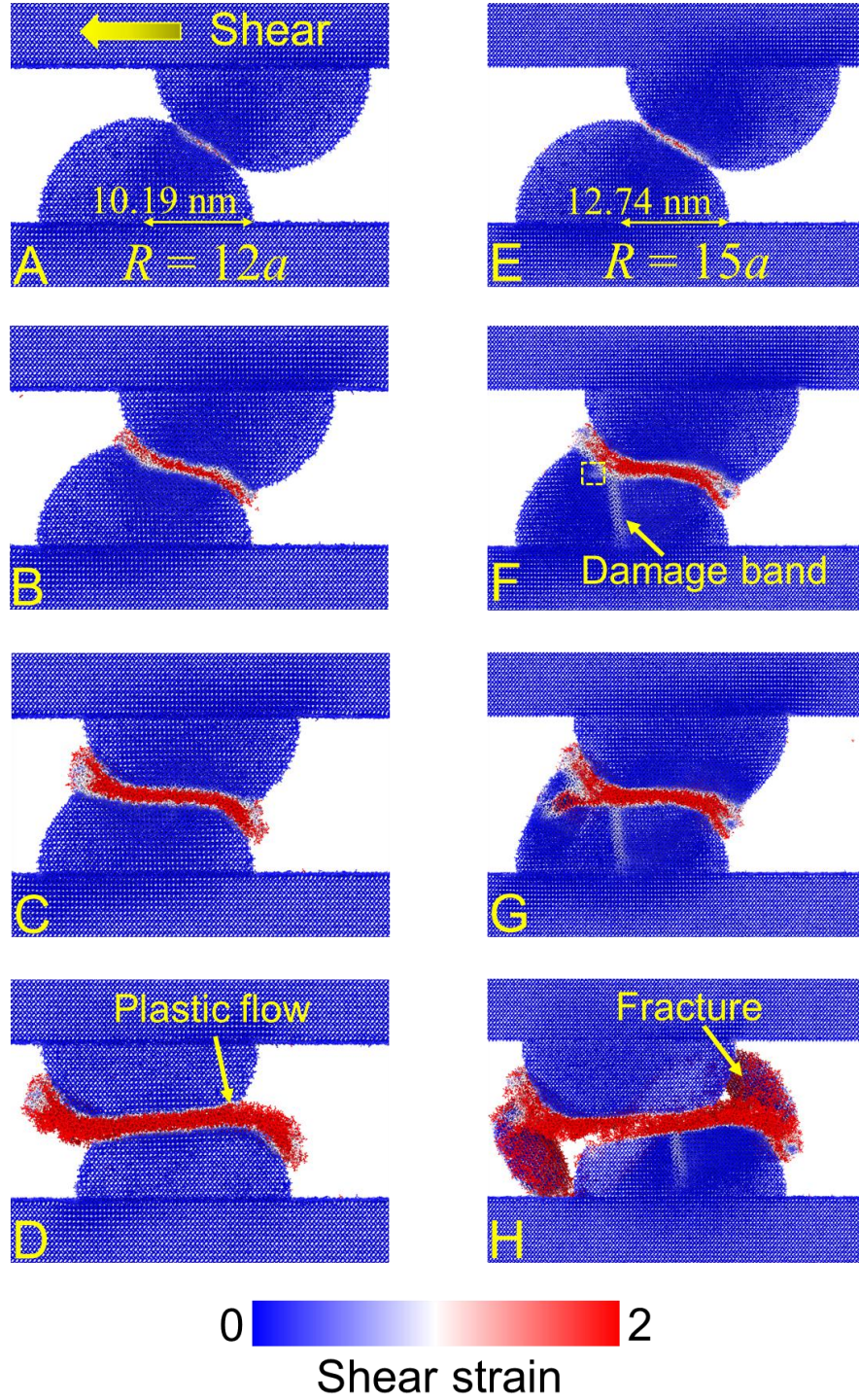


Figure 5. 2. Two typical cases involving plastic and fracture failure modes for the case of Case II ($\Delta H = R/2$) with $R = 12a$ (A-D) and $R = 15a$ (E-H), visualized by OVITO (Stukowski, 2010). Snapshots from A-D correspond to $L = 7$ nm, 10.5 nm, 14 nm, and 21.5 nm, respectively. Snapshots from E-H correspond to $L = 9.75$ nm, 14.75 nm, 16 nm, and 29 nm, respectively.

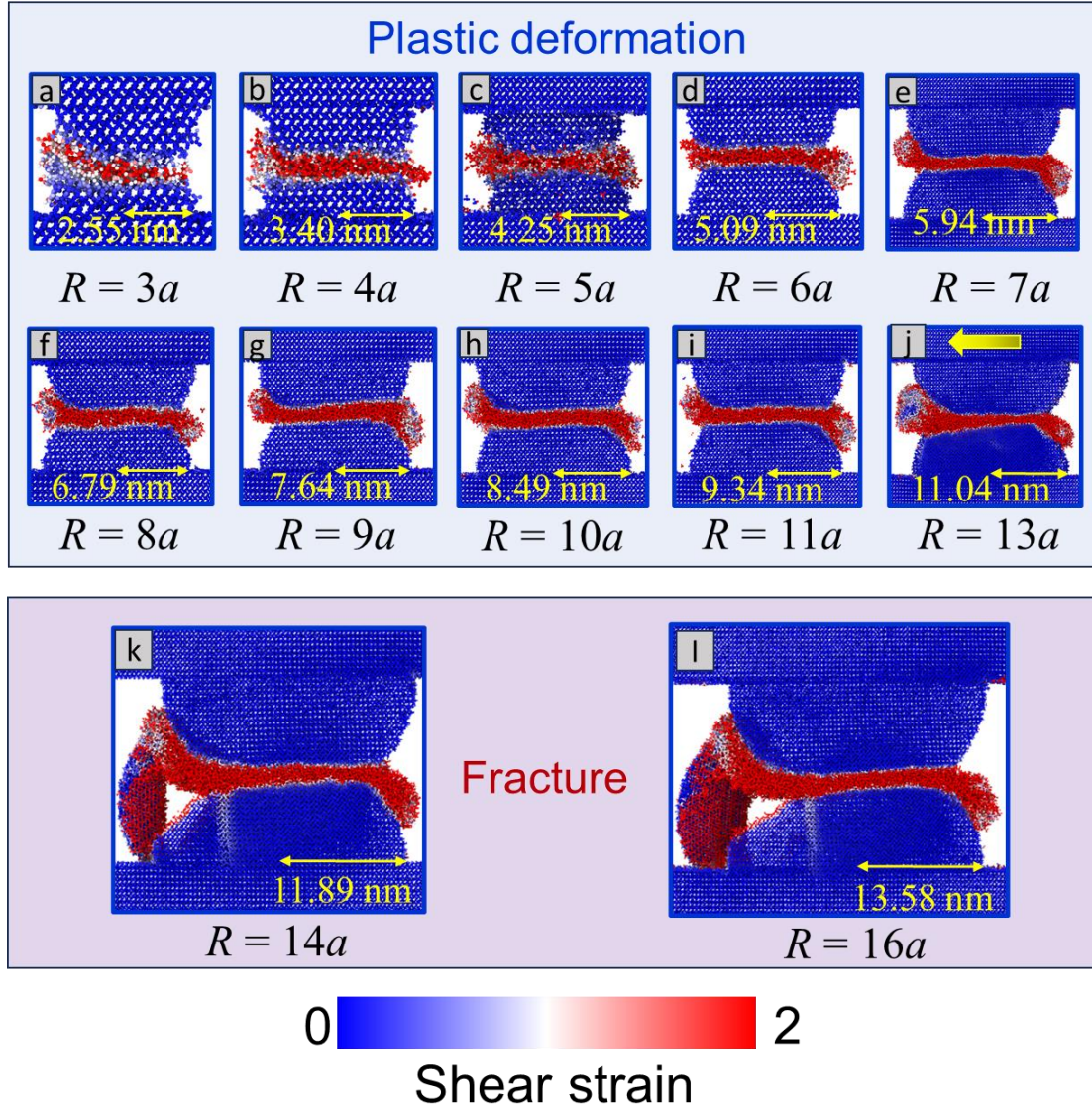


Figure 5. 3. Snapshots of asperity wear failure for the case of $\Delta H = R/2$ with R ranging from $3a$ to $16a$ ($a \sim 1$) under CS-like condition, except for $R = 12a$ and $R = 15a$. The loading distance from a to l is 4.5 nm, 6.25 nm, 8.25 nm, 9.5 nm, 10.5 nm, 12.5 nm, 14 nm, 15.25 nm, 16.75 nm, 20 nm, 20.75 nm, 24.5 nm respectively. The light blue background indicates plastic deformation, while the light purple denotes the cases of fracture. The shear strain ranges from 0 to 2. The yellow arrow under each subfigure indicates the radius scale. The subsequent figures follow the same color scheme and shear strain ranges.

For Case I ($\Delta H = R$) condition, the models from $R = 3a$ to $12a$ are computed. In

Figure 5.4, two typical cases involving plastic and fracture failure modes for $R = 3a$ and $R = 12a$ are shown. Other cases are shown in Figure 5.5. As observed, the elastic stage (Figure 5.4AC) and plastic wear mechanisms (Figure 5.4B) are similar to those for Case II. Notable differences arise in the fracture stage. As shown in Figure 5.4D, after the elastic stage, a localized amorphization or damage band forms inside the asperity. It typically develops within a region corresponding to the high-stress zone described in Hertzian contact (Johnson, 1985), coexisting with the surrounding elastic region. Here, the amorphous band (dash line in Figure 5.4D) forms an angle with the contact interface, which is similar to a notch inside the asperity. Therefore, with further shear loading, the crack initiates from the damage band (Figure 5.4E), ultimately resulting in the wear particle formation under mixed tensile-shear stresses (Figure 5.4F).

Therefore, the failure of α -quartz asperities occurs in two different modes: plastic flow and fracture at both Case I and Case II conditions.

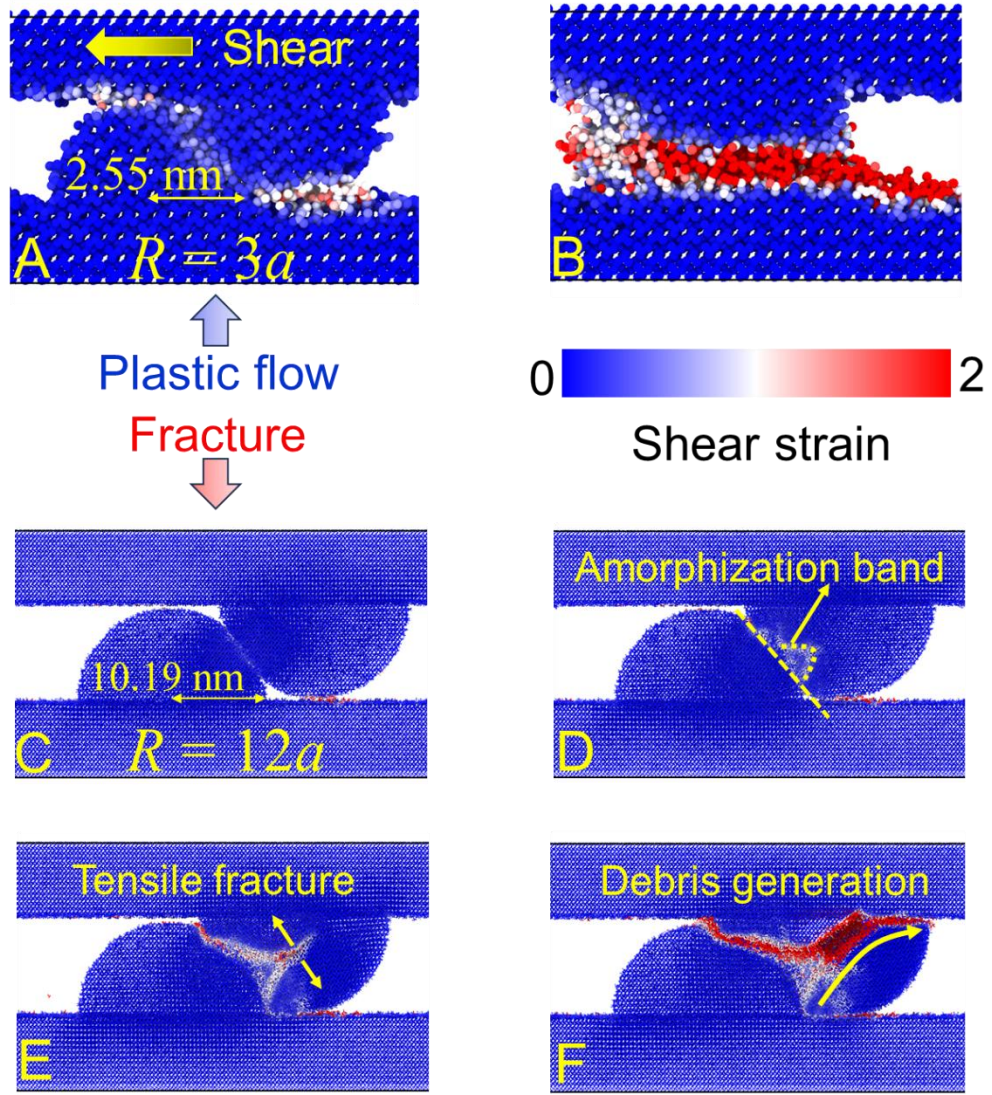


Figure 5. 4. Typical cases involving plastic and fracture failure modes for Case I ($\Delta H = R$) with $R = 3a$ (A-B) and $R = 12a$ (C-F). Snapshots A and B correspond to $L = 1.25$ nm and 4.75 nm, respectively. Snapshots C-F correspond to $L = 3$ nm, 4.5 nm, 5.5 nm, and 7.75 nm, respectively.

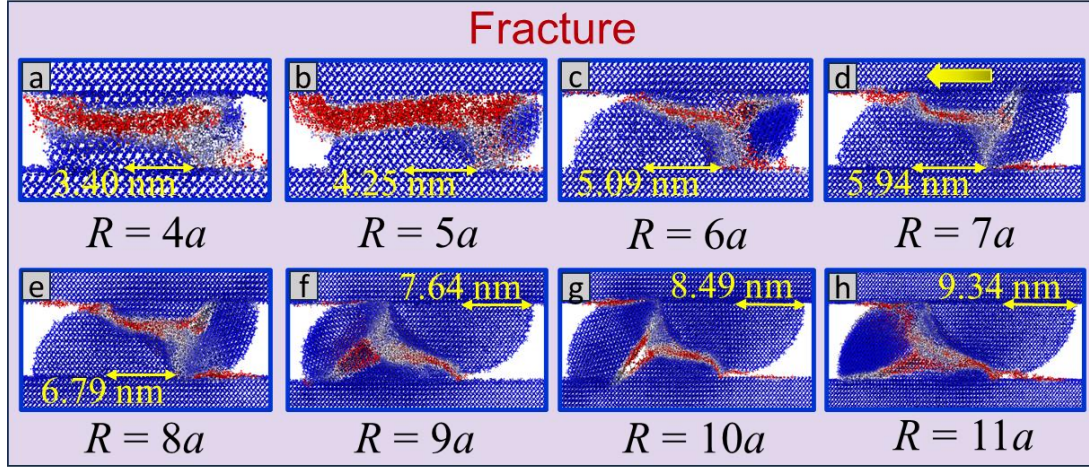


Figure 5.5. Snapshots of asperity wear failure for the case of $\Delta H = R$ under CS-like condition, with R ranging from $4a$ to $11a$ (a ~ h). The loading distance from a to h is 5 nm, 8 nm, 4.5 nm, 4.5 nm, 5.25 nm, 6 nm, 5.75 nm, 6.25 nm respectively.

5.4.2 CL condition

Under CL condition, Figure 5.6A-D shows two representative results for $F_n = 20$ nN and 80 nN, at $R = 8a$. Other F_n cases are shown in Figure 5.7. Figure 5.6E-H shows two representative cases when $F_n = 120$ nN and 150 nN, which includes plastic flow with damage band at $R = 12a$. Other failure cases under different F_n are shown in Figure 5.8. In Figure 5.9, all the failure cases at $R = 4a$ under $F_n = 10$ nN ~ 60 nN are shown. As observed in Figure 5.6A-D and Figures 5.7-5.9, the wear failure of asperities involves plastic and fracture modes depending on F_n . Under relatively low F_n (e.g., 20 nN in Figure 5.6A), the plastic wear dominates and is characterized by surface amorphization. Asperity dilation in the normal direction or relative shear along the contact interface is accompanied in this case (e.g., Figure 5.6A-B). In contrast, higher F_n will generally lead to fracture continuously (e.g., Figure 5.6C-D and Figure 5.7). Meanwhile, the asperity dilation will be limited during shear loading. Instead, the contact area and atomic shear strain inside asperities increase accordingly, which resembles the contact process under Case I of the CS-like condition. Therefore, the subsequent formation of the amorphization band within the asperity, the mode of crack propagation as well as

particle generation, proceed through a mechanism similar to the fracture cases observed at Case I under CS-like condition.

However, it should be noted that plastic wear under CL condition can also occur with internal damage beneath the contact surface during initial asperity collision (Figure 5.6EG and Figure 5.8). Such features are commonly observed in an intermediate normal-force range (e.g., about 100 ~ 150 nN for $R = 12a$). This range lies slightly below the threshold for the asperity fracture, yet above the regime where only plastic wear is observed without visible internal damage as typically shown in Figure 5.6A. Moreover, in this intermediate regime, where plastic wear with internal damage band is observed, should be related to asperity radius R , as the maximum value in the intermediate force range at $R = 4a$ (around 30 nN) and $R = 8a$ (around 60 nN) is far smaller than that at $R = 12a$ (about 150 nN). Here, maximum F_n value of intermediate regime is roughly provided, as estimating more precise force range would require more computations. Additionally, fracture can occur sporadically in the intermediate regime (e.g., the case at $F_n = 130$ nN shown in Figure 5.8). This phenomenon may originate from thermal fluctuations of surface atoms commonly observed in MD simulations (Umeno et al., 2010; Zhang et al., 2019), where local atomic kinetic energy and stress distribution near the contact region fluctuate accordingly, causing sporadic variations in the mechanical behavior. The effects could be significant especially near the critical failure state. This explanation also applies to the subsequent fluctuations in the critical maximum shear force observed in the next section. Nevertheless, the simulation results remain statistically significant, as the failure transition of asperities under different normal loading regimes at different asperity sizes is overall differentiated clearly.

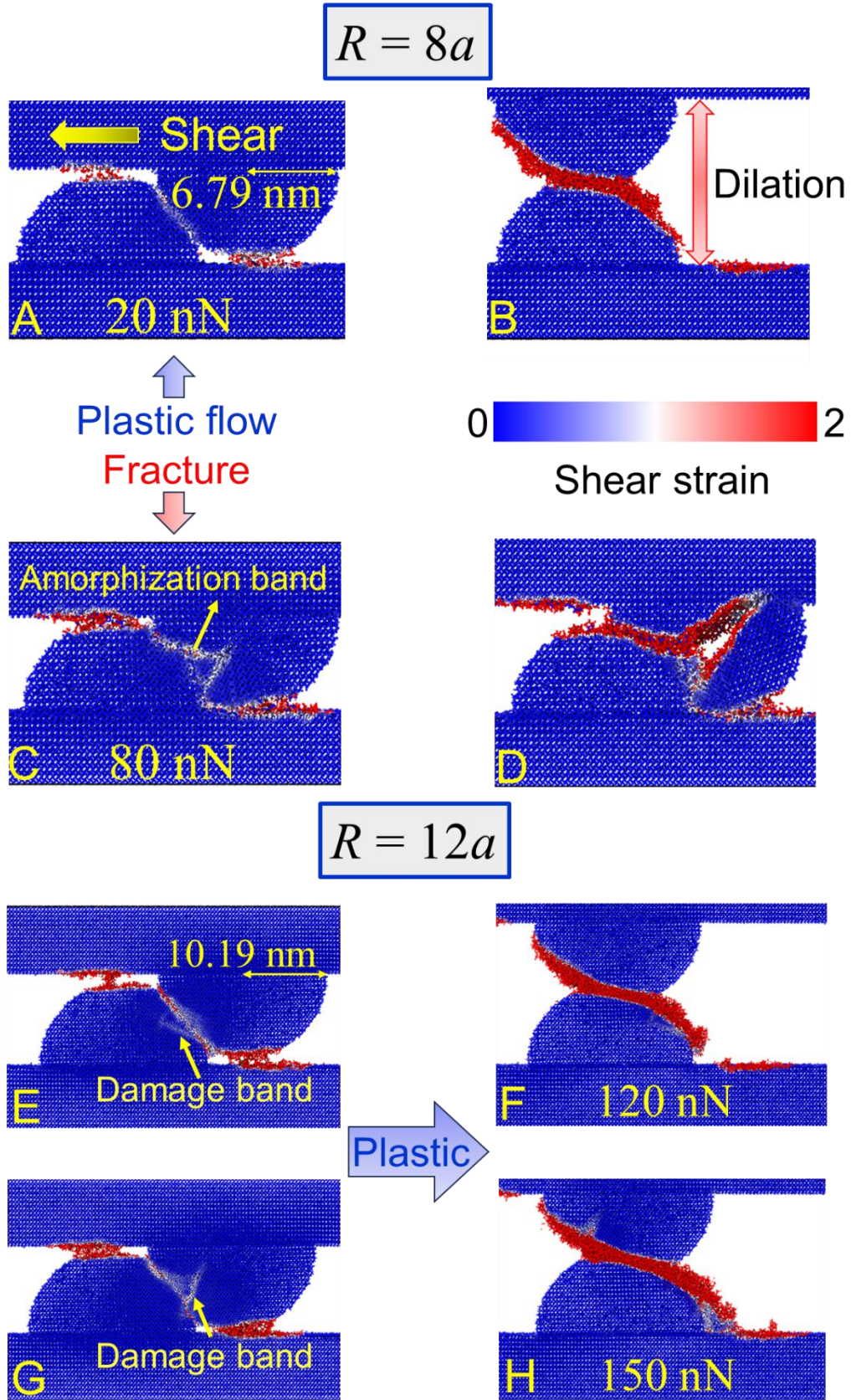
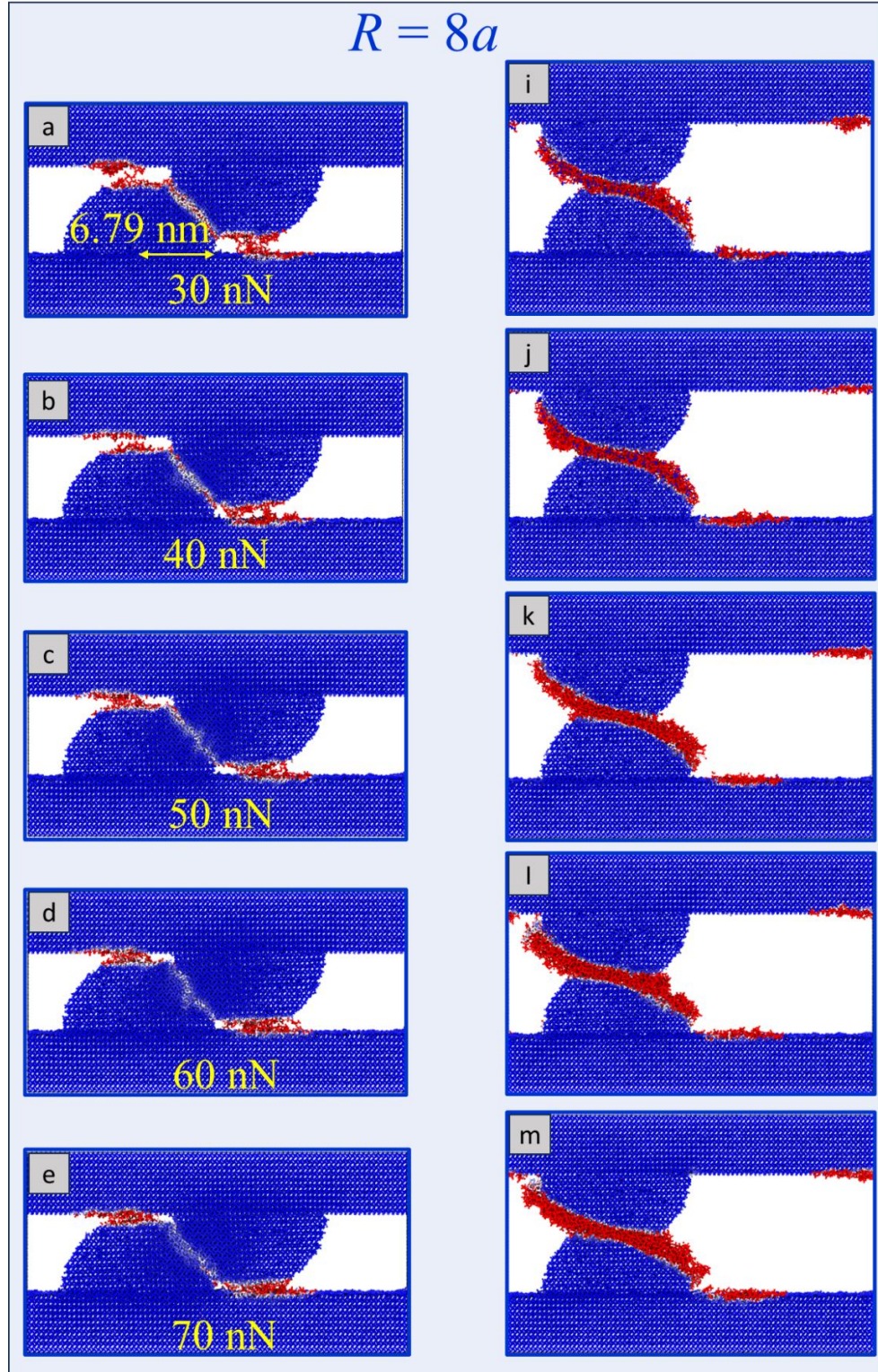


Figure 5. 6. Representative cases of plastic and fracture failure modes at $R = 8a$ under $F_n = 20$ nN (AB) and 80 nN (CD), and plastic wear with initial internal damage at $R =$

12a under $F_n = 120$ nN (EF) and 150 nN (GH). Snapshots of A, B, C and D correspond to $L = 2$ nm, 12.5 nm, 3 nm and 12.5 nm, respectively. Snapshots of E, F, G, and H correspond to $L = 4.25$ nm, 17.5 nm, 4.25 nm, and 17.5 nm, respectively.



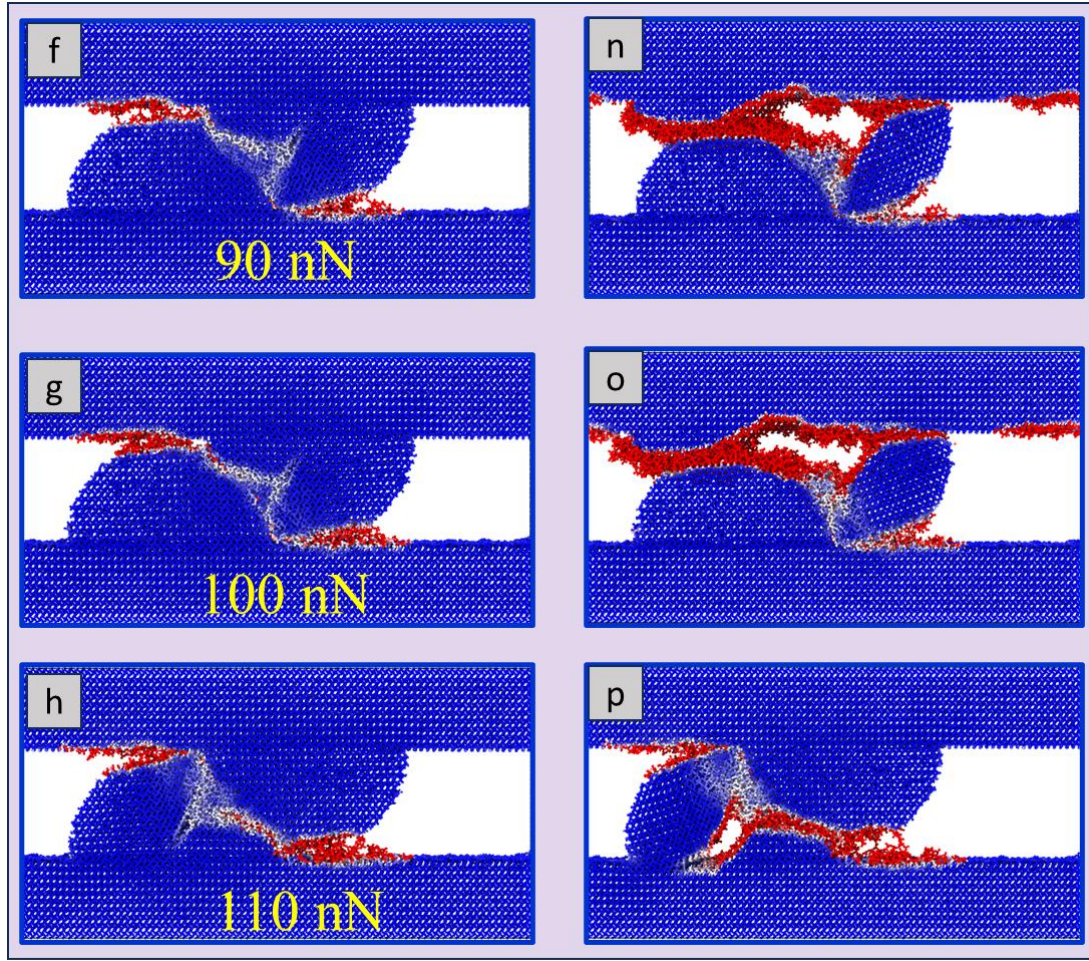


Figure 5. 7. Snapshots of asperity wear failure for the case of $R = 8a$ under CL condition, subjected to normal forces ranging from 20 nN to 110 nN (a~p), except for 20 nN and 80 nN. The loading distance in the left figures (a ~ e) is 2.75 nm and 3.25 nm (f ~ g) as well as 3.75 nm (h). The loading distance in the right figures (i ~ o) is 12.5 nm and 5 nm (p).

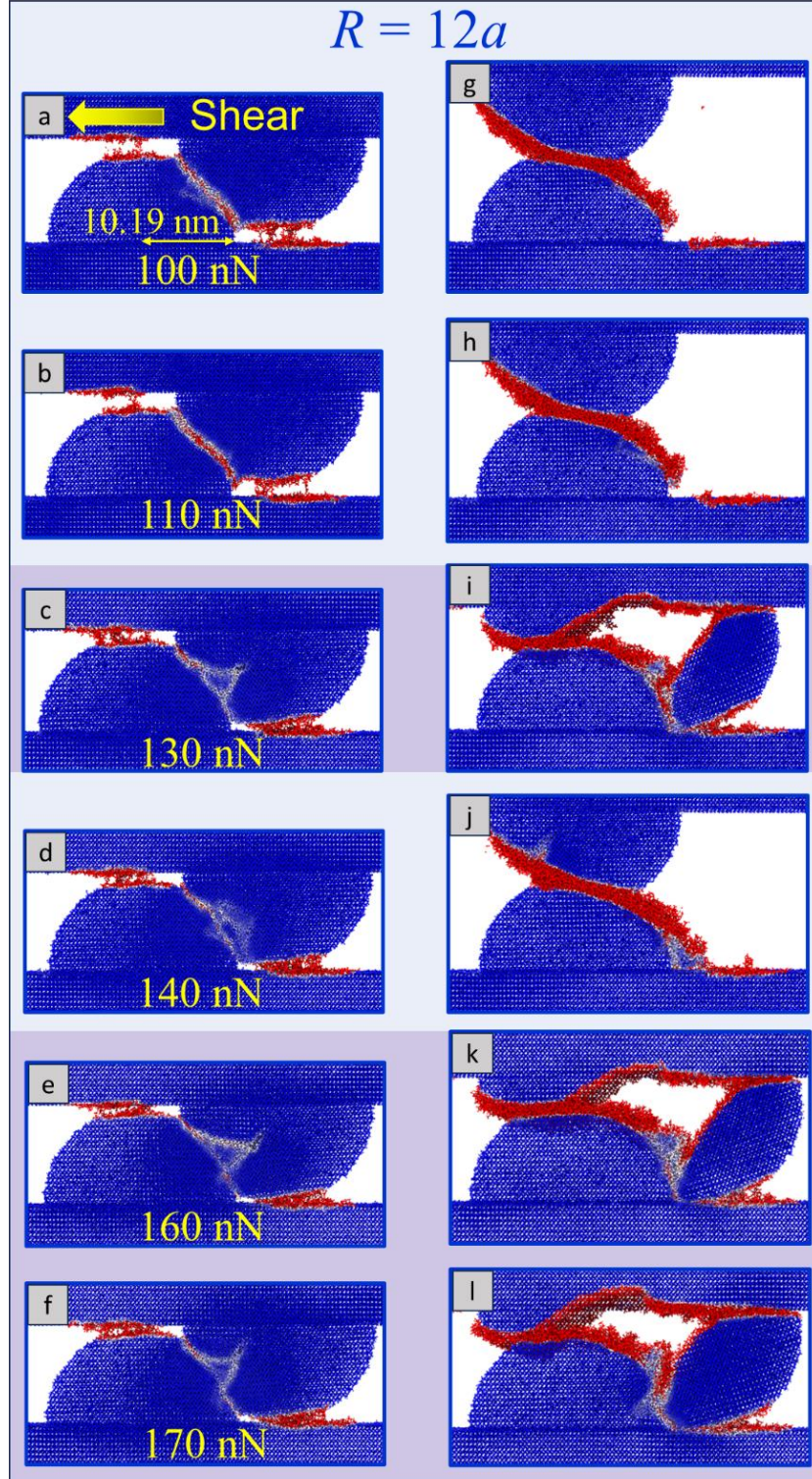


Figure 5. 8. Snapshots of asperity wear failure for the case of $R = 12a$ under CL condition, subjected to normal forces ranging from 100 nN to 170 nN (a~l), except for 120 nN and 150 nN. The loading distance in the left figures (a ~ f) is 4.25 nm and 17.75 nm in the right figures (g ~ l).

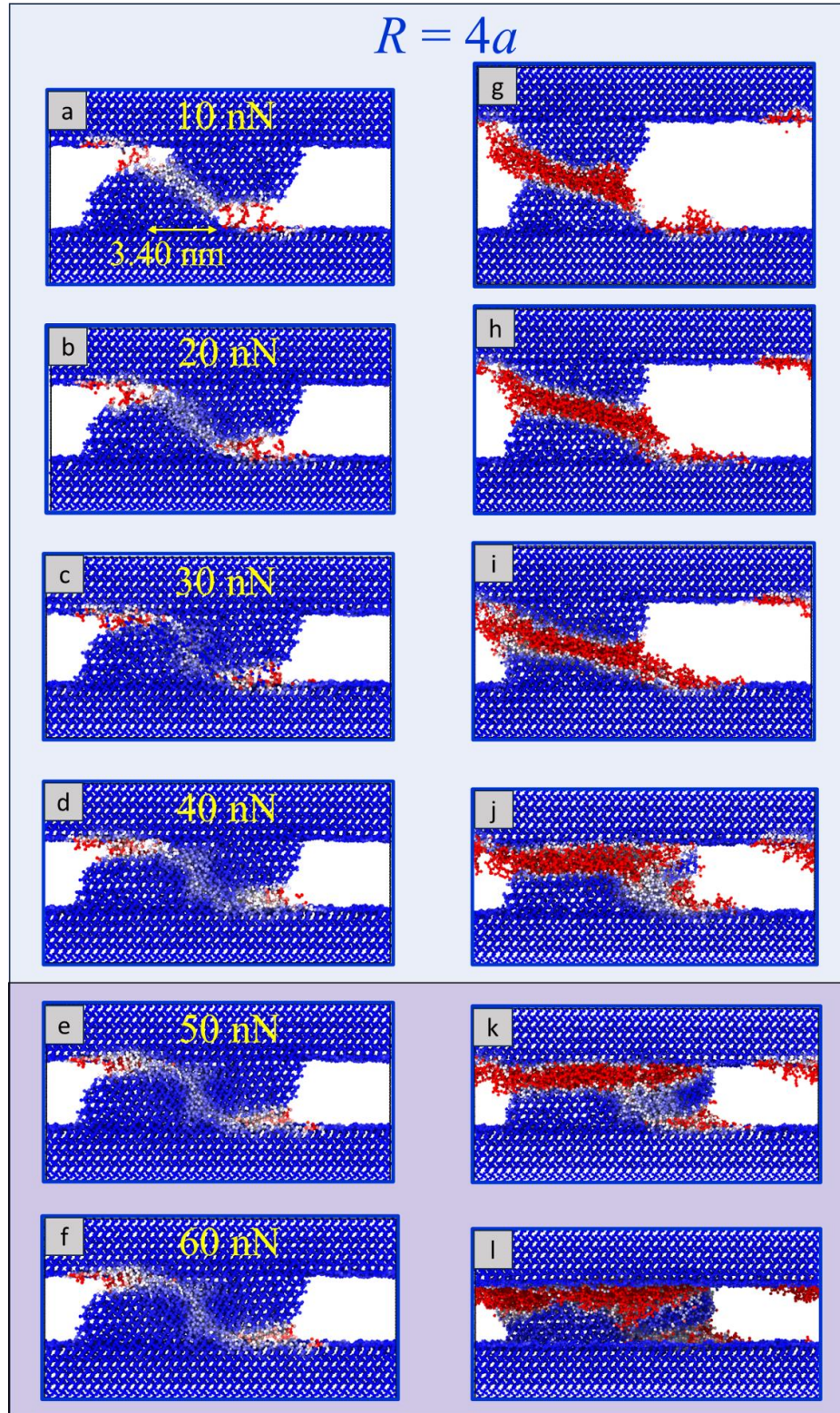


Figure 5. 9. Snapshots of asperity wear failure for the case of $R = 4a$ under CL condition, subjected to normal forces ranging from 10 nN to 60 nN (a~l). The loading distance in the left figures (a ~ f) is 2 nm and 6 nm in the right figures (g ~ l).

5.5 Failure Mode Transition Prediction

Figure 5.10 presents all cases of asperity wear failure modes under CS-like condition, including both plastic wear and fracture. The asperity failure modes are mapped by the height ratio ($\Delta H/R$) versus relative asperity radius n ($=R/a$). As observed, $\Delta H/R$ corresponding to fracture inversely correlates with R/a . Asperity with smaller size requires larger height ratio for fracture to occur. When $\Delta H/R$ is 0.5, the threshold asperity radius for fracture is 11.89 nm ($R/a = 14$). In contrast, when $\Delta H/R$ is 1, fracture consistently emerges when R is larger than only 2.55 nm ($R/a = 3$), which also indicates that asperity fracture is not observed at extremely small asperity sizes. Despite the absence of simulations for $R > 12a$ (Case I) and $R > 16a$ (Case II) in Figure 5.10, fracture is expected to consistently occur as supported by consistent fracture observations at previous cases.

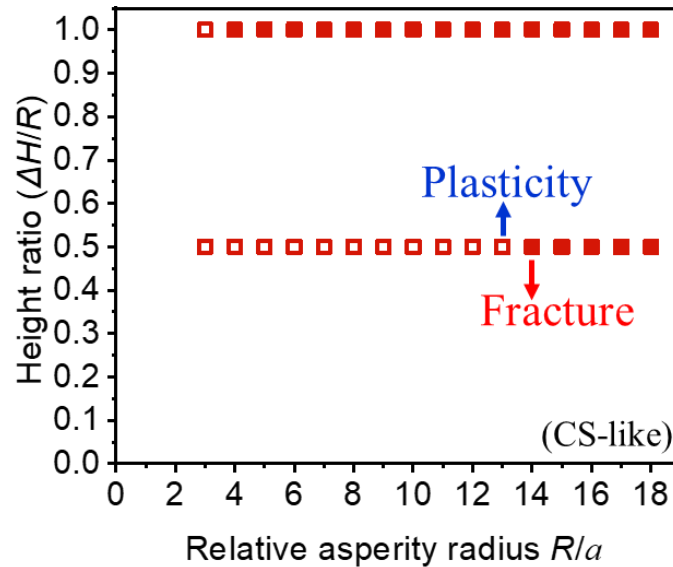


Figure 5. 10. The conditions under which asperity plastic wear and fracture occur under CS-like condition (constant normal stiffness-like condition). Open squares represent the cases for plastic wear and solid ones represent the cases of fracture.

Furthermore, in Figure 5.11, the failure mode transition under CL condition at the cases of (a) $R = 4a$, (b) $R = 8a$ and (c) $R = 12a$ is shown, where the maximum tangential shear force F_{tm} versus the normal force F_n is presented. Figure 5.11d shows the nominal maximum shear stress (t_{nm}) defined as $F_{tm}/(L_x * L_y)$ versus the nominal normal stress (s_n) defined as $F_n/(L_x * L_y)$ for all cases. As shown in Figure 5.11a-c, maximum shear force F_{tm} increases with F_n under all cases. Different critical thresholds exist under different asperity sizes, above which fracture occurs. Otherwise, plastic wear dominates. Notably, F_{tm} at the fracture cases of $R = 4a$, $8a$ and $12a$ observed under CS-like condition ($\Delta H = R$) is also close to the F_{tm} under CL condition. This suggests that F_{tm} may serve as an effective indicator for the failure transition under both CS-like and CL conditions.

When examining t_{nm} as a function of s_n for the cases of $R = 4a$, $R = 8a$, and $R = 12a$ in Figure 5.11d, all the data are on the same line, indicating that self-similarity exists in these simulation results. In addition, as R increases, the critical t_{nm} , which is the nominal maximum shear stress at the transition from plastic wear to fracture, appears to converge. This may provide reliable insights for the upscaling of the simulation results. The size effect observed for smaller asperities ($R = 4a$) is likely attributed to that the fracture process is accompanied by partial plastic deformation. Here, the gradient of the fitting curve between t_{nm} and s_n for all CL cases is also provided. The gradients (ξ) between t_{nm} and s_n for three cases ($R = 4a$, $8a$ and $12a$) are 0.81, 1.30 and 1.34, respectively. Actually, ξ is considered as the coefficient of friction for nanoscale asperity contacts.

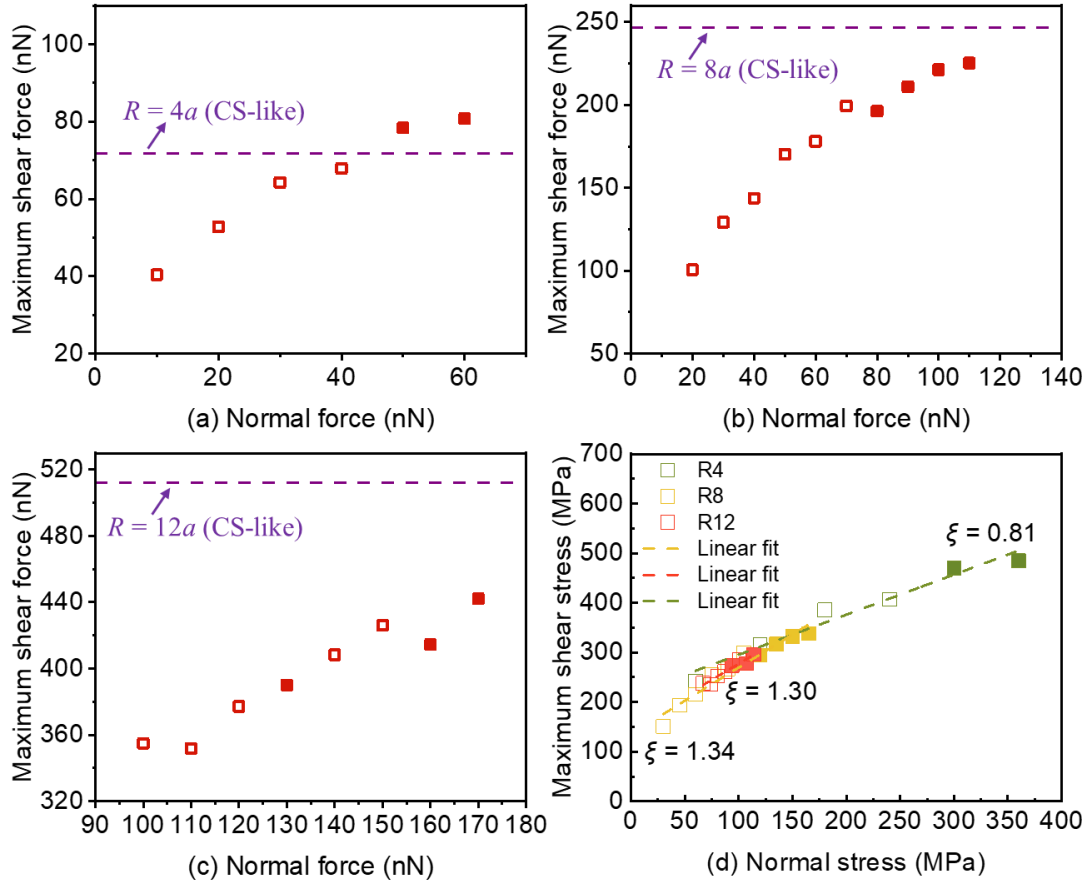


Figure 5. 11. The conditions under which asperity smoothing wear and fracture occur under CL condition. The maximum tangential shear force F_{tm} versus the normal force F_n is presented at (a) $R = 4a$, (b) $R = 8a$ and (c) $R = 12a$. (d) The nominal maximum shear stress (t_{nm}) defined as $F_{tm}/(L_x * L_y)$ versus the nominal normal stress (s_n) defined as $F_n/(L_x * L_y)$. The open triangle and square represent the case of plastic deformation. The solid ones represent the case of fracture.

5.6 Wear Volume Prediction

The generation of debris from asperity fracture or plastic flow should be accompanied by energy dissipation and transfer (De Moerlooze et al., 2011; Garcia-Suarez et al., 2023). Establishing the relationship between the wear volume and friction work is crucial for understanding seismic energy dissipation. Holm (1946) proposed a wear model related to the real contact area and flow pressure at atomic scale. Moreover, wear models involving thermal activation and energy barriers have also been developed

to predict the atomic-scale wear volume (Wang et al., 2021a; Wang et al., 2021b). However, these models are primarily applicable to the smoothing or plastic deformation cases. Hence, it is necessary to develop the wear model for fractured asperities.

Here, it is observed that Eq. (4.1) remains applicable for predicting the total wear volume of fractured α -quartz asperities (Figure 5.12). The scaling factor q for the fractured α -quartz asperities is estimated about 5.53 GPa, which could be related to the uniaxial strength recorded at about 8.23 GPa (Li and Fukuyama, 2025). Notably, q was also reported to be the lesser of the bulk shear strength and the junction shear strength in MD simulation for the grooving cases of asperity fracture (Aghababaei et al., 2017). However, the linear relationship may be disrupted when the temperature effect is obvious (Hirose et al., 2012).

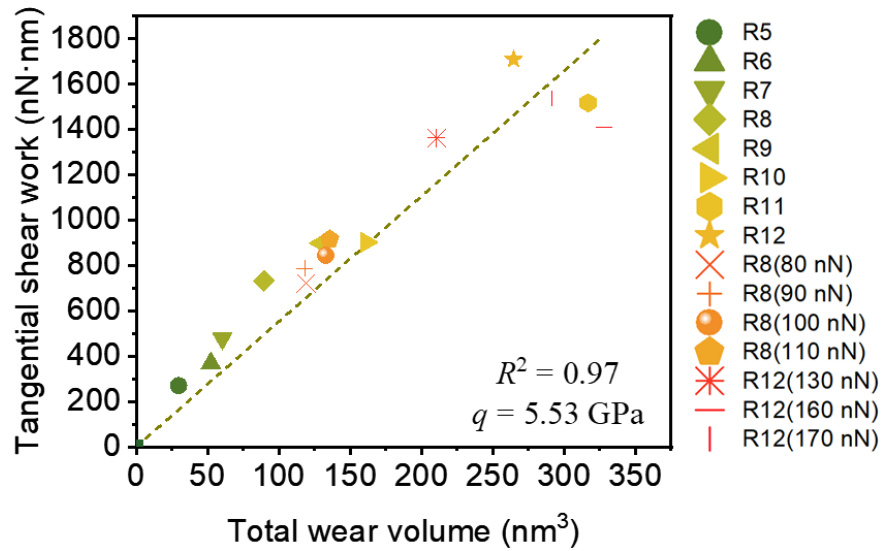


Figure 5. 12. The linear relationship between the total wear volume and tangential shear work for typical asperity fracture cases. Here, R5 stands for $R = 5a$ for Case I of the CS-like condition and so on. R8 (80nN) stands for CL case with $F_n = 80$ nN and so on.

5.7 Discussion

5.7.1 Comparison with prior nanoscale observation

The results reveal that under both CS-like and CL conditions, nanoscale α -quartz asperity wear failure is characterized by adhesive wear (Candela & Brodsky, 2016). The wear failure of nanoscale α -quartz asperities generally exhibits a transition from plastic

flow to fracture but is influenced by asperity radius and contact configuration. These results expand the earlier view favoring the plastic deformation at the nanoscale rock asperities during fault slip (Candela & Brodsky, 2016), which also offer a complementary perspective on twin-mediated plastic-to-brittle transition mechanism (Siman-Tov et al., 2013). However, it should be noted that this study primarily focuses on the failure mode transition of rock asperities without surface grooves. In contrast, earlier molecular dynamics studies in tribology revealed the plastic-to-fracture transition under grooving conditions (Aghababaei et al., 2016, 2017), which significantly advanced the understanding of nanoscale asperity failure mode transition, particularly by informing the critical length scale for groove formation on faults (Candela & Brodsky, 2016).

Furthermore, when comparing the present results with Li & Fukuyama (2025) on the ductile-to-brittle transition of α -quartz asperities under normal loading, the crack propagation paths within the asperity and the mechanisms of debris formation are substantially different. Under normal loading condition of Li & Fukuyama (2025), meridian fractures can develop due to the effect of Poisson effect under centrosymmetric contact, resulting in radially distributed fragments along multiple fracture planes. In contrast, under shear loading in the present study, debris formation occurs more uniformly and is primarily aligned along a single fracture plane within the asperity in the present study. These observations suggest that the loading or contact boundary condition can profoundly influence the underlying failure mechanisms of nanoscale rock asperities. These observations should be considered in theoretical modeling to more comprehensively capture the various types of ductile-to-brittle transitions in the future.

5.7.2 Failure mode transition mechanism

It is deemed that the wear failure transition of asperities is related to the local contact stress evolution and bulk yielding strength, as the yield-induced damage band is consistently observed in the fracture cases. Here, the local contact stress could refer to

the von Mises stress (σ_{VM}) (Laithy et al, 2019). For convenience, the local contact stress evolution and the yielding process are illustrated by considering the theoretical solution for normal contact between two spheres.

According to Hertzian contact theory, the surface pressure distribution at the contact interface between two spheres can be expressed as ($\chi \geq 0$) (Johnson, 1985):

$$p(\chi) = p_0 \sqrt{1 - \left(\frac{\chi}{\rho}\right)^2} \quad (5.1)$$

where p is the surface pressure; p_0 is the maximum surface pressure; χ is the distance from the center; ρ is the contact radius. However, as the maximum value of σ_{VM} typically occurs at a certain depth below the contact surface (Johnson, 1985), the subsurface stress distributions need to be considered. For simplicity, the stress components below the centerline ($\chi = 0$) are presented as follows (Johnson, 1985):

$$\sigma_x = \sigma_y = -p_0 \left[(1 + \nu) \left(1 - \frac{z}{\rho} \tan^{-1} \left(\frac{\rho}{z} \right) \right) - \frac{1}{2} \left(1 + \frac{z^2}{\rho^2} \right)^{-1} \right] \quad (5.2)$$

$$\sigma_z = -p_0 \left(1 + \frac{z^2}{\rho^2} \right)^{-1} \quad (5.3)$$

where ν is the Poisson's ratio and z is the depth below the contact surface. Then, by substituting Eq. (5.2) and Eq. (5.3) into the Von Mises stress expression, σ_{VM} of the subsurface can be written in the form of Eq. (5.4).

$$\sigma_{VM} = p_0 \left\{ \frac{3}{2} \left(1 + \frac{z^2}{\rho^2} \right)^{-1} - (1 + \nu) \left[\left(1 - \frac{\rho}{z} \tan^{-1} \left(\frac{\rho}{z} \right) \right) \right] \right\} \quad (5.4)$$

Here, in Eq. (5.4), p_0 and ρ can be further expressed as functions that are positively proportional to the nominal strain ε_n , which is defined by overlapping distance ΔH divided by asperity radius R (see also in Figure 1.2b). Therefore, σ_{VM} can be represented as a function solely dependent on ε_n for a given material. By numerical analysis, one can observe that σ_{VM} generally increases with ε_n (Johnson, 1985; Kumar et al, 2015). This indicates that during the collision process, asperities will undergo strain accumulation. As the strain increases, the subsurface stress (e.g. σ_{VM}) within the asperity also rises accordingly. Once the stress reaches the material's yield strength (Li & Fukuyama, 2025), damage bands begin to form.

However, the formation of damage bands is in the initial stage of the failure transition.

Whether the transition to asperity fracture occurs depends on the competition between the rising contact stress and the strength of the damaged asperity. As observed in Figure 5.6, in the intermediate regime under CL condition, damage bands may form without actual fracture, resulting instead in plastic wear of asperities. This occurs because the stress caused by loading is insufficient to reach the strength (Ritchie et al., 1973) in the damaged asperity. Therefore, a larger F_n is often required to enhance adhesion between asperities and increase the local contact stress to a critical level for fracture initiation. However, it is worth noting that the morphology of damage bands within the asperity can vary (Figure 5.8), which may in turn influence the strength of the asperity.

5.7.3 Formation mechanism of vertical damage bands

A nearly vertical damage layer occurs at $\Delta H = R/2$ under CS-like condition. This phenomenon is fundamentally different from the 45° cracks at the asperity root reported in previous studies (Aghababaei et al., 2017). Firstly, it could be associated with the increased normal contact force F_n . As shown in Figure 5.13, F_n increases with L for both $R = 12a$ and $R = 16a$ cases. In the fracture case ($R = 16a$), F_n exceeds the peak value for asperity fracture observed in previous studies of the normal contact (Li & Fukuyama, 2025), whereas in plastic deformation case ($R = 12a$), F_n is significantly lower than the critical peak force F_{tm} .

Moreover, the occurrence of this phenomenon is coupled with the morphological irregularities of the contact interface. Two typical cases are compared under Case II of CS-like condition; one is without vertical damage ($R = 12a$) and the other is with vertical damage ($R = 15a$) (Figure 5.14). Contact surface profile and damage plane are selected by using the alpha-shape method (probe sphere radius is 0.5 nm) (Lou et al., 2013) and the von Mises strain criterion (> 0.5) is adopted. Here, the surface atoms (red part) involved in the contact between asperities in Figure 5.14 are almost entirely covered to reconstruct the contact profile. As can be seen, the contact profile for $R = 12a$ appears relatively smooth compared with that at $R = 15a$ (Figure 5.14AC). Importantly, the contact profile at $R = 15a$ displays a pronounced lift-up at the sliding

front, producing a relative height difference of the contact profile (Figure 5.14B and shallow depression in Figure 5.14D). This indicates that the contact surfaces of the asperities undergo obvious non-uniform compression in the normal direction, which induces relative shear (Figure 5.14B) and results in vertical defects. Given the brittle nature of α -quartz, the defect will propagate downward and forward (x direction) under the combined effect of shear and normal loading. Ultimately, it forms the planar damage layer inside asperities. However, it should be noted that α -quartz exhibits significant anisotropy, with fracture surface energy depending on the crystallographic orientation (Molaei, 2022). Therefore, the formation mechanism of the damage layer may change, or alternative mechanisms may arise, depending on the crystal orientations.

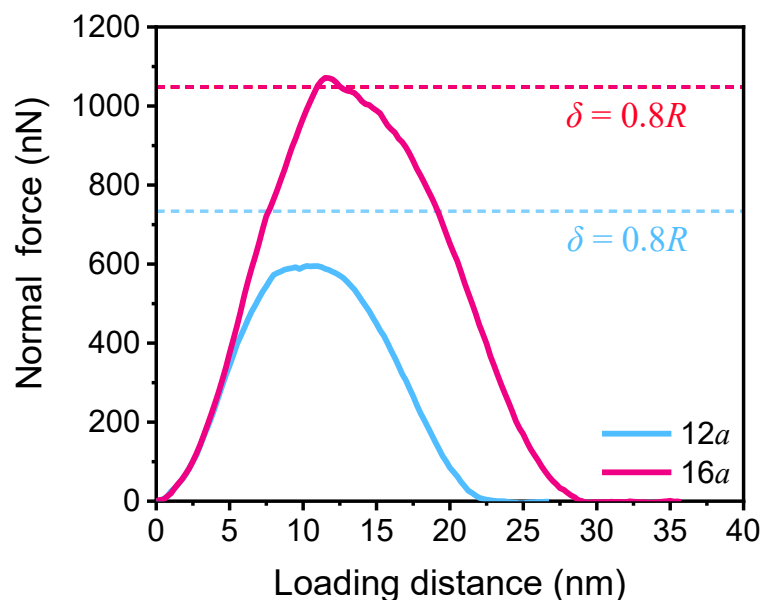


Figure 5. 13. The normal force F_n (nN) as a function of loading distance L (nm) under the case of $R = 12a$ and $R = 16a$. The dotted lines are the corresponding maximum normal force estimated from Li & Fukuyama (2025) for the case of $r = 0.8R$. r is the horizontal offset distance between two asperity tops.

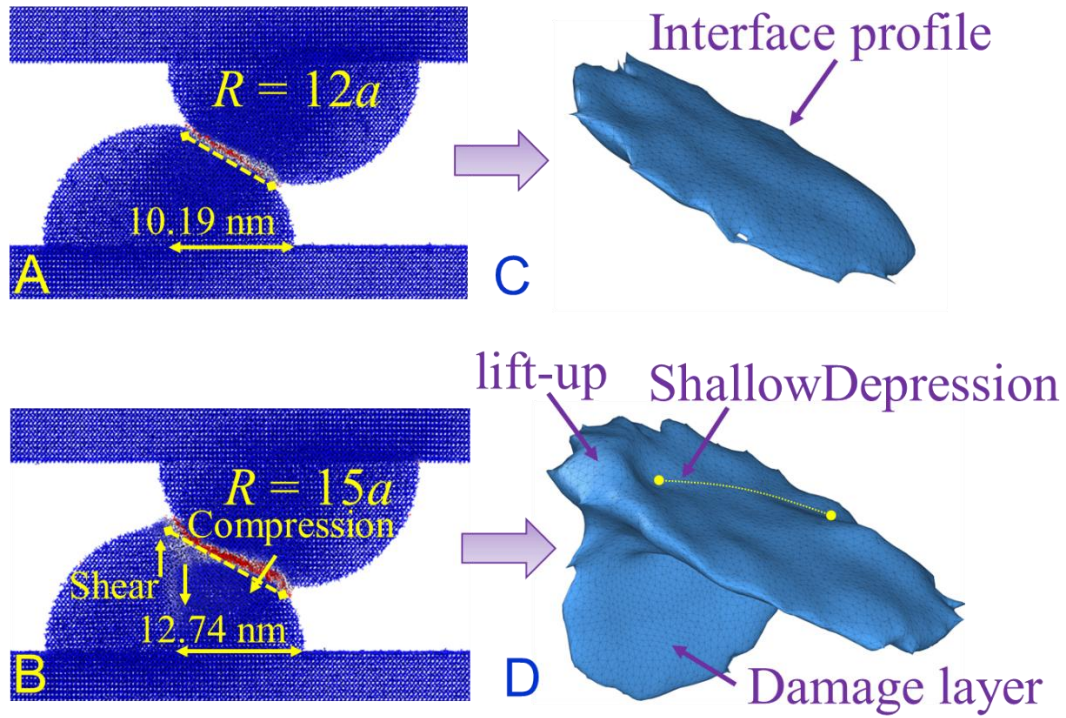


Figure 5. 14. The contact profiles and damage band from two cases under Case II of CS-like condition. (A) $R = 12a$ (no vertical damage) and (B) $R = 15a$ (vertical damage). (C) The contact profile of $R = 12a$ and (D) the contact profile and damage layer of $R = 15a$. The scale bars in (A) and (B) indicate the asperity radius. The ends of yellow dash lines in A (length of about 9.29 nm) and B (length of about 13.98 nm) represent the size of contact profile in C and D.

5.7.4 Grooving and non-grooving mechanism

In simulation results, asperity fracture overall precedes surface fracture on a substratum, preventing from groove formation (Figure 5.15). As another failure mode, asperity fracture with surface grooves has been reported by Aghababaei et al. (2016, 2017). Therefore, the asperity fracture can be categorized into two cases: grooving and non-grooving cases. The transition from non-grooving to grooving cases should be related to the critical fracture stress at the asperity root, which is associated with tensile fracture and depends on the angle θ_c (Figure 5.15). Here, θ_c can be interpreted as the crack angle formed between the asperity boundary and the substratum surface (Malekan, 2023). Although a theoretical expression from the non-grooving to grooving transition

remains highly challenging, as it involves many factors such as the asperity contact configuration, boundary condition, interfacial properties, and material strength heterogeneity, a useful semi-empirical formula was proposed by Aghababaei et al. (2016). The fracture initiation was considered to be related to the interfacial shear strength and the bulk shear strength of asperities. Therefore, groove formation was modeled by considering the relation between the bulk and junction shear strengths and the balance between elastic strain energy and fracture surface energy as follows (Aghababaei et al., 2016):

$$\alpha \cdot \frac{\sigma_j^2}{2G} \cdot \frac{\pi(D)^3}{6} = \beta \cdot (\Delta w \cdot \frac{\pi(D)^2}{4}) \quad (5.5)$$

where σ_j is the lesser of the bulk shear strength and the interfacial junction shear strength; α and β are the shape factors; G , D , and Δw are the shear modulus, junction size and fracture surface energy, respectively. Then, the groove formation can be generally linked to a critical junction length during asperity collision (Aghababaei, et al., 2016).

It is worth noting that the critical junction length defined in previous studies corresponds to the strong adhesion force required to detach the asperity from the substrate (Aghababaei et al., 2016). In simulations of non-grooving case under both boundary conditions (CS-like and CL) of this thesis, the asperity fracture cases in Figure 5.10 and Figure 5.11 can also be related to critical junction lengths. However, the length is primarily correlated with the condition that the subsurface stress reaches the strength of damaged asperity. Therefore, the underlying meaning is different. Moreover, as shown in Figure 5.16, under CS-like condition when $\Delta H = R$, the critical contact length before fracture is about 4.20 nm ($R = 5a$). In contrast, when the asperity size increases to $R = 12a$ at $\Delta H = R/2$, the contact length increases to about 9.81 nm, but plastic deformation dominates. Therefore, in the non-groove case of α -quartz asperities, the critical length should vary with different contact configurations due to heterogeneous material properties. More computational cases are needed in the future to characterize the distribution of the values.

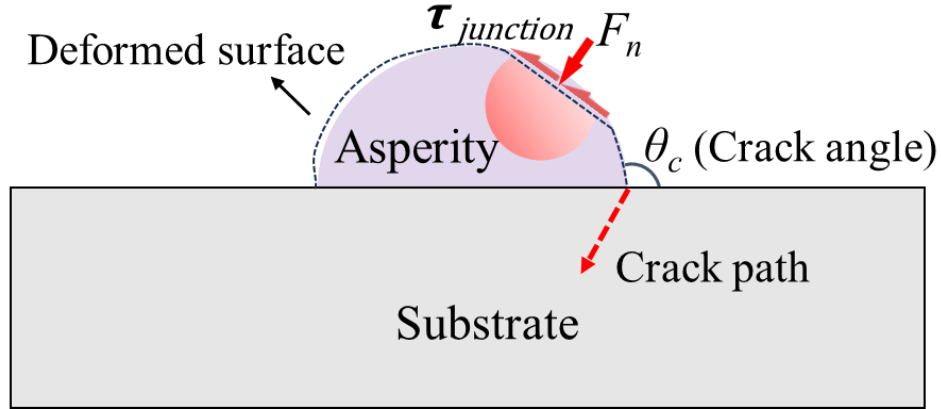


Figure 5. 15. Schematic illustration of asperity fracture modes. Red shade indicates stress concentration.

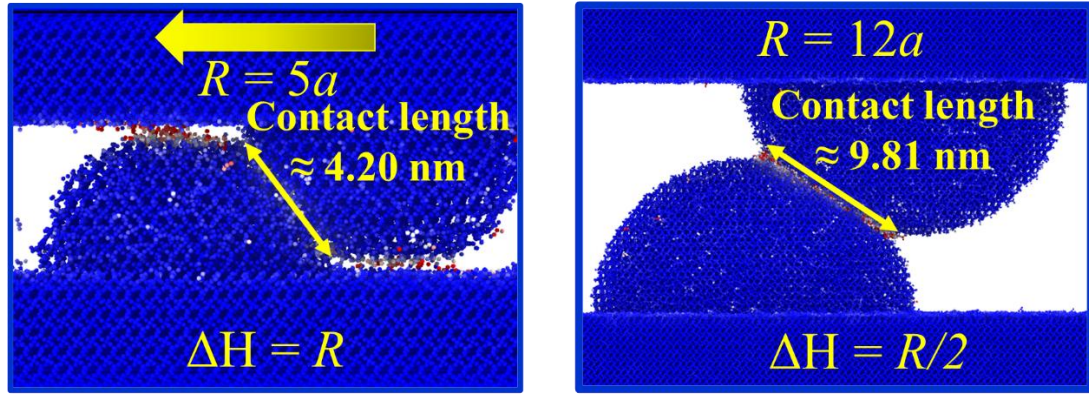


Figure 5. 16. The typical contact length measured at $R = 5a$ (Case I) and $R = 12a$ (Case II) under CS-like condition. Here, the junction length can also be the projection of contact length onto the x -axis.

5.7.5 Friction evolution under different failure modes

Finally, the evolution of tangential shear force F_t under various asperity radii and contact configurations under CS-like condition is presented in Figure 5.17. As seen, both F_{tm} and the weakening distance increase with R . The weakening distance is defined as the distance between the peak and final tangential shear forces. Moreover, the evolution of nanoscale shear force in all single-asperity cases exhibits a slip-weakening behavior, analogous to that described in macroscopic slip-weakening model (Scholz and Aviles, 1986). However, at the microscale, the weakening reflects multiple

mechanisms, including the overcoming of interfacial adhesive forces in plastic cases and the release of fracture energy in fracture cases. Moreover, it is also observed that variations in contact configuration give rise to different F_{tm} as typically illustrated at $R = 12a$, differing by over a hundred nanonewtons (351.6 nN for RH12 and 512.3 nN for R12). From this case, it is also evident that the wear failure mode significantly influences the friction force drop (after F_{tm}). The post-peak force slope becomes steeper in fracture cases (e.g., R12) than in plastic ones (e.g., RH12) at the nanoscale. These results can offer important insights into the multiscale friction modeling, where the understanding of dynamic rupture process at the microscale can also be informed (Wu & Barbot, 2025).

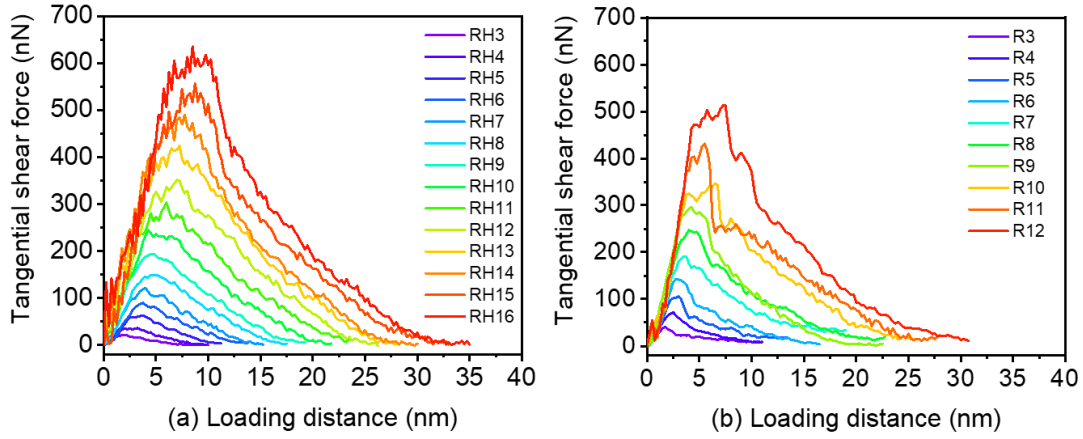


Figure 5. 17. The tangential shear force (F_t) as a function of loading distance (L) under various asperity radius and contact configurations under CS-like condition for the case of (a) $\Delta H = R/2$ (Case I) and (b) $\Delta H = R$ (Case II). R3 stands for $R = 3a$, and the others follow the same pattern. RH stands for the case $\Delta H = R/2$.

5.8 Conclusion

In summary, it is confirmed that both plastic flow and fracture of α -quartz asperities can occur during nanoscale friction. In the plastic wear case, the amorphization of surface atoms during sliding becomes the primary mode of energy dissipation. In contrast, in the fracture case, distinct damage bands typically emerge inside the asperity but the generation of damage bands depends on contact configurations and asperity size.

The occurrence of fracture can be fundamentally attributed that the local contact stress exceeds the critical fracture stress of damaged α -quartz asperities during frictional sliding. Moreover, it is observed that under CS-like condition, asperity with smaller radius requires larger height ratio for fracture to occur. Under CL condition, the failure transition can be reflected by the peak tangential shear force. Finally, the fracture-induced total wear volume of nanoscale α -quartz asperities linearly scales with the total tangential shear work.

CHAPTER VI

Particle Wear and Its Role in Friction

6.1 Introduction

This chapter aims to clarify the frictional wear mechanisms of nanoscale gouge particles and their role in the evolution of fault shear strength. A series of nanoscale single-particle wear processes of α -quartz are simulated under different asperity intervals, particle sizes, contact configurations and the normal forces, where the corresponding wear damage and wear volume of gouge particles, as well as the impact of particle wear damage on the friction coefficient are also discussed. The results indicate that higher normal forces can induce particle breakage over a short loading distance, while the lower normal forces lead to smoothing wear over longer distance. For smoothing wear cases, the wear volume increases linearly with loading distance in a stable mode. In contrast, in fracture cases, stable, sub-stable, and fracture stages of wear volume evolution exist with the sub-stable stage marked by superlinear wear volume growth. The wear volume of particles in both stable and sub-stable wear stages can be predicted by tangential shear work, as the shear work scales well with the wear volume. Finally, the particle size, asperity interval, normal force and contact configuration can influence the lifetime of α -quartz gouge particles, and particle fracture can lead to an immediate increase in friction coefficient rather than a decrease. These findings are crucial for understanding nanoscale friction and wear mechanisms in faults containing gouge particles, contributing to the explanation of the microscopic origins of macroscopic frictional behavior of faults.

6.2 Numerical Model

Figure 6.1 illustrates the crystal structure of α -quartz and the friction model. As seen, the friction system contains two rectangular friction blocks composed of asperity walls and a spherical gouge particle. The asperities with identical radius ($R = 4a$) were arranged on the upper and lower friction surfaces in the blocks. They were aligned in parallel along the X - and Y -axes with equal spacing ($\lambda_1 = \lambda_2 = 2.5R$) (Figure 6.1c-d). The center of the particle was positioned to coincide with the body center formed by the

four upper and four lower asperity centers, resulting in a total of eight contact surfaces initially (Figure 6.1c-d). Here, the particle radius R_b was set to $5a$ in initial setup.

Overall, the effect of particle size (R_b), asperity spacing (λ_1), and the normal force (F_n) on the particle wear mechanism is investigated by increasing R_b from $5a$ to $6a$, λ_1 from $2.5R$ to $3R$ as well as F_n from 35 nN to 70 nN in the increment of 5 nN. Additionally, the influence of contact configuration of particles on the particle wear mechanism is also examined by locating the particle at the center to coincide with the middle line in the side view (dotted circle in Figure 6.1d), where four contact surfaces were formed in initial setup. Here, other simulation conditions remained consistent with the initial setup but F_n from 35 nN to 50 nN. Table 6.1 shows the model description and simulation parameters.

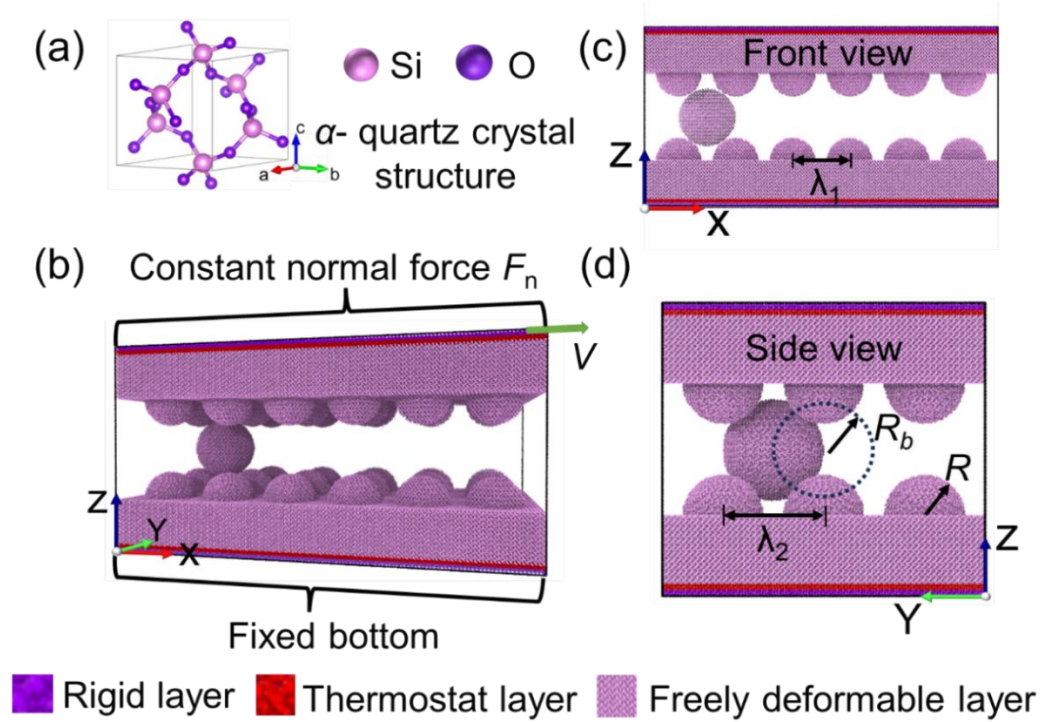


Figure 6. 1. Materials and simulation model. (a) The crystal structure of α -quartz. (b) The oblique view of the friction model. (c) The front view (X-Z plane) of the friction model. (d) The side view (Y-Z plane) of the friction model. The dotted circle is the middle contact case. L_x and L_y are fixed at $15R$ and $7.5R$ and the thickness of both substrates in the z -direction is fixed at $2R$.

Table 6. 1. The model description and simulation parameters. Model 1 serves as the reference, while Models from 2 to 4 change the particle size, asperity interval, and particle location, respectively.

Model Name	Particle Location	R_b	λ_1	λ_2
Model 1	Trough	$5a$	$2.5R$	$2.5R$
Model 2	Trough	$6a$	$2.5R$	$2.5R$
Model 3	Trough	$5a$	$3.0R$	$2.5R$
Model 4	Ridge	$5a$	$2.5R$	$2.5R$

6.3 Simulation Procedure

The simulation procedure is also similar to that in Chapter IV. The loading velocity was set to 30 m/s, which has been considered appropriate in molecular dynamics simulations, balancing accuracy with computational resource demands (Brilliantov et al., 2023).

6.4 Wear Damage and Wear Volume of Particles

6.4.1 Computation results for Model 1

Figure 6.2 illustrates the typical wear processes of nanoscale α -quartz particles (see Table 6.1 for detailed configuration) under various normal forces (40 nN, 50 nN, 60 nN, and 70 nN).

As can be seen, all the cases undergo the adhesive wear but the wear mechanisms of α -quartz particles exhibit a clear dependence on the applied normal force. At relatively low normal forces (40 nN and 50 nN), the wear of nanoscale α -quartz particles predominantly involves the smoothing wear process within a finite loading distance. However, as the normal force increases (e.g., 70 nN), particle breakage occurs. Notably, this can also be reflected in Figure 6.3a where the particle wear volume evolution is shown as a function of loading distance under various normal forces (35 nN~70 nN). As seen, the wear volume of α -quartz particles generally increases with the normal force.

The particle breakage can lead to a sharp increase in the wear volume under the normal forces of 65 nN and 70 nN, whereas the non-breakage wear process (smoothing wear) results in a relatively stable wear volume evolution. It should be noted that the wear volume evolution in the breakage cases (65 nN and 70 nN) can be further divided into three distinct stages, as exemplified under a normal force of 70 nN in Figure 6.3a. Stage I is a stable wear stage with a linear increase in the wear volume, followed by a sub-stable wear stage with the superlinear wear volume increase (Stage II). Finally, the severe wear (breakage) stage (Stage III) occurs, characterized by an abrupt increase in the wear volume. In comparison, at relatively lower normal forces (35 nN~60 nN), the particles only experience Stage I due to insufficient loading distances. Here, L_c can be defined as the critical loading distance required for particle breakage, which is estimated from the visualized particle strain and the distinct inflection point in the wear volume evolution. As observed, when the normal force increases, L_c decreases, where the breakage occurs at approximately 75 nm and 59.25 nm for $F_n = 65$ nN and $F_n = 70$ nN, respectively.

Furthermore, corresponding specific wear rate w_s is calculated in Figure 6.3b. In Stage I, the average w_s is calculated up to $L = 42.75$ nm for the cases from $F_n = 35$ nN to 70 nN. In Stage II, the average w_s is evaluated for L between approximately 51.75 nm and 59.25 nm for the cases of $F_n = 65$ nN and 70 nN. As can be seen, the average w_s in Stage I is approximately 4.43×10^{-3} ($\text{nm}^3/\text{nN} \cdot \text{nm}$) for all normal forces, with the order of 10^{-3} ($\text{nm}^3/\text{nN} \cdot \text{nm}$). The value in Stage II is approximately 1.22×10^{-2} ($\text{nm}^3/\text{nN} \cdot \text{nm}$), with the order of 10^{-2} ($\text{nm}^3/\text{nN} \cdot \text{nm}$), larger than that in Stage I. In contrast, the average w_s can reach the magnitude of the order of 10^{-1} ($\text{nm}^3/\text{nN} \cdot \text{nm}$) during Stage III (59.25 nm ~ 60 nm), showing the serious wear state of particles.

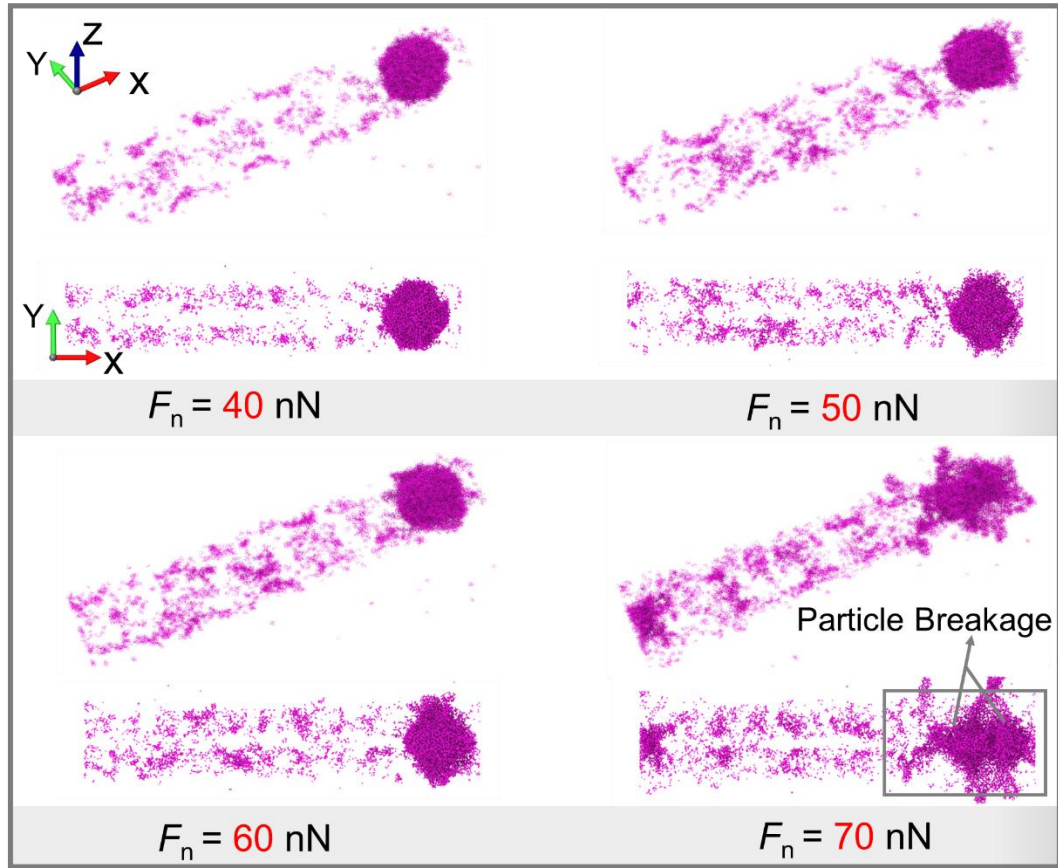


Figure 6. 2. The typical wear processes of α -quartz particles in Model 1 under various normal forces (40 nN, 50 nN, and 60 nN, 70 nN) at the loading distance of about 75 nm. The color density represents the distribution of detached atoms from the particle on the friction surfaces. The two snapshots represent the 3-D view (upper one) and 2-D view (lower one) of the particle trace.

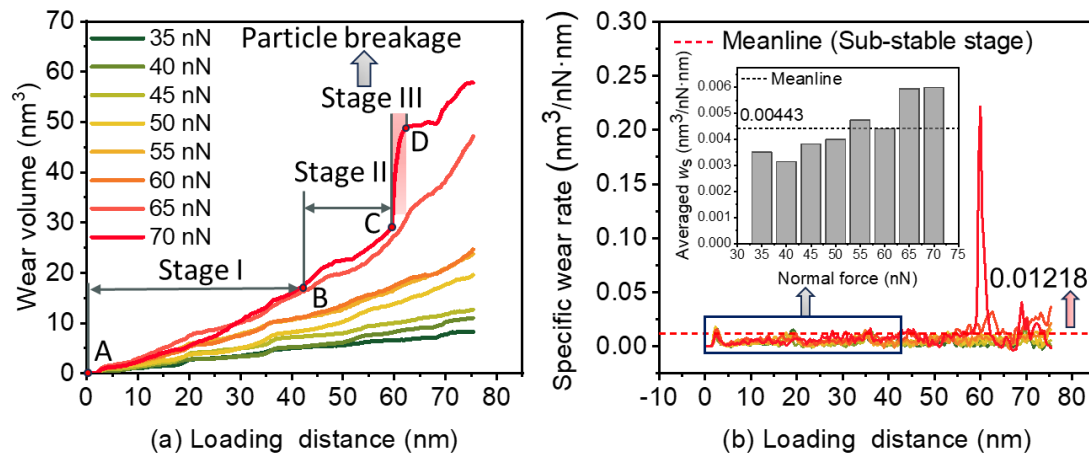


Figure 6. 3. The wear volume and specific wear rate versus loading distance for Model 1. (a) The wear volume as a function of loading distance under varying normal forces

from 35 nN to 70 nN in Model 1. (b) The specific wear rate as a function of loading distance under varying normal forces from 35 nN to 70 nN. The insert figure is the average specific wear rate in the stable wear stage.

6.4.2 Computation results for Model 2

Figure 6.4 illustrates the typical wear processes of nanoscale α -quartz particles with $R_b = 6a$ (Model 2 in Table 1) under various normal forces (40 nN, 50 nN, 60 nN, and 70 nN). These results indicate an obvious size dependence by comparing with the Model 1 results. Specifically, all the cases in Model 2 undergo smoothing wear without breakage while some breakage occurs in Model 1. Additionally, as shown in Figure 6.5a, the particle wear volume evolution follows a linear increase with loading distance, indicating stable wear stages (Stage I) under all normal forces. Therefore, the critical sliding distance also increases with particle size. It should be noted that the positive relation between the wear volume and the normal force still holds in Model 2.

Furthermore, w_s is shown in Figure 6.5b for all normal force cases. The average w_s of Model 2 ($R_b = 6a$) is 3.39×10^{-3} ($\text{nm}^3/\text{nN} \cdot \text{nm}$) estimated from $L = 0$ to 42.75 nm, which remains the same order of magnitude as that of Model 1 ($R_b = 5a$) in Stage I. Here, it is worth noting that the local peaks in Figure 6.5b primarily occur due to the collisions between the particle and asperities. They are associated with the adsorption and repulsion between atoms, which consequently lead to the local fluctuations of w_s .

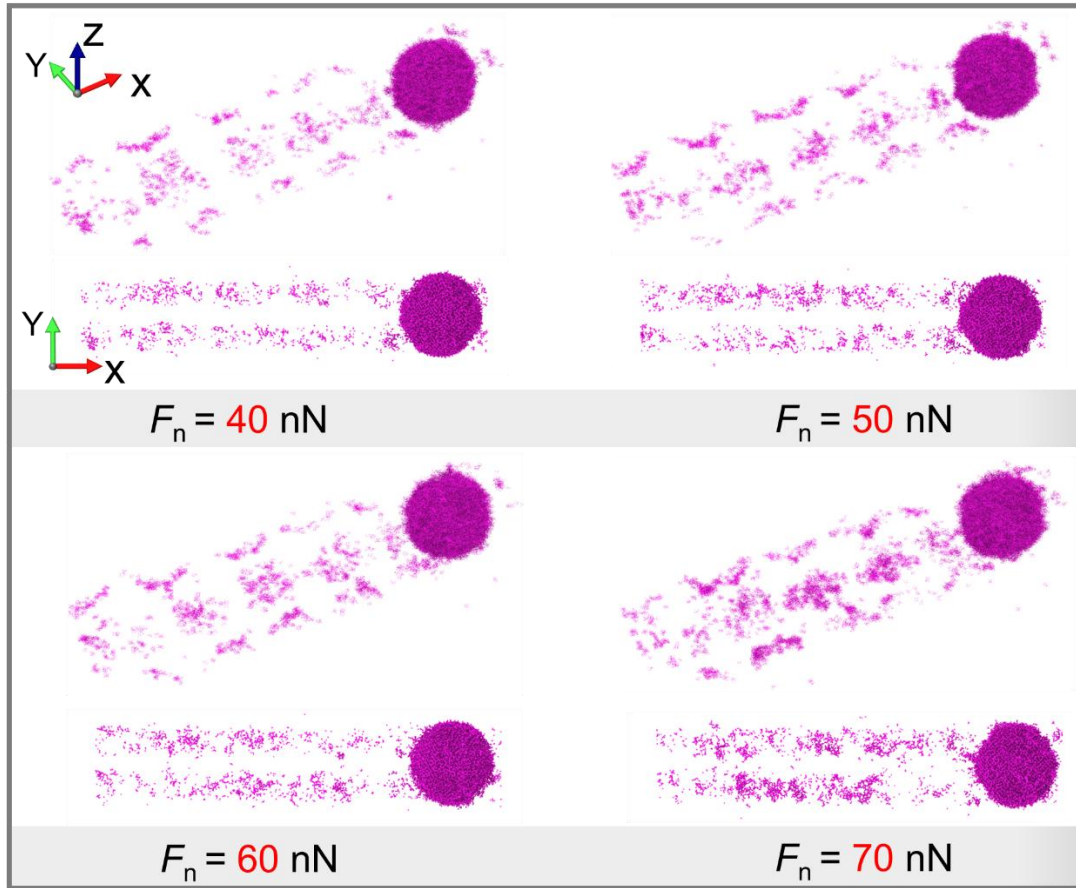


Figure 6. 4. The typical wear processes of α -quartz particles in Model 2 under various normal forces (40 nN, 50 nN, 60 nN, and 70 nN) at the loading distance of about 75nm.

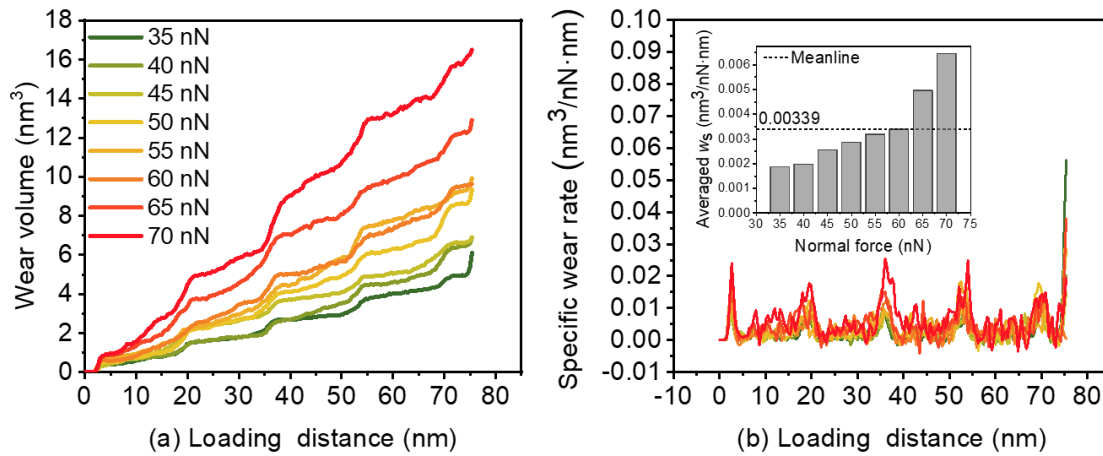


Figure 6. 5. The wear volume and specific wear rate versus loading distance for Model 2. (a) The wear volume as a function of loading distance under varying normal forces from 35 nN to 70 nN in Model 2. (b) The specific wear rate as a function of loading distance under varying normal forces from 35 nN to 70 nN. The insert figure shows the average w_s in Stage I.

6.4.3 Computation results for Model 3

Figure 6.6 shows the typical wear results of nanoscale α -quartz particles for $\lambda_1 = 3R$ (Model 3) under various normal forces (40 nN, 50 nN, 60 nN, and 70 nN). Figure 6.7 shows w_s for normal forces from 35 nN to 70 nN. It is observed that the particle still experiences smoothing wear and fracture depending on the normal force when $\lambda_1 = 3R$. However, increasing the asperity interval can influence the failure condition of the particle. Specifically, the particle breakage can occur at 60 nN when $\lambda_1 = 3R$ (Figure 6.6 and Figure 6.7a), but it is smoothing wear mode when $\lambda_1 = 2.5R$ (Figure 6.2). Here, the critical slip distance L_c varies with the normal force, ranging from approximately 48 nm to 71.25 nm for 60 nN $\sim$ 70 nN, respectively (Table 6.2). They are smaller than those of Model 1 ($\lambda_1 = 2.5R$).

However, it should be noted that increasing the asperity interval appears to have an insignificant effect on the average w_s in Stage I, with a value of $4.26 \times 10^{-3} \text{ nm}^3/\text{nN} \cdot \text{nm}$ recorded, which is similar to that observed in Model 1 ($\lambda_1 = 2.5R$). Moreover, the sub-stable wear stage before breakage (Stage II) still exists in Model 3, where w_s is relatively larger than that for Model 1, with the value of $1.32 \times 10^{-2} \text{ nm}^3/\text{nN} \cdot \text{nm}$.

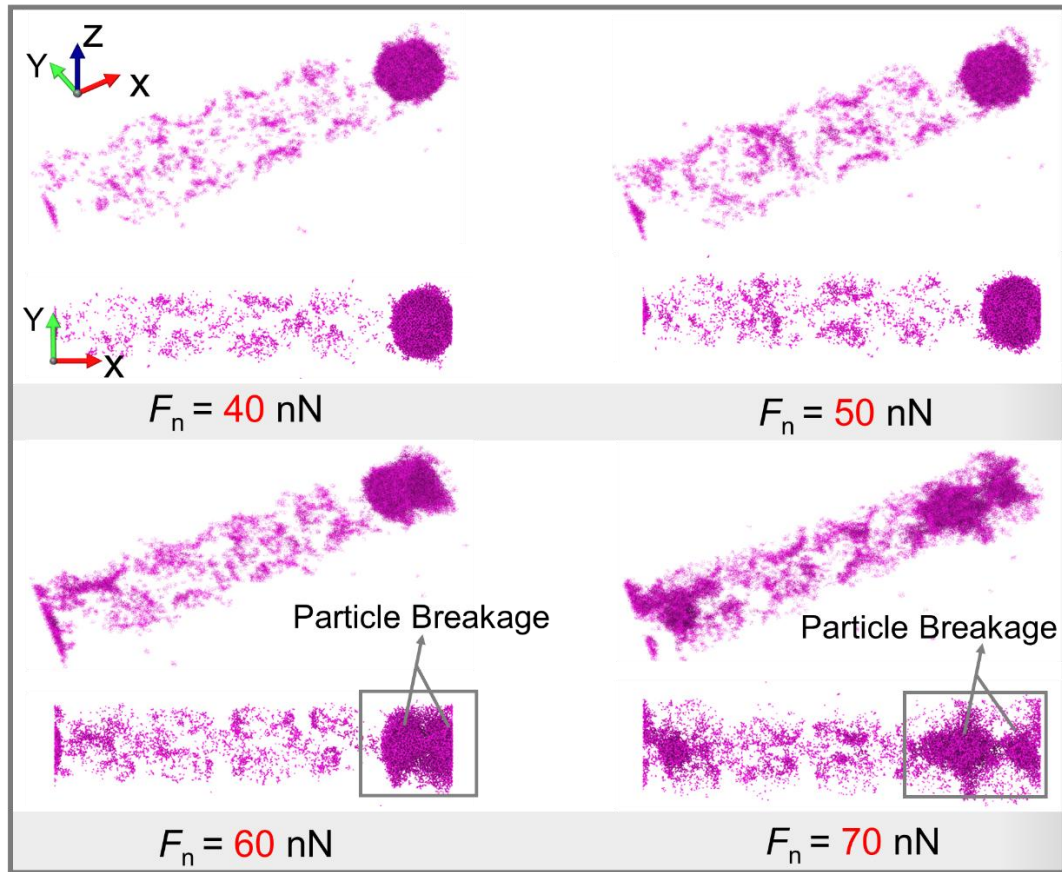


Figure 6. 6. The typical wear processes of α -quartz particles under various normal forces (40 nN, 50 nN, 60 nN, and 70 nN) in Model 3 at the loading distance of about 75nm.

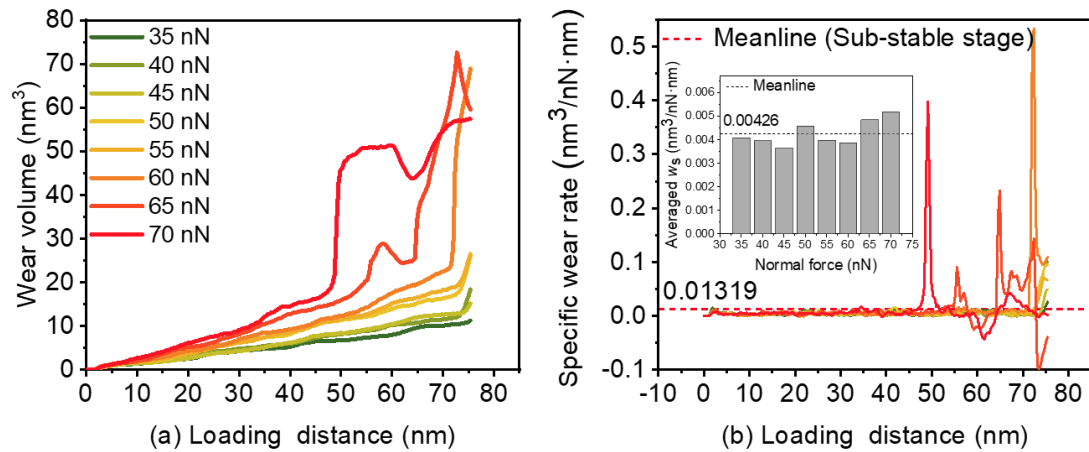


Figure 6. 7. The wear volume and specific wear rate versus loading distance for Model 3. (a) The wear volume as a function of loading distance under varying normal forces from 35 nN to 70 nN in Model 3. (b) The specific wear rate as a function of loading distance under varying normal forces from 35 nN to 70 nN.

6.4.4 Computation results for Model 4

Figure 6.8 shows the typical wear results of nanoscale α -quartz particles in Model 4 under various normal forces (42.5 nN, 45 nN, 47.5 nN, and 50 nN) where the particle is initially located along the asperity centers (ridge) shown as the dotted circle in Figure 6.1d. Figure 6.9 shows the corresponding wear volume from 35 nN to 50 nN and w_s for 35 nN and 40 nN cases. It is important to note that in the ridge case (Model 4), the particle trajectory can deviate and come into contact with adjacent asperities to form the trough case. Therefore, in Figure 6.9b, the cases for $F_n = 35$ nN and 40 nN are only shown which did not deviate the trace for the comparison of trough cases (Model 1). Moreover, in Tables 6.2 and 6.3, L_c and the average w_s for Stages I and II from Models 1 to 4 are summarized.

As shown in Figures 6.8 and 6.9a, the contact configuration has a significant effect on the wear behavior of particles. In the ridge case (Model 4), the particle breakage can occur at 47.5 nN, which is quite smaller than that for the trough case (Model 1). Moreover, the particle breakage can occur at significantly shorter loading distance than those in the trough case (Table 6.2), such as $L_c = 17.63$ nm at $F_n = 50$ nN in Model 4 but $L_c > 75$ nm in Model 1, demonstrating the high sensitivity of particle fracture to the normal force. This could be attributed that rolling path deviation in the ridge case can gradually shift the loading (contact) points from particle center to the edge along Y-axis. Meanwhile, the effective load-bearing volume is also be reduced. These changes will result in elevated stress concentration in the edge zone of particles, making them reach the failure threshold earlier. Therefore, the accelerated wear of particles is observed.

However, in Figure 6.9b, the average w_s in Stage I is approximately 2.94×10^{-3} ($\text{nm}^3/\text{nN} \cdot \text{nm}$) and 3.29×10^{-3} ($\text{nm}^3/\text{nN} \cdot \text{nm}$) for $F_n = 35$ nN and $F_n = 40$ nN cases, respectively (Table 6.3). Averaging was done from $L = 0$ to 21 nm. These values are close to that for the trough case (Model 1) under the same loading distance (3.39×10^{-3} $\text{nm}^3/\text{nN} \cdot \text{nm}$ and 3.37×10^{-3} $\text{nm}^3/\text{nN} \cdot \text{nm}$).

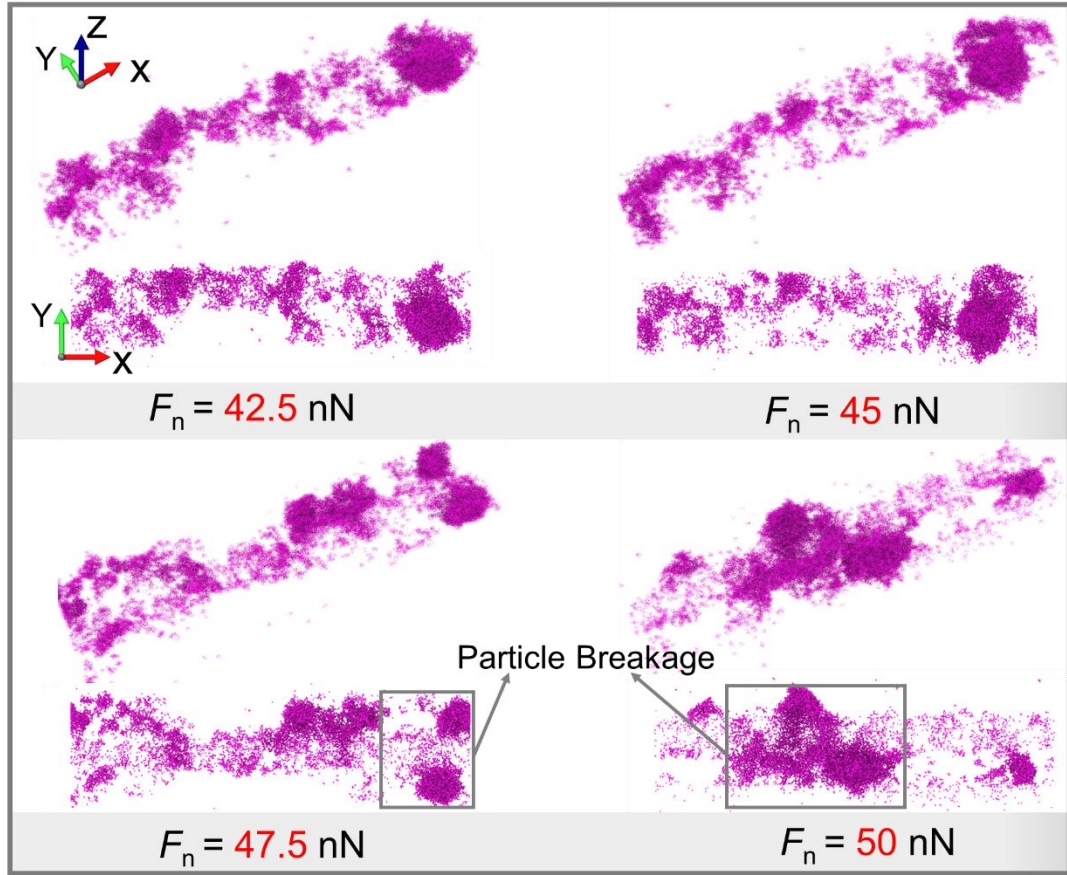


Figure 6. 8. The typical wear processes of α -quartz particles under various normal forces (42.5 nN, 45 nN, 47.5 nN, and 50 nN) in Model 4 at the loading distance of about 75 nm.

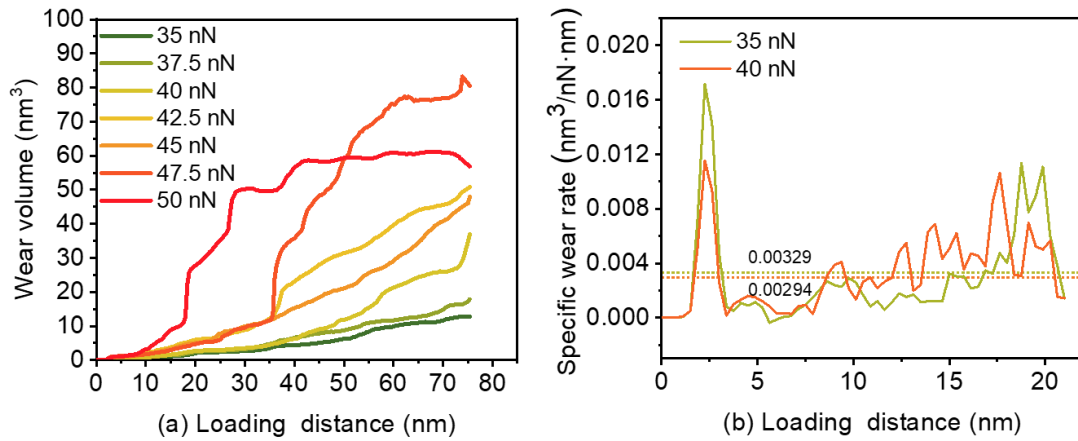


Figure 6. 9. The wear volume and specific wear rate versus loading distance for Model 4. (a) The wear volume as a function of loading distance under varying normal forces from 35 nN to 70 nN in Model 4. (b) The specific wear rate as a function of loading distance at the normal force of $F_n = 35$ nN and $F_n = 40$ nN respectively.

Table 6. 2. The critical sliding distance (L_c) from Model 1 to Model 4 under different normal forces (F_n).

F_n (nN)	L_c (nm)			
	Model 1	Model 2	Model 3	Model 4
42.5	—	—	—	35.25
45	—	—	—	—
47.5	—	—	—	35.25
50	—	—	—	17.63
60	—	—	71.25	—
65	75	—	55.13	—
70	59.25	—	48	—

Table 6. 3. The average w_s in stable and sub-stable wear modes from Model 1 to Model 4. The representative value of w_s is determined as the mean of the all averages.

Wear mode	Average w_s (nm ³ /nN·nm)			
	Model 1	Model 2	Model 3	Model 4
Stable	4.43×10^{-3}	3.39×10^{-3}	4.26×10^{-3}	3.14×10^{-3}
Sub-stable	1.22×10^{-2}	—	1.32×10^{-2}	—

6.5 Friction Coefficient

Figure 6.10 illustrates the typical evolution of the tangential shear force and friction coefficient averaged for 75nm (μ_a) for the trough cases. The tangential shear force is estimated by calculating the forces acting on the thermostat and rigid layers and considered as the friction force here. μ_a is linearly fitted by excluding the final two data points in the case of nonlinear increase. As shown in Figure 6.10, the friction force exhibits a stick-slip behavior during sliding, with the peak force arising from interlocking with asperities. Moreover, as the normal force increases, the friction force in the system also increases, consistent with macroscopical experimental observations (Byerlee, 1978). However, it should be noted that μ_a becomes uniform where the wear volume evolves linearly (Figure 6.10d). In contrast, when the particle fracture occurs, μ_a exhibits an increasing trend (Figures 6.10b and 6.10f). Notably, in Figure 6.10bdf,

the asperity gap and particle size also affect the friction coefficient. When $\lambda_1 = 2.5R$ and $R_b = 5a$ (Model 1), μ_a in the linear increase stage is at 0.51, larger than 0.47 recorded at $\lambda_1 = 3R$ and $R_b = 5a$ (Model 3). When $\lambda_1 = 2.5R$ and $R_b = 6a$ (Model 2), the friction coefficient is at 0.39, indicating a strong lubrication effect of the particle on the friction surfaces. Here, the average μ_a under different models is summarized in Table 6.4.

Table 6. 4. The average μ_a in the linear increase stage from Model 1 to Mode 3.

	Model 1	Model 2	Model 3	Model 4
μ_a	0.51	0.39	0.47	—

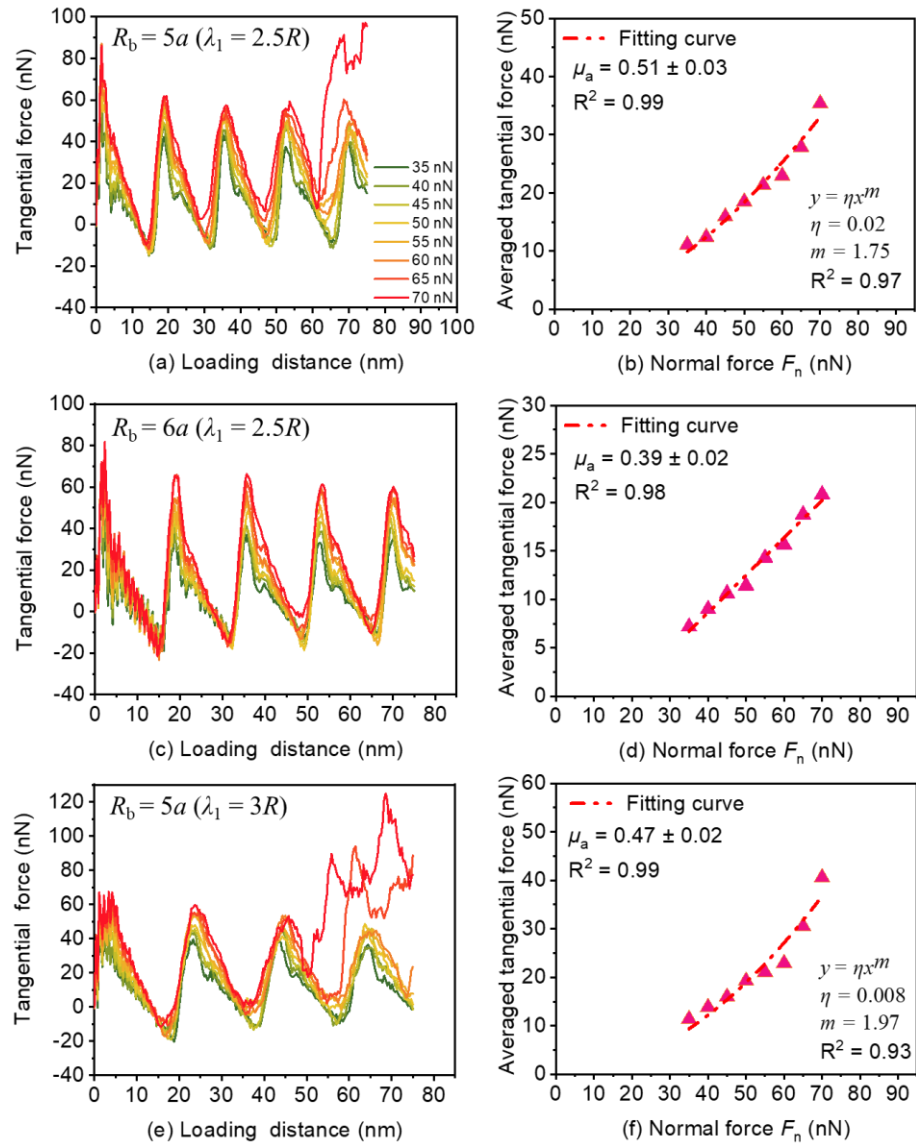


Figure 6. 10. The tangential shear force as a function of loading distance at the case of

(a) Model 1; (c) Model 2; (e) Model 3. The averaged tangential shear force as a function of the normal force at the case of (b) Model 1; (d) Model 2; (f) Model 3.

6.6 Wear Volume Prediction

Here, it is also observed that the nanoscale wear volume of α -quartz particles during Stages I (stable) and II (sub-stable) can be well predicted using the tangential shear work shown in Eq. (4.1). As typically shown in Figure 6.11, the tangential shear work scales well with the wear volume in both wear stages, which could be viewed as a reliable predictor for the particle wear loss.

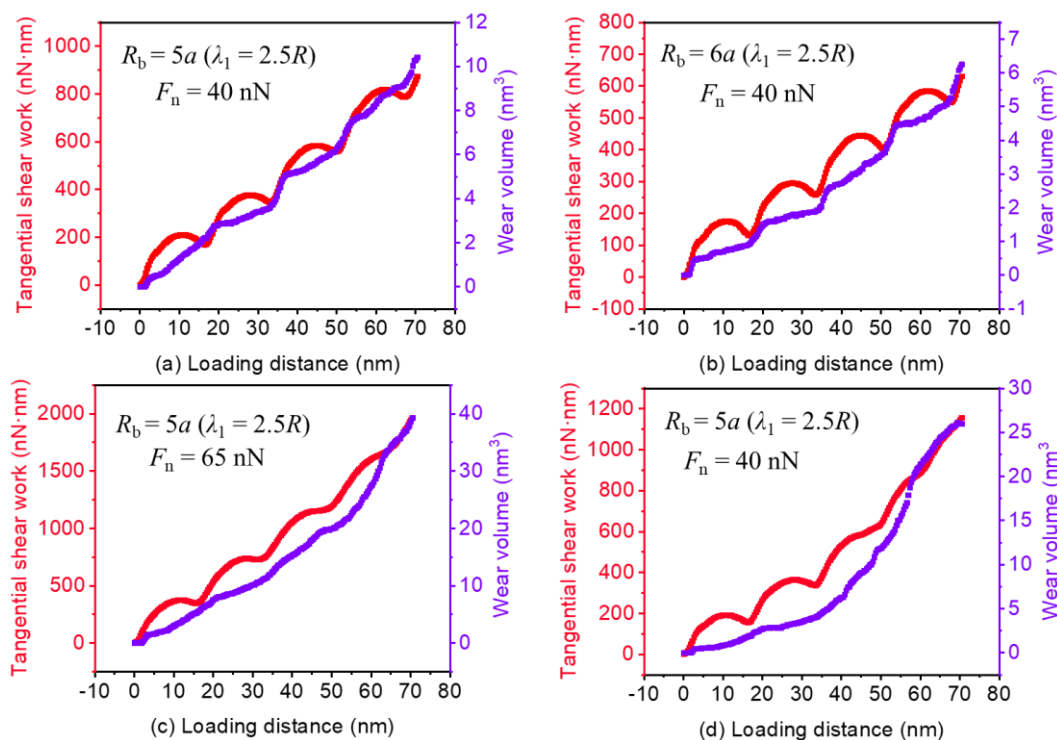


Figure 6. 11. The wear volume and tangential shear work as a function of loading distance at typical wear cases for (a) Model 1, (b) Model 2, (c) Model 1 and (d) Model 4. Red lines indicate tangential shear work and purple lines are wear volume.

6.7 Discussion

It is observed that under all cases, the normal force is positively related with the wear volume. This phenomenon could be attributed to the larger contact area and stronger adhesive force between a particle and asperities. As shown in Figure 6.12, the contact

length between a particle and asperities increases with increasing F_n , which can lead to an increase in the frequency of atomic wear events as more atomic contacts are constructed. Furthermore, the increasing normal force can enhance the interatomic forces due to closer interatomic distances, elevating the adhesive force between a particle and asperities. This can make surface atoms more likely to be separated from the surface. Therefore, the enlarged contact length and stronger adhesion force contribute together to the increase of wear volume under increasing F_n . This may also account for the accelerated failure of nanoscale α -quartz particles under higher F_n .

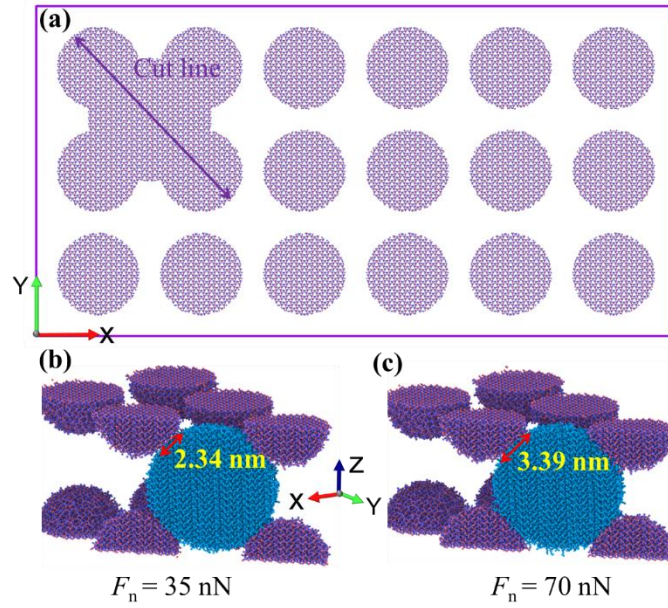


Figure 6. 12. The contact length under different normal forces in Model 2. (a) The 2-D cut view in the XY-plane for Model 2. The 3-D cut view under the normal force of (b) 35 nN and under the normal force of (c) 70 nN, along the cut line shown in (a). Red arrows indicate the contact length.

Furthermore, under the high F_n , particle breakage occurs within short loading distance L . It is deemed that the occurrence of particle fracture is related to the reduction of particle volume, since smaller particles have lower load-bearing capacity, which is consistent with previous observations (Issa et al., 2020). Moreover, as shown in Figure 6.13, the particle breakage primarily results from tensile strain inside, where the crack path typically develops vertically, leading to splitting failure. This failure mode

resembles the fracture pattern observed in Brazilian splitting tests. Here, the critical von Mises shear strain for fracture initiation is around 0.2, which could be comparable to the fracture strain of α -quartz under uniaxial simulation in MD reported by Issa et al. (2020).

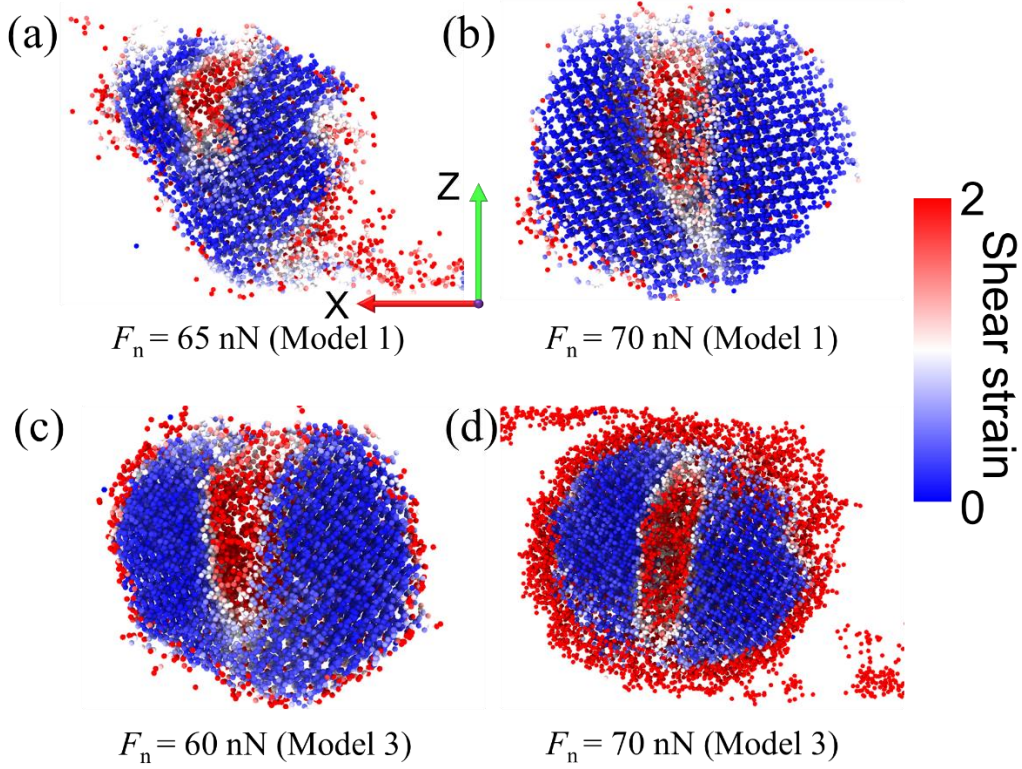


Figure 6. 13. The Von Mises shear strain of the typical cases of particle fracture for (a) $F_n = 65$ nN and (b) 70 nN of Model 1 and (c) $F_n = 60$ nN and (d) 70 nN for Model 3. Here, the cross-section of the fractured particles is shown where most of the worn atoms have been removed. The fractured particles are about at the loading distance of L_c .

Moreover, the occurrence of particle fracture should also be related to the dynamic shape changes induced by wear (Cho et al., 2006; Kock and Huhn, 2007; Zhang et al., 2020). As shown in Figure 6.14, when the normal force is 70 nN (Model 1), the particle appears rhomboidal in both of the XY and YZ projections before fracture. In contrast, when $F_n = 70$ nN (Model 3), the particle exhibits an elliptical shape in the YZ projection. These shape changes have been considered significant to altering the distribution and concentration of contact stresses within particles (Antony & Kuhn, 2004; Abe, & Mair,

2009; Athanassiadis et al., 2014), which need to be further considered in the future studies.

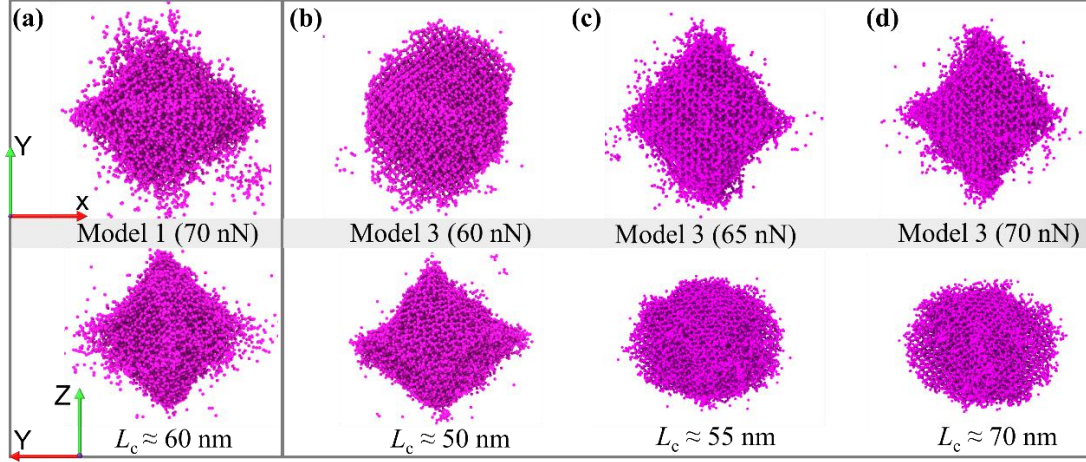


Figure 6. 14. The typical wear surface morphology and critical loading distance of nanoscale α -quartz particles under (a) Model 1 for $F_n = 70$ nN; (b) Model 3 for 60 nN; (c) Model 3 for 65 nN; (d) Model 3 for 70 nN. Here, the upper figure is the XY view of the particle morphology, where the lower one is the corresponding YZ view.

Furthermore, I also attempt to explain why particle fracture leads to an increase, rather than an immediate decrease in friction coefficient. I show two typical cases (Case 1 and Case 2) in Figure 6.15. In both cases, rolling friction dominates during the initial slip stage prior to particle breakage (Stages I and II). The friction force primarily arises by overcoming rolling resistance. Then, particle splitting occurs, generating two fragments.

In Case I (Figure 6.15a), while the left fragment sticks and rotates in place, the right slides and continues moving laterally as shear displacement increases. Therefore, the system needs to overcome the tensile adhesion force F_{adh} between the vertically fractured surfaces, which serves as the primary source of shear resistance. Moreover, since F_{adh} is positively correlated with the contact area, the shear force F generated by fracture surface adhesion should be much greater than the rolling resistance that typically involves only a small part of contact area. As a result, more energy is required to overcome the F_{adh} during slip, leading to a higher friction force.

Furthermore, in Case 2 (Figure 6.15b), particle fracture can also cause both fragments to stick and rotate in place simultaneously. In this mode, the fragments initially exhibit relative sliding along the fractured interface, perpendicular to a normal force F'_n (Figure 6.15b). Due to the large interfacial friction area, the resulting friction force should also be greater than the rolling resistance. Moreover, this mode of fragment motion can eventually lead to the cessation of relative sliding due to limited shear space, where further compression between the fragments will occur, inducing secondary fragmentation. At this stage, the friction force is primarily related to the particle bulk strength, which can also lead to higher shear resistance compared to the rolling mode.

Therefore, the overall increase in friction force after particle breakage can be largely attributed to the generation of fragments that introduces higher frictional resistance due to interfacial shear strength, interfacial adhesion strength, and particle bulk strength during slip. It is worth noting that the shortening displacement between the two plates (Δh , see Figure 6.15) is observed as a result of particle fracture in all cases (Figure 6.16). This Δh is coupled with the shear loading displacement, jointly adjusting the motion direction and interaction modes of fragments and playing a crucial role in the evolution of friction force.

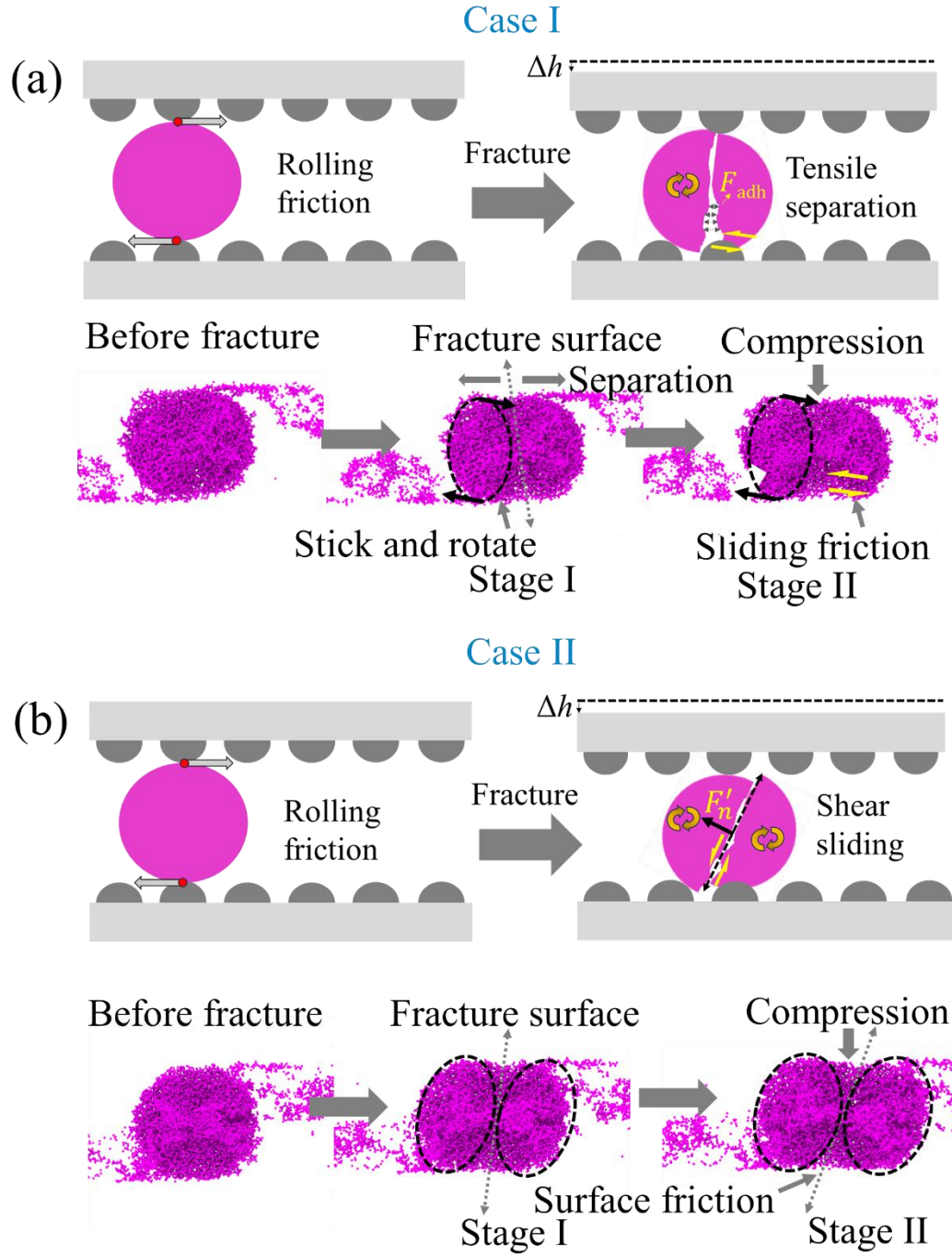


Figure 6. 15. The typical fragment motion after fracture under the normal force of 70 nN for two typical cases. (a) Case 1 is observed in Model 1 and (b) Case 2 is observed in Model 3. Here, the top raw in (a) and (b) is the schematic illustration of the computation results at the bottom raw.

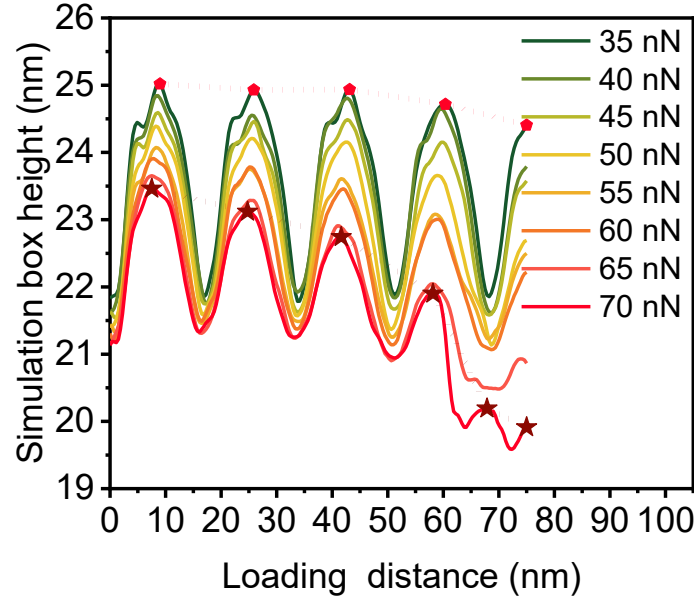


Figure 6. 16. The simulation box height as a function of loading distance at the case of Model 1 between $F_n = 35$ nN and 70 nN. The red solid circles and brown stars are the peak values of box height under every collision between asperities and the particle, respectively.

6.8 Conclusion

In summary, the results reveal that in all cases, the wear volume of particles increases as increasing the normal force, but the wear volume evolution depends on the wear damage state of the particle. Specifically, in the case of particle fracture, the wear state can be categorized as stable, sub-stable, and fracture stages, where the first two stages exhibit linear and superlinear increases in wear volume, respectively. In contrast, for smoothing wear case, the stable wear stage (Stage I) persists over longer distances. In the sub-stable wear stage (Stage II), the specific wear rate of α -quartz gouge particles is on the order of $10^{-2} \text{ nm}^3/\text{nN}\cdot\text{nm}$, while it is on the order of $10^{-3} \text{ nm}^3/\text{nN}\cdot\text{nm}$ in Stage I. However, the wear volume in both wear stages can be predicted by the tangential shear work as it scales well with the wear volume.

Furthermore, the particle breakage can occur within short L under high F_n , while the smoothing wear dominates within longer L under relatively low F_n . Therefore, L_c

required for particle breakage decreases with increasing F_n . Notably, L_c can be significantly influenced by particle size, contact configuration, and asperity interval, especially the former two factors. A larger particle typically exhibits a larger L_c under the same normal force, excluding the cases with extremely high normal forces. In contrast, variations in contact configuration can markedly reduce L_c and trigger particle fracture under low normal forces. It should be noted that the latter conclusion is based on the cases where the particle and asperities are initial contact in a centrosymmetric manner, which may differ under other initial contact configurations. Finally, it is observed that particle fracture leads to an immediate increase in friction coefficient rather than a decrease, indicating a fault strengthening trend.

CHAPTER VII

Discussion

In this thesis, three-dimensional nonequilibrium molecular dynamics (MD) simulations are employed to investigate the nanoscale normal contact and friction wear mechanisms of a pair of α -quartz asperities, and the wear mechanisms of a single α -quartz particle interacting with asperity walls during friction.

7.1 Asperity Contact

Firstly, in the study of normal contact behavior typically occurring prior to fault slip, it was found that fracture can occur during the compression of nanoscale α -quartz asperities, a result that contrasts with conventional assumptions of elastic or elastoplastic contact deformation in rock asperities. This highlights the need for further investigation into rock friction and wear, as models in these areas often focus on asperity deformation but traditionally assume it as elastic or plastic (Brown & Scholz, 1986; Wang & Scholz, 1994; Tang et al., 2017; Zhao et al., 2020). Specifically, it is well understood that the friction strength and wear volume of rocks are governed by the real contact area of asperities (Wang & Scholz, 1994; Aharonov & Scholz, 2018; Verberne et al., 2020; Nielsen et al., 2021). The traditional models predict an increase in the contact area as the normal force increases (Johnson, 1985; Chang et al., 1987; Zhao et al., 2000; Kogut & Etsion, 2002). However, this prediction can be disrupted when the fracture occurs, as it changes energy dissipation and the contact state of asperities, causing significant fluctuations in the real contact area. Therefore, in comparison with the traditional unbroken assumption of asperities, fractured asperities can exhibit considerable variability in terms of the friction strength and wear behavior. Here, an interesting point should be noted that previous studies on asperity wear have typically assumed that material loss occurs during friction stage (Archard, 1953; Wang & Scholz, 1994). In contrast, the results in this thesis demonstrate that the wear of α -quartz asperities can initiate even during contact stage, with material loss ranging from fine debris generated by plastic flow to larger particle-like fragments. This phenomenon presents a fundamentally different understanding from the previous wear mechanisms and holds significant implications for wear studies. Therefore, future studies can further

link the contact fracture of asperities to the modeling of friction as well as asperity wear on faults. Moreover, since this thesis focuses exclusively on spherical asperities, future work could explore non-spherical or fractal-featured asperities to better characterize the contact mechanics of individual asperities (Figure 7.1). On the other hand, the actual contact behavior of faults involves complex multiscale interactions among numerous asperities. While single-asperity contact models can provide valuable foundational insights, they are insufficient to fully capture these complexities. Hence, future research should also incorporate multiscale surface roughness (Figure 7.1) and collective asperity interactions to advance the comprehensive understanding of fault contact mechanisms.

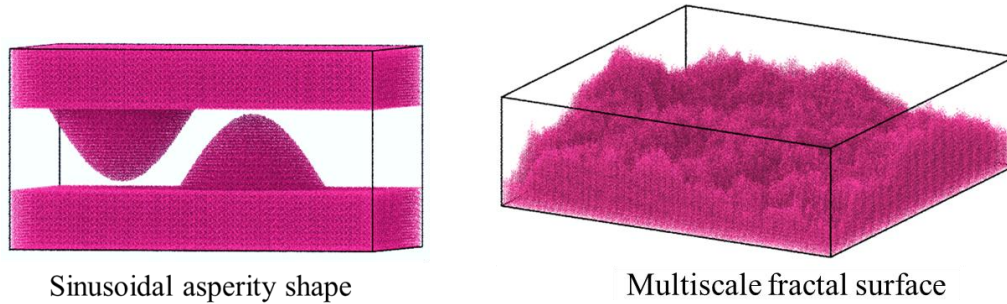


Figure 7. 1. The non-spherical asperities and fractal surface.

7.2 Asperity Friction Wear

When clarifying the single-asperity wear mechanisms typically occurring during fault slip, it was observed that both plastic deformation and fracture can occur in α -quartz asperities during nanoscale friction, extending earlier views of plastic-dominated and mixed plastic–brittle failure modes. Besides, the particle can be generated at the asperity radius only larger than 2.55 nm. These results hold significant implications for accurately estimating the fracture energy along a fault during earthquakes, which often needs to identify the minimum size of gouge particles generated from asperities during fault slip (Chou et al., 2014). However, it is worth noting that the fracture cases explored in this thesis are limited to non-groove scenarios, possibly due to the anisotropic

strength of α -quartz. Therefore, future work should consider a broader range of crystallographic orientations to examine the condition leading to groove formation and the particle size could change with crystallographic orientations. Notably, there is currently no unified and theoretical framework to explain the formation of grooves on asperities. While prior studies have suggested that groove initiation corresponds to the maximum shear strength of material (Aghababaei et al., 2017), this interpretation is primarily based on numerical simulations and lacks of a solid physical foundation. Whether this conclusion can be applied to explain the groove formation in geological materials remains to be investigated.

On the other hand, in the single-asperity friction wear chapters, it was observed that the wear volume in both plastic and fracture cases scales linearly with the tangential shear work, providing a quantitative basis for predicting wear volume at the nanoscale. However, a closer examination of the plastic wear case reveals that the evolution of wear volume with loading distance deviates from the linear trend predicted by the macroscopic wear model. This discrepancy underscores the need to further investigate the multiscale mechanisms governing asperity wear during friction, in order to bridge the gap between nanoscale observations and macroscopical models. Moreover, although the wear model introduced in this thesis exhibits strong predictive capability, the linearity between the wear volume and tangential shear work may break down under conditions where thermal effects become significant (Hirose et al., 2012). Therefore, further validation across a broader range of temperature is required to assess its general applicability.

Furthermore, the single-asperity wear process at the fracture case in Chapter V can also be viewed as the contact deformation process of asperities. Compared to the contact case under the normal loading discussed in Chapter III, the cases examined in Chapter V are primarily under shear loading. Nevertheless, as shown in Chapter V, shear-induced contact fracture can, in some contact configurations, be strongly coupled with the normal deformation in Chapter III. Hence, the normal contact deformation

discussed in Chapter III provides a critical foundation for understanding the shear-induced fracture behavior.

Overall, the single-asperity wear process, whether dominated by fracture or plastic deformation, involves interactions between asperities. Therefore, similar to the outlook presented in Figure 7.1, future studies should also consider the effects of asperity geometry, multiscale surface features, and multi-asperity interactions to comprehensively understand the two-body wear mechanisms on faults.

7.3 Particle Friction Wear

Moreover, since the single-asperity friction wear can lead to the formation of nanoscale gouge particles, this thesis also explored the mechanism of particle wear during friction. It reveals that nanoscale gouge particles can evolve from plastic wear to fracture with increasing loading distance. Stable wear prior to fracture has limited impact on the friction coefficient, but continuing volume loss eventually causes particle breakage and then leads to a significant increase in friction coefficient. These findings deepen the understanding of the role of wear damage state of nanoscale particles in fault strength evolution, which has been poorly understood in previous studies. On the other hand, the wear volume of particles was observed to scale linearly with the tangential shear work in the stable and sub-stable wear stages, which helps to establish a unified understanding of wear volume prediction from two-body to third-body friction processes. However, it should be noted that these observations are from the frictional wear of a single α -quartz gouge particle at the nanoscale. In natural faults, the third-body friction process generally involves complex interactions among multiple and multiscale gouge particles (Reches and Dewers, 2005; Mizoguchi et al., 2009). To better approximate natural fault conditions, future work could incorporate multiple particles with different sizes between host rocks to explore the coupled effects of multi-particle fractures on the macroscopic friction (Figure 7.2). Additionally, progressively increasing the thickness of gouge particles in the future may help reveal the full evolution of frictional behavior of faults (Figure 7.2). Since the computation resources

are limited to simulate a large number of particles and a wide size distribution by MD method, more detailed studies could be done in the future by the development of advanced parallel computing techniques and coarse-grained force fields to efficiently simulate larger third-body friction systems, which also contributes to the studies of larger-scale contact and tribological systems.

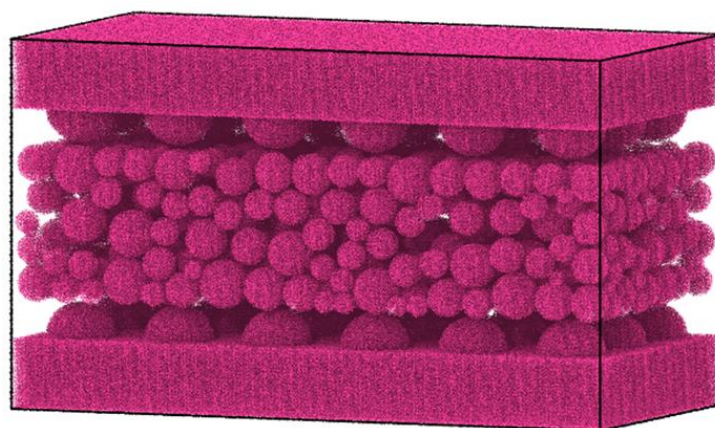


Figure 7. 2. Multiple gouge particles with different sizes between rocks.

7.4 Complex Geological Settings

This thesis focuses only on the dry contact and dry friction in the absence of fluid or gas media on faults. However, in geological settings such as subduction zones or engineered scenarios involving CO₂ injection and hydraulic fracturing near faults, fluids and gases can infiltrate fault zones, significantly altering the contact and frictional mechanisms of faults by complex physical and chemical processes such as pressure solution and fluid overpressure. Therefore, future studies can incorporate these media into the dry cases during simulation to reveal the mechanical behavior of faults under more complex geological environments. On the other hand, it should be noted that in molecular dynamics (MD) simulations, interatomic potential modeling has matured relatively and a wide range of geological materials in seismic zones can be modeled currently. These include rock minerals such as olivine and calcite, as well as clay minerals like kaolinite, illite, and montmorillonite. Future research can further investigate the influence of these geological minerals on fault rheology. Finally, all

simulations in this thesis were performed under ambient temperature and pressure. Future work will explore fault contact and slip behavior under high-temperature and high-pressure conditions, thereby contributing to a more comprehensive understanding of the mechanisms underlying earthquakes of different depths and types.

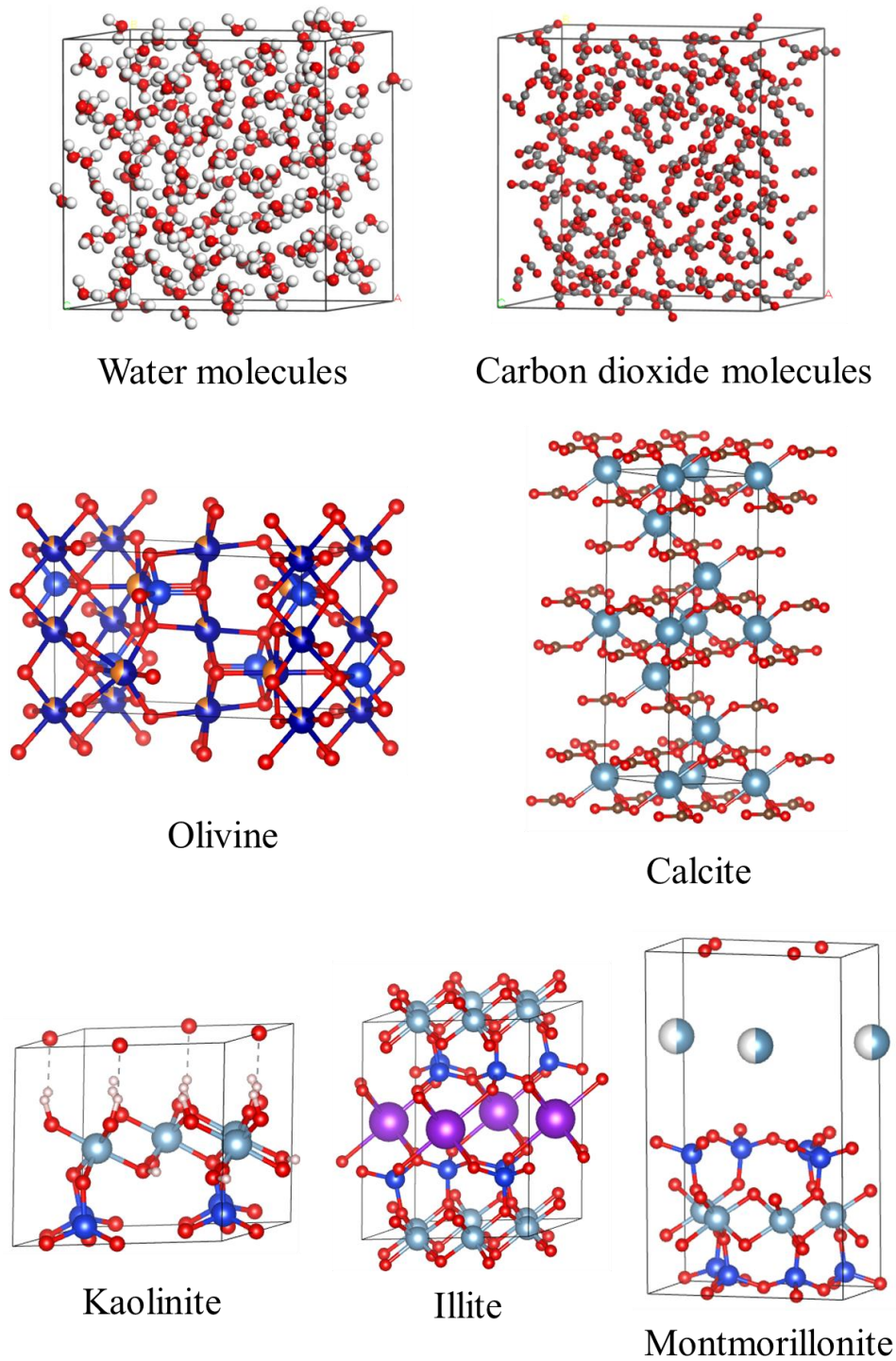


Figure 7. 3. Typical geological materials, along with gas and fluid molecules.

CHAPTER VIII

Conclusion

This thesis has investigated the contact and friction wear mechanisms of single-asperity contact of α -quartz as well as the friction wear mechanisms of a single α -quartz particle against asperity walls at the nanoscale, by employing the three-dimensional nonequilibrium molecular dynamics (MD) method.

During the investigation of the contact behavior, it was observed that fracture occurs in nanoscale α -quartz asperities during the contact process, which is inconsistent with the traditional assumptions of elastic and elastoplastic deformation for rock asperities. Additionally, asperity size and contact configuration significantly influence the failure mechanisms of α -quartz asperities, particularly the transition from plasticity-dominant failure to fracture damage. Besides, a multiscale disparity exists, as macroscopic contact models are limited in their ability to predict the nanoscale contact behavior of α -quartz asperities in terms of the evolution of normal contact force versus interference distance.

Moreover, during the investigation of single-asperity plastic wear mechanisms, it was identified that there is a positive correlation between the normal force and the shear damage zone or wear volume in plastic wear cases, while the wear volume and asperity damage exhibit a negative correlation with the high loading velocity. At low normal forces, wear primarily occurs through interfacial bonding and shear traction. In contrast, high normal forces lead to cluster detachment via layered shear motion, with the larger forces resulting in the removal of larger material clumps. Additionally, the wear volume shows a nonlinear positive correlation with the normal force and a nonlinear negative correlation with high loading velocity.

When further investigating the failure mode transition from plasticity to fracture of asperities, it was confirmed that both plasticity and fracture of α -quartz asperities can occur during nanoscale friction, where the occurrence of fracture can be fundamentally attributed that the local contact stress exceeds the critical fracture stress of damaged α -quartz asperities during frictional sliding. Moreover, it was observed that under CS-like condition, asperity with smaller radius requires larger height ratio for fracture to occur. Additionally, the peak shear force was identified as an effective indicator of the

transition between plastic- and fracture-dominated failure modes under both CS-like and CL conditions. For wear volume, both plastic and fracture-induced wear of nanoscale α -quartz asperities scale linearly with the tangential shear work.

Finally, during the investigation of particle wear mechanisms, it was observed that the normal force governs the damage state of α -quartz particles and the wear volume evolution depends on the damage mode. For fractured particles, wear progresses through stable (linear increase), sub-stable (superlinear increase), and fracture stages. In contrast, smoothing wear without particle fracture maintains a stable stage. Notably, the specific wear rate differs by an order of magnitude between sub-stable ($10^{-2} \text{ nm}^3/\text{nN}\cdot\text{nm}$) and stable ($10^{-3} \text{ nm}^3/\text{nN}\cdot\text{nm}$) stages, but the wear volume in both stages correlates proportionally with tangential shear work. Moreover, particle breakage occurs at short loading distances under high normal forces, while smoothing dominates at longer distances with lower forces. The critical breakage distance decreases with the increasing normal force and is strongly influenced by particle size and particle contact configuration. Finally, it was identified that particle fracture elevates the friction coefficient by disrupting low-resistance rolling motion. The resulting fragments can introduce additional higher shear resistance components, involving the shear and tensile adhesive strengths of fractured surfaces as well as particle bulk strength during slip.

REFERENCES

- Abbott, E.J., Firestone, F.A. (1933). ‘Specifying surface quality – a method based on accurate measurement and comparison. *Journal of Mechanical Engineering*. 55, 9, 569-572
- Abe, S., & Mair, K. (2009). Effects of gouge fragment shape on fault friction: New 3D modelling results. *Geophysical Research Letters*, 36(23).
- Abdelbary, A. (2020). Extreme tribology: fundamentals and challenges. *CRC press*.
- Adams, G. G., & Nosonovsky, M. (2000). Contact modeling—forces. *Tribology international*, 33(5-6), 431-442.
- Aghababaei, R., Warner, D. H., & Molinari, J. F. (2016). Critical length scale controls adhesive wear mechanisms. *Nature communications*, 7(1), 11816.
- Aghababaei, R., Warner, D. H., & Molinari, J. F. (2017). On the debris-level origins of adhesive wear. *Proceedings of the National Academy of Sciences*, 114(30), 7935-7940.
- Aharonov, E., & Scholz, C. H. (2018). A physics-based rock friction constitutive law: Steady state friction. *Journal of Geophysical Research: Solid Earth*, 123(2), 1591-1614.
- Antony, S. J., & Kuhn, M. R. (2004). Influence of particle shape on granular contact signatures and shear strength: new insights from simulations. *International Journal of Solids and Structures*, 41(21), 5863-5870.
- Archard, J. (1953). Contact and rubbing of flat surfaces. *Journal of applied physics*, 24(8), 981-988.
- Arnaud, P., Baydoun, S., & Fouvry, S. (2021). Modeling adhesive and abrasive wear phenomena in fretting interfaces: A multiphysics approach coupling friction energy, third body and contact oxygenation concepts. *Tribology International*, 161, 107077.
- Athanassiadis, A. G., Miskin, M. Z., Kaplan, P., Rodenberg, N., Lee, S. H., Merritt, J., ... & Jaeger, H. M. (2014). Particle shape effects on the stress response of granular packings. *Soft Matter*, 10(1), 48-59.
- Badt, N., Hatzor, Y. H., Toussaint, R., & Sagy, A. (2016). Geometrical evolution of interlocked rough slip surfaces: The role of normal stress. *Earth and Planetary Science Letters*, 443, 153-161.
- Balasubramanian, A. (2017). Quartz Group of Minerals. *Centre For Advanced Studies In Earth Science University Of Mysore*.
- Beeler, N. M., & Hickman, S. H. (2001). A note on contact stress and closure in models of rock joints and faults. *Geophysical research letters*, 28(4), 607-610.

- Beeler, N. M. (2023). On the scale-dependence of fault surface roughness. *Journal of Geophysical Research: Solid Earth*, 128(2), e2022JB024856.
- Bedford, J. D., & Faulkner, D. R. (2021). The role of grain size and effective normal stress on localization and the frictional stability of simulated quartz gouge. *Geophysical Research Letters*, 48(7), e2020GL092023.
- Boneh, Y., Sagy, A., & Reches, Z. (2013). Frictional strength and wear-rate of carbonate faults during high-velocity, steady-state sliding. *Earth and Planetary Science Letters*, 381, 127-137.
- Boneh, Y., Chang, J. C., Lockner, D. A., & Reches, Z. (2014). Evolution of wear and friction along experimental faults. *Pure and Applied Geophysics*, 171, 3125-3141.
- Boneh, Y., & Reches, Z. E. (2018). Geotribology-Friction, wear, and lubrication of faults. *Tectonophysics*, 733, 171-181.
- Bhaskaran, H., Gotsmann, B., Sebastian, A., Drechsler, U., Lantz, M. A., Despont, M., & Sridharan, K. (2010). Ultralow nanoscale wear through atom-by-atom attrition in silicon-containing diamond-like carbon. *Nature nanotechnology*, 5(3), 181-185.
- Bhamra, J. S., Ewen, J. P., Latorre, C. A., Bomidi, J. A., Bird, M. W., & Dini, D. (2023). Atomic-scale insights into the tribochemical wear of diamond on quartz surfaces. *Applied Surface Science*, 639, 158152.
- Brace, W. F., & Byerlee, J. D. (1966). Stick-slip as a mechanism for earthquakes. *Science*, 153(3739), 990-992.
- Branicio, P. S., Rino, J. P., Gan, C. K., & Tsuzuki, H. (2009). Interaction potential for indium phosphide: a molecular dynamics and first-principles study of the elastic constants, generalized stacking fault and surface energies. *Journal of Physics: Condensed Matter*, 21(9), 095002.
- Brown, S. R., & Scholz, C. H. (1986). Closure of rock joints. *Journal of Geophysical Research: Solid Earth*, 91(B5), 4939-4948.
- Broughton, J. Q., Meli, C. A., Vashishta, P., & Kalia, R. K. (1997). Direct atomistic simulation of quartz crystal oscillators: Bulk properties and nanoscale devices. *Physical Review B: Condensed Matter and Materials Physics*, 56(2), 611-618.
- Brilliantov, N. V., Tsukanov, A. A., Grebenko, A. K., Nasibulin, A. G., & Ostanin, I. A. (2023). Atomistic Mechanism of Friction-Force Independence on the Normal Load and Other Friction Laws for Dynamic Structural Superlubricity. *Physical review letters*, 131(26), 266201.
- Byerlee, J. (1978). Friction of rocks. *Pure and applied geophysics*, 116(4), 615-626.
- Candela, T., Renard, F., Klinger, Y., Mair, K., Schmittbuhl, J., & Brodsky, E. E. (2012). Roughness of fault surfaces over nine decades of length scales. *Journal of Geophysical Research: Solid Earth*, 117(B8).

- Candela, T., & Brodsky, E. E. (2016). The minimum scale of grooving on faults. *Geology*, 44(8), 603-606.
- Casas, N., Mollon, G., & Daouadji, A. (2022). DEM analyses of cemented granular fault gouges at the onset of seismic sliding: peak strength, development of shear zones and kinematics. *Pure and Applied Geophysics*, 179(2), 679-707.
- Chang, W. R., Etsion, I., & Bogoy, D. B. (1987). An elastic-plastic model for the contact of rough surfaces. *Journal of tribology*, 109(2), 257-263.
- Cho, G. C., Dodds, J., & Santamarina, J. C. (2006). Particle shape effects on packing density, stiffness, and strength: natural and crushed sands. *Journal of geotechnical and geoenvironmental engineering*, 132(5), 591-602.
- Chen, X., Madden, A. S., Bickmore, B. R., & Reches, Z. E. (2013). Dynamic weakening by nanoscale smoothing during high-velocity fault slip. *Geology*, 41(7), 739-742.
- Chou, Y. M., Song, S. R., Tsao, T. M., Lin, C. S., Wang, M. K., Lee, J. J., & Chen, F. J. (2014). Identification and tectonic implications of nano-particle quartz (< 50 nm) by synchrotron X-ray diffraction in the Chelungpu fault gouge, Taiwan. *Tectonophysics*, 619, 36-43.
- Clavier, G., Desbiens, N., Bourasseau, E., Lachet, V., Brusselle-Dupend, N., & Rousseau, B. (2017). Computation of elastic constants of solids using molecular simulation: comparison of constant volume and constant pressure ensemble methods. *Molecular Simulation*, 43(17), 1413-1422.
- Dascher-Cousineau, K., Kirkpatrick, J. D., & Cooke, M. L. (2018). Smoothing of fault slip surfaces by scale-invariant wear. *Journal of Geophysical Research: Solid Earth*, 123(9), 7913-7930.
- De Moerlooze, K., Al-Bender, F., & Van Brussel, H. (2011). A novel energy-based generic wear model at the asperity level. *Wear*, 270(11-12), 760-770.
- De Paola, N. (2013). Nano-powder coating can make fault surfaces smooth and shiny: implications for fault mechanics?. *Geology*, 41(6), 719-720.
- Dickel, D., Nitol, M., & Barrett, C. D. (2021). LAMMPS implementation of rapid artificial neural network derived interatomic potentials. *Computational Materials Science*, 196, 110481.
- Fabbro, S., Araujo, L. M., Engel, J., Kondratiuk, J., Kuffa, M., & Wegener, K. (2021). Abrasive and adhesive wear behaviour of metallic bonds in a synthetic slurry test for wear prediction in reinforced concrete. *Wear*, 476, 203690.
- Francis, H. A. (1976). Phenomenological analysis of plastic spherical indentation. *Journal of Engineering Materials and Technology*, 98(3): 272-281.
- Fukuyama, E., Muramatsu, I., & Mikumo, T. (2007). Seismic moment of the 1891 Nobi, Japan, earthquake estimated from historical seismograms. *Earth, planets and*

space, 59, 553-559.

- Ganose, A. M., Park, J., Faghaninia, A., Woods-Robinson, R., Persson, K. A., & Jain, A. (2021). Efficient calculation of carrier scattering rates from first principles. *Nature communications*, 12(1), 2222.
- Garcia-Suarez, J., Brink, T., Molinari, J.F. (2023). Breakdown of Reye's theory in nanoscale wear. *Journal of the Mechanics and Physics of Solids*, 173, 105236.
- Greenwood, J. A., & Williamson, J. P. (1966). Contact of nominally flat surfaces. *Proceedings of the royal society of London. Series A. Mathematical and physical sciences*, 295(1442), 300-319.
- Götze, J., Pan, Y., & Müller, A. (2021). Mineralogy and mineral chemistry of quartz: A review. *mineralogical magazine*, 85(5), 639-664.
- Handzel-Powierza, Z., Klimczak, T., & Polijaniuk, A. (1992). On the experimental verification of the Greenwood-Williamson model for the contact of rough surfaces. *Wear*, 154(1), 115-124.
- Hirose, T., Mizoguchi, K., & Shimamoto, T. (2012). Wear processes in rocks at slow to high slip rates. *Journal of Structural Geology*, 38, 102-116.
- Holm, R. (1946). Electrical Contacts. Stockholm. *H. Gerbers*.
- Hoover, W. G. (1985). Canonical dynamics: Equilibrium phase-space distributions. *Physical review A*, 31(3), 1695.
- Issa, H. K., Taherizadeh, A., & Maleki, A. (2020). Atomistic-level study of the mechanical behavior of amorphous and crystalline silica nanoparticles. *Ceramics international*, 46(13), 21647-21656.
- Ikari, M. J., & Conin, M. (2024). Dependence of simulated fault gouge frictional behavior on mineral surface chemistry quantified by cation exchange capacity. *Geochemistry, Geophysics, Geosystems*, 25(9), e2024GC011678.
- Jacobs, T. D., & Carpick, R. W. (2013). Nanoscale wear as a stress-assisted chemical reaction. *Nature nanotechnology*, 8(2), 108-112.
- Jia, Z., Jin, Z., Marchandon, M., Ulrich, T., Gabriel, A. A., Fan, W., ... & Fialko, Y. (2023). The complex dynamics of the 2023 Kahramanmaraş, Turkey, M w 7.8-7.7 earthquake doublet. *Science*, 381(6661), 985-990.
- Johnson, K. L. (1985). Contact mechanics, *Cambridge University Press*.
- Kajita, S., Pacini, A., Losi, G., Kikkawa, N., & Righi, M. C. (2023). Accurate Multiscale Simulation of Frictional Interfaces by Quantum Mechanics/Green's Function Molecular Dynamics. *Journal of Chemical Theory and Computation*, 19(15), 5176-5188.
- Kogut, L., & Etsion, I. (2002). Elastic-plastic contact analysis of a sphere and a rigid flat. *Journal of Applied Mechanics*, 69(5), 657-662.

- Kock, I., & Huhn, K. (2007). Influence of particle shape on the frictional strength of sediments—a numerical case study. *Sedimentary Geology*, 196(1-4), 217-233.
- Koketsu, K., & Miyake, H. (2008). A seismological overview of long-period ground motion. *Journal of Seismology*, 12, 133-143.
- Koudriachova, M. V., Beckers, J. V. L., & De Leeuw, S. W. (2001). Computer simulation of the quartz surface: a combined ab initio and empirical potential approach. *Computational materials science*, 20(3-4), 381-386.
- Kumar, R., & Dhiman, S. (2013). A study of sliding wear behaviors of Al-7075 alloy and Al-7075 hybrid composite by response surface methodology analysis. *Materials & Design*, 50, 351-359.
- Kumar Pal, R., Morton, J., Wang, E., Lambros, J., & Geubelle, P. H. (2015). Impact response of elasto-plastic granular chains containing an intruder particle. *Journal of Applied Mechanics*, 82(1), 011002.
- Lantz, M. A., Wiesmann, D., & Gotsmann, B. (2009). Dynamic superlubricity and the elimination of wear on the nanoscale. *Nature nanotechnology*, 4(9), 586-591.
- Laithy, M. E., Wang, L., Harvey, T. J., Vierneusel, B., Correns, M., & Blass, T. (2019). Further understanding of rolling contact fatigue in rolling element bearings-a review. *Tribology International*, 140, 105849.
- Li, Q., Tullis, T. E., Goldsby, D., & Carpick, R. W. (2011). Frictional ageing from interfacial bonding and the origins of rate and state friction. *Nature*, 480(7376), 233-236.
- Li, S., & Fukuyama, E. (2025). Nanoscale contact behavior of α -quartz asperities—A molecular dynamics approach. *Computers and Geotechnics*, 183, 107239.
- Lou, S., Jiang, X., & Scott, P. J. (2013). Application of the morphological alpha shape method to the extraction of topographical features from engineering surfaces. *Measurement*, 46(2), 1002-1008.
- Marone, C. (1998). Laboratory-derived friction laws and their application to seismic faulting. *Annual Review of Earth and Planetary Sciences*, 26(1), 643-696.
- Martys, N. S., & Mountain, R. D. (1999). Velocity Verlet algorithm for dissipative-particle-dynamics-based models of suspensions. *Physical Review E*, 59(3), 3733.
- Ma, Z., Gamage, R. P., & Zhang, C. (2021). Mechanical properties of α -quartz using nanoindentation tests and molecular dynamics simulations. *International Journal of Rock Mechanics and Mining Sciences*, 147, 104878.
- Malekan, M. (2023). Transition from plastic shearing to fracture of asperity junctions: role of a critical aspect ratio. *Tribology Letters*, 71(1), 26.
- Ma, X. Y., Zhu, L. F., Zou, X., & Kang, X. (2023). Investigation of the interface stick-slip friction behavior of clay nanoplatelets by molecular dynamics

- simulations. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 679, 132601.
- McClimon, J. B., Hilbert, J., Lukes, J. R., & Carpick, R. W. (2020). Nanoscale run-in of silicon oxide-doped hydrogenated amorphous carbon: dependence of interfacial shear strength on sliding length and humidity. *Tribology Letters*, 68, 1-14.
- Mizoguchi, K., Hirose, T., Shimamoto, T., & Fukuyama, E. (2009). High-velocity frictional behavior and microstructure evolution of fault gouge obtained from Nojima fault, southwest Japan. *Tectonophysics*, 471(3-4), 285-296.
- Mizoguchi, K., & Fukuyama, E. (2010). Laboratory measurements of rock friction at subseismic slip velocities. *International Journal of Rock Mechanics and Mining Sciences*, 47(8), 1363-1371.
- Milanese, E., Brink, T., Aghababaei, R., & Molinari, J. F. (2019). Emergence of self-affine surfaces during adhesive wear. *Nature communications*, 10(1), 1116.
- Mo, Y., Turner, K. T., & Szlufarska, I. (2009). Friction laws at the nanoscale. *Nature*, 457(7233), 1116-1119.
- Momma, K., & Izumi, F. (2011). VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data. *Journal of applied crystallography*, 44(6), 1272-1276.
- Molinari, J. F., Aghababaei, R., Brink, T., Frérot, L., & Milanese, E. (2018). Adhesive wear mechanisms uncovered by atomistic simulations. *Friction*, 6, 245-259.
- Molaei, F. (2022). Understanding the anisotropic mechanical behavior of single-crystalline alpha quartz from the insight of molecular dynamics. *Journal of Geophysical Research: Solid Earth*, 127(6), e2021JB023681.
- Mulvihill, D. M., Kartal, M. E., Nowell, D., & Hills, D. A. (2011). An elastic-plastic asperity interaction model for sliding friction. *Tribology international*, 44(12), 1679-1694.
- Nakano, A., Kalia, R. K., & Vashishta, P. (1994). First sharp diffraction peak and intermediate-range order in amorphous silica: finite-size effects in molecular dynamics simulations. *Journal of non-crystalline solids*, 171(2), 157-163.
- Nielsen, S., Spagnuolo, E., Violay, M., & Di Toro, G. (2021). Thermal weakening friction during seismic slip: experiments and models with heat sources and sinks. *Journal of Geophysical Research: Solid Earth*, 126(5), e2020JB020652.
- Nosé, S. (1984). A unified formulation of the constant temperature molecular dynamics methods. *The Journal of chemical physics*, 81(1), 511-519.
- Otsuka, S., Kimata, S., Sasajima, Y., & Ishikawa, N. (2024). Molecular Dynamics Simulation of High-Energy Beam Irradiation of SiO₂ Single Crystal with Three Different Morphologies: No Free Surface, with a Free Surface, and Thin

- Films. *ECS Journal of Solid State Science and Technology*, 13(11), 114005.
- Parab, N. D., Guo, Z., Hudspeth, M. C., Claus, B. J., Fezzaa, K., Sun, T., & Chen, W. W. (2017). Fracture mechanisms of glass particles under dynamic compression. *International Journal of Impact Engineering*, 106, 146-154.
- Pham-Ba, S., & Molinari, J. F. (2021). Creation and evolution of roughness on silica under unlubricated wear. *Wear*, 472, 203648.
- Pitarka, A., Irikura, K., Iwata, T., & Sekiguchi, H. (1998). Three-dimensional simulation of the near-fault ground motion for the 1995 Hyogo-ken Nanbu (Kobe), Japan, earthquake. *Bulletin of the Seismological Society of America*, 88(2), 428-440.
- Pugliese, G., Tavares, S. M. O., Ciulli, E., & Ferreira, L. A. (2008). Rough contacts between actual engineering surfaces: Part II. Contact mechanics. *Wear*, 264(11-12), 1116-1128.
- Ramalho, A. (2010). A reliability model for friction and wear experimental data. *Wear*, 269(3-4), 213-223.
- Reye, T (1860) Zur theorie der zapfenreibung. *J Der Civilingenieur*, 4, 235–255.
- Reches, Z. E., & Dewers, T. A. (2005). Gouge formation by dynamic pulverization during earthquake rupture. *Earth and Planetary Science Letters*, 235(1-2), 361-374.
- Ritchie, R. O., Knott, J. F., & Rice, J. R. (1973). On the relationship between critical tensile stress and fracture toughness in mild steel. *Journal of the Mechanics and Physics of Solids*, 21(6), 395-410.
- Rubino, V., Lapusta, N., & Rosakis, A. J. (2022). Intermittent lab earthquakes in dynamically weakening fault gouge. *Nature*, 606(7916), 922-929.
- Sagy, A., & Brodsky, E. E. (2009). Geometric and rheological asperities in an exposed fault zone. *Journal of Geophysical Research: Solid Earth*, 114(B2).
- Sato, T., Ishida, T., Jalabert, L., & Fujita, H. (2012). Real-time transmission electron microscope observation of nanofriction at a single Ag asperity. *Nanotechnology*, 23(50), 505701.
- Sato, T., Milne, Z. B., Nomura, M., Sasaki, N., Carpick, R. W., & Fujita, H. (2022). Ultrahigh strength and shear-assisted separation of sliding nanocontacts studied in situ. *Nature communications*, 13(1), 2551.
- Scholz, C. H., & Aviles, C. A. (1986). The fractal geometry of faults and faulting. *Earthquake Source Mechanics*, 37, 147-155.
- Scholz, C.H. (1987). Wear and gouge formation in brittle faulting. *Geology*, 15, 493e495.
- Scholz, C. H. (1998). Earthquakes and friction laws. *Nature*, 391(6662), 37-42.

- Schreijäg, S., Kaufmann, D., Wenk, M., Kraft, O., & Mönig, R. (2015). Size and microstructural effects in the mechanical response of α -Fe and low alloyed steel. *Acta Materialia*, 97, 94-104.
- Shimizu, F., Ogata, S., & Li, J. (2007). Theory of shear banding in metallic glasses and molecular dynamics calculations. *Materials transactions*, 48(11), 2923-2927.
- Siman-Tov, S., Aharonov, E., Sagy, A., & Emmanuel, S. (2013). Nanograins form carbonate fault mirrors. *Geology*, 41(6), 703-706.
- Spikes, H. (2018). Stress-augmented thermal activation: Tribology feels the force. *Friction*, 6, 1-31.
- Stesky, R. M., & Hannan, S. S. (1989). A new theory for the static contact between rough, unmated surfaces in non-elastically deforming rock and its implications for rock friction. *Journal of structural geology*, 11(7), 787-798.
- Stukowski, A. (2010). Visualization and analysis of atomistic simulation data with OVITO—the Open Visualization Tool. *Modelling and simulation in materials science and engineering*, 18(1), 015012.
- Strozewski, B., Sly, M. K., Flores, K. M., & Skemer, P. (2021). Viscoplastic rheology of α -quartz investigated by nanoindentation. *Journal of Geophysical Research: Solid Earth*, 126(9), e2021JB022229.
- Svenningsson, I., & Tatar, K. (2021). On the mechanism of three-body adhesive wear in turning. *The International Journal of Advanced Manufacturing Technology*, 113(11), 3457-3472.
- Tang, Z. C., Xia, C. C., Jiao, Y. Y., & Wong, L. N. Y. (2016). Closure model with asperity interaction in normal contact for rock joint. *International Journal of Rock Mechanics and Mining Sciences*, 83, 170-173.
- Tang, Z. C., Jiao, Y. Y., & Wong, L. N. Y. (2017). Theoretical model with multi-asperity interaction for the closure behavior of rock joint. *International Journal of Rock Mechanics and Mining Sciences*, 97, 15-23.
- Thompson, A. P., Aktulga, H. M., Berger, R., Bolintineanu, D. S., Brown, W. M., Crozier, P. S., ... & Plimpton, S. J. (2022). LAMMPS—a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Computer physics communications*, 271, 108171.
- Tobias, D. J., Martyna, G. J., & Klein, M. L. (1993). Molecular dynamics simulations of a protein in the canonical ensemble. *The Journal of Physical Chemistry*, 97(49), 12959-12966.
- Tucker, M. G., Keen, D. A., & Dove, M. T. (2001). A detailed structural characterization of quartz on heating through the α - β phase transition. *Mineralogical Magazine*, 65(4), 489-507.

- Umeno, Y., Shimada, T., & Kitamura, T. (2010). Dislocation nucleation in a thin Cu film from molecular dynamics simulations: instability activation by thermal fluctuations. *Physical Review B—Condensed Matter and Materials Physics*, 82(10), 104108.
- Vashishta, P., Kalia, R. K., Rino, J. P., & Ebbsjö, I. (1990). Interaction potential for SiO₂: A molecular-dynamics study of structural correlations. *Physical Review B*, 41(17), 12197–12209.
- Vashishta, P., Kalia, R. K., Nakano, A., & Rino, J. P. (2008). Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina. *Journal of Applied Physics*, 103(8).
- Van de Walle, C. G., & Neugebauer, J. (2004). First-principles calculations for defects and impurities: Applications to III-nitrides. *Journal of applied physics*, 95(8), 3851-3879.
- Vadgama, B. N., Jackson, R. L., & Harris, D. K. (2015). Molecular scale analysis of dry sliding copper asperities. *Applied nanoscience*, 5, 469-480.
- Vakis, A. I., Yastrebov, V. A., Scheibert, J., Nicola, L., Dini, D., Minfray, C., ... & Ciavarella, M. (2018). Modeling and simulation in tribology across scales: An overview. *Tribology International*, 125, 169-199.
- Verberne, B. A., van den Ende, M. P., Chen, J., Niemeijer, A. R., & Spiers, C. J. (2020). The physics of fault friction: Insights from experiments on simulated gouges at low shearing velocities. *Solid Earth*, 11(6), 2075-2095.
- Wang, W., & Scholz, C. H. (1994). Wear processes during frictional sliding of rock: a theoretical and experimental study. *Journal of Geophysical Research: Solid Earth*, 99(B4), 6789-6799.
- Wang, W., Dietzel, D., & Schirmeisen, A. (2021a). Thermal activation of nanoscale wear. *Physical Review Letters*, 126(19), 196101.
- Wang, Y., Xu, J., Ootani, Y., Ozawa, N., Adachi, K., & Kubo, M. (2021b). Non-empirical law for nanoscale atom-by-atom wear. *Advanced Science*, 8(2), 2002827.
- Wu B, Barbot S. Evolution of the real area of contact during laboratory earthquakes. *Proceedings of the National Academy of Sciences*. 2025 Jun 10;122(23):e2410496122.
- Xie, W., Liu, C., Jiang, D., & Jin, J. (2021). Inelastic contact behaviors of nanosized single-asperity and multi-asperity on α -Fe surface: molecular dynamic simulations. *International Journal of Mechanical Sciences*, 204, 106569.
- Yang, H. (2014). *Multiscale chemo-mechanical mechanics of high-capacity anode materials in lithium-ion nano-batteries*. The Pennsylvania State University.
- Yan, Y. T., & Wang, S. W. (2023). Simulation investigation of mechanical and failure

- characteristics of jointed rock with different shapes of joint asperities under compression loading. *Computational Particle Mechanics*, 10(1), 45-59.
- Zhao, Y., Maietta, D. M., & Chang, L. (2000). An asperity microcontact model incorporating the transition from elastic deformation to fully plastic flow. *Journal of Tribology*, 122(1), 86-93.
- Zhao, Z. (2013). Gouge particle evolution in a rock fracture undergoing shear: a microscopic DEM study. *Rock mechanics and rock engineering*, 46, 1461-1479.
- Zheng, X., Zhu, H., Kosasih, B., & Tieu, A. K. (2013). A molecular dynamics simulation of boundary lubrication: The effect of n-alkanes chain length and normal load. *Wear*, 301(1-2), 62-69.
- Zhang, J. (2017). Phase transformation in two-dimensional crystalline silica under compressive loading. *Physical Chemistry Chemical Physics*, 19(12), 8478-8484.
- Zhao, S., Evans, T. M., & Zhou, X. (2018). Effects of curvature-related DEM contact model on the macro-and micro-mechanical behaviours of granular soils. *Géotechnique*, 68(12), 1085-1098.
- Zhang, Y., Sprittles, J. E., & Lockerby, D. A. (2019). Molecular simulation of thin liquid films: Thermal fluctuations and instability. *Physical Review E*, 100(2), 023108.
- Zhao, Y., Wang, C. L., & Bi, J. (2020). Analysis of fractured rock permeability evolution under unloading conditions by the model of elastoplastic contact between rough surfaces. *Rock Mechanics and Rock Engineering*, 53, 5795-5808.
- Zhang, X., Baudet, B. A., & Yao, T. (2020). The influence of particle shape and mineralogy on the particle strength, breakage and compressibility. *International Journal of Geo-Engineering*, 11, 1-10.
- Zhou, X. P., & Zhang, J. Z. (2021). Damage progression and acoustic emission in brittle failure of granite and sandstone. *International Journal of Rock Mechanics and Mining Sciences*, 143, 104789.