

Micromechanics of solid-surface contact suspension and its role in friction

by

Shuman Xia

M. Sc. Applied Mathematics, Brown University, 2008

B. Sc. Theoretical and Applied Mechanics, Beijing University, 2003

A dissertation submitted in partial fulfillment of the
requirements for the Degree of Doctor of Philosophy
in the Division of Engineering at Brown University

Providence, Rhode Island

May, 2008

© Copyright 2008 by Shuman Xia

This dissertation by Shuman Xia is accepted in its present form by
the Division of Engineering as satisfying the dissertation requirement
for the degree of Doctor of Philosophy.

Date _____

Professor Kyung-Suk Kim, Advisor

Recommended to the Graduate Council

Date _____

Professor Allan F. Bower, Reader

Date _____

Professor Pradeep R. Guduru, Reader

Approved by the Graduate Council

Date _____

Professor Sheila Bonde
Dean of the Graduate School

Vita

Shuman Xia was born on December 10, 1981, in Jingzhou, Hubei, P. R. China. He attended Beijing University in 1999, where he received his B. Sc. degree in Theoretical and Applied Mechanics, and graduated with honors from both Beijing University and Beijing Municipal Commission of Education in 2003. He entered the Solid Mechanics program at Brown University in September, 2003. He was awarded an M. Sc. in Applied Mathematics in May, 2008.

Acknowledgements

My utmost gratitude goes to my thesis advisor, Prof. Kyung-Suk Kim, for his inspiring and invaluable guidance throughout my PhD journey. This thesis would not be possible without his support, encouragement and advice. Deep gratitude is also due to the members of the thesis committee, Prof. Allan Bower and Prof. Pradeep Guduru, for their insightful comments and suggestions leading to significant improvement in the quality of this work.

Part of my research work was undertaken in collaboration with research scientists at the General Motors R&D center. I wish to express my indebtedness to my collaborators, Dr. Yue Qi, Dr. Tom Perry, Dr. Yang-Tse Cheng, Dr. Leo Lev and Dr. Anil Sachdev. I also wish to acknowledge the generous funding provided by General Motors through the GM/Brown collaborative research lab.

I would like to thank all of the professors in the Solid Mechanics group. They created a rigorous academic environment which fostered my growth as an independent scientist. I also wish to thank the current and former members of Nano- and Micromechanics Laboratory, Brian Burke, Dr. Qunyang Li, Yisoo Pyon, Dr. Huck Beng Chew, Dr. Yanfei Gao and Dr. Jun Lou. They made my stay at Brown both enjoyable and intellectually stimulating. I am grateful to my fellow graduate students, Dr. Yuan Lin, Julie Waters, Vinay Gill, Nikhil Medhekar and Dr. Wei Guo, for their friendship and helpful assistances. Special thanks also go to Charles Vickers, Dr. Christopher Bull and Brian Corkum, who provided me with the much needed

technical help.

Last, but not least, I thank my wife and my parents and sister in China for their continuous and unconditional support.

Contents

Signature Page	iii
Vita	iv
Acknowledgements	v
Table of Contents	vii
List of Tables	x
List of Figures	xi
1 INTRODUCTION	1
1.1 Background and overview	1
1.2 Outlines of the present work	5
2 SCALE DEPENDENT CONTACT STRENGTH OF NANO-ASPERITIES	7
2.1 Introduction	7
2.2 Problem definition	10
2.3 Asymptotic analysis of contact strength	11
2.4 A full numerical solution	18

2.5	Discussions	23
2.6	Chapter summary	26
	Appendix A	27
3	SUSPENSION RESISTANCE OF REINFORCEMENT PARTICLES IN METAL MATRIX COMPOSITES	29
3.1	Introduction	29
3.2	Problem definition of particle nanoindentation	34
3.2.1	Generic configuration of particle nanoindentation	34
3.2.2	Canonical response of particle nanoindentation	36
3.3	Experiment	39
3.3.1	Experimental procedure	39
3.3.2	Experimental results	41
3.4	Finite element analysis	48
3.4.1	Finite element model	48
3.4.2	Finite element analysis with a perfectly bonded interface . . .	49
3.4.3	Finite element analysis with interface failure	52
3.5	Discussions	55
3.6	Chapter summary	61
	Appendix B	63
4	EXPERIMENTAL STUDY ON MICRO-SLIP FRICTION LAWS OF ROUGH SURFACES	67
4.1	Introduction	67
4.2	Experimental procedures	70
4.3	Experiment results	73
4.4	Discussions	82

4.5 Chapter summary	84
Bibliography	85

List of Tables

3.1	Comparison between the material properties measured in the current work and the atomistic estimations	58
-----	--	----

List of Figures

2.1	A schematic of the dislocation structure in gold pyramids subjected to contact loading.	10
2.2	The asymptotic stress field (a) near the contact edge is decomposed into two sub-fields: the stress field (b) of a wedge containing an edge dislocation without external load and the stress field (c) of the loaded wedge without a dislocation. The no-slip and frictionless contact conditions between the punch and the wedge top surface are considered.	12
2.3	Asymptotic solution of size-dependent contact strength for various values of η/b . (a) No slip contact; (b) Frictionless contact.	16
2.4	The integration surface of 3-D M-integral for the calculation of dislocation configurational force	17
2.5	The decomposition of the elastostatic field of the 3-D dislocation model	20
2.6	Comparison between the asymptotic and full numerical results for $\eta/b = 2$. (a) No slip contact; (b) Frictionless contact.	22
2.7	Comparison of the model result with the MD (Ward 2008) and experimental (Wang <i>et al.</i> 2006) results. Frictionless contact condition and $\eta/b = 1.25$ are used to obtained the asymptotic solution.	23
2.8	A planar dislocation loop.	27

3.1	(a) A schematic of a nanoindentation test of an elastic particle embedded in a ductile metal matrix; (b) Optical microscope image of the cross-section microstructure of the hypoeutectic Al/Si alloy. A silicon particle selected for a nanoindentation test is shown inside the circle.	35
3.2	(a) The indentation load function applied on the silicon particles; (b) Indentation curves of three particles with different H/D of 2.10 (Particle 1), 0.76 (Particle 2) and 0.45 (Particle 3).	42
3.3	AFM images of Particle 2 before (a) and after (b) indentation and Particle 3 before (c) and after (d) indentation. The small bump on the top surface of Particle 2 before indentation was a cluster of colloidal silica particles. It was removed from the top surface before nanoindentation test by rubbing the surface with the indenter tip.	44
3.4	(a) Decomposition of the total indentation response of Particle 1 into the elastic and plastic parts; (b) Plastic indentation response of Particle 1 after subtraction of the elastic part.	45
3.5	(a) Characterization of $p - \bar{h}_p$ curves by three quantities, the yield PI-pressure, p_Y , the hardening index, n , and the reverse-yield PI-pressure drop, Δp . Experimental relationship of (b) yield PI-pressure versus particle aspect ratio; (c) hardening index versus particle aspect ratio; (d) reverse yield PI-pressure versus particle aspect ratio. The error bars in (d) are given by varying the fitting range of the unloading portion for the elastic displacement calculation.	47
3.6	Comparison of the yield PI-pressure versus particle aspect ratio between experiment and simulation.	50
3.7	Contour plots of the Von Mises stress with a perfectly bonded interface.	51

3.8	Comparison of the hardening index versus particle aspect ratio between experiment and simulation.	53
3.9	Contour plots of σ_{11} and σ_{12} of particle indentation ($H/D = 2.5$) simulated with NILS-CZM during unloading (10x magnification of the displacement in the radial direction).	56
3.10	Comparison of reverse yield PI-pressure versus particle aspect ratio between experiment and simulation.	57
3.11	(a) A schematic of a Mode I cohesive crack with cohesive length of a ; (b) A model configuration of the exterior cohesive zone model; (c) Scaling law of CZM strength with respect to finite element size. . . .	64
4.1	(a) A schematic of the test configuration; (b) a close view of the loading device; (c) an experimental ESPI system for 2-D displacement field measurement. The loading device in (c) is switched from left to right for ease of experimental operation. The data presented in Section 4.3 will be consistent with the schematic as shown in (a).	71
4.2	Raw phase fringe maps for each loading step. (a) Horizontal; (b) vertical.	74
4.3	Smoothed phase fringe maps for each loading step. (a) Horizontal; (b) vertical.	75
4.4	Raw displacement fields unwrapped from the smoothed fringe fields. (a) Horizontal displacement field; (b) vertical displacement field. . . .	77
4.5	Displacement fields smoothed with the FEM equilibrium algorithm. (a) Horizontal displacement field; (b) vertical displacement field. . . .	77
4.6	Displacement profiles along the interface. (a) Horizontal; (b) vertical.	79
4.7	Stress fields calculated from the smoothed displacement fields. (a) σ_{12} field; (b) σ_{22} field.	79

4.8	(a) Traction distribution along the interface; (b) distribution of ratio of shear stress to pressure along the interface; (c) slip distance profile along the interface; (d) ratio of shear stress to pressure as a function of slip distance.	81
4.9	The relationship between normal pressure and penetration depth. The data points are obtained at $x= 0$ mm during the first ten steps with normal loading.	82

Chapter 1

INTRODUCTION

1.1 Background and overview

Solid surface suspension, which is interpreted as supporting solid surfaces with discrete contact spots, is emerging as a new discipline in surface science and engineering. Solid surface suspension is governed by the size-dependent asperity hardness and multi-frequency surface roughness. Applications of the solid surface suspension technique are twofold: (1) to design solid surfaces with low conformation resistance for nano-imprinting; (2) to make materials with high contact strength for anti-adhesion and/or friction and wear reduction. This work presented in this thesis is mainly motivated by the latter.

There are numerous studies showing that solid surface suspension improves tribological performance. For example, a recent study (Jay *et al.* 2007) has shown that the friction of mammalian joints at low slip rates and high pressure is not mainly governed by hydrodynamic lubrication of the synovial fluid. Instead, the boundary lubrication is primarily achieved by surface suspension with a special type of protein called lubricin. The lubricin can support the cartilage surfaces to avoid bare

cartilage-cartilage contact up to a very high pressure (18 MPa). As a consequence of this suspension, a very low friction coefficient on the order of 0.001 is attainable. Li (2008) conducted a series of AFM friction experiments by sliding a gold-coated micro-sphere with nano-roughness undulations against a flat mica surface. He found that the frictional resistance of the micro-sphere was much smaller than the anticipated value for a smooth contact. Based on this work, one can draw a conclusion that, small-scale friction can be reduced by increasing roughness when the adhesive friction mechanism is dominant.

As a new research subject, solid surface suspension can find its theoretical basis closely tied to the comprehensive research on contact and friction of rough surfaces. Nearly all solid surfaces, natural or man-made, are rough at the microscopic scale. Intimate contact and friction of rough surfaces occurs only at the summits of the asperities. Bowden and Tabor addressed the role of roughness in friction in the early 1950s (Bowden and Tabor 1950). They separated the total frictional force into the ploughing force term and the adhesive force term. The first term is proportional to the real contact area with the proportionality constant being the asperity shear strength. The calculation of the second term requires the relationship between the contact area and the normal load. Archard (1957) obtained this relationship for non-adhesive elastic contact with hierarchical spectra of roughness. He found that, when the hierarchical order of asperities increases, the dependence of contact area on normal load approaches a linear relationship. A different approach based on statistical asperity height distribution was taken by Greenwood and Williamson (1966) to get an approximately linear relationship between the normal load and real contact area. Besides these geometric aspects of roughness, adhesion effects have been also included in modeling rough surface friction via the JKR model (Johnson *et al.* 1971; Fuller and Tabor 1975, Chowdhury and Ghosh 1994), the DMT model (Derjaguin *et al.* 1975;

Chang *et al.* 1988) and the Maugis model (Maugis 1992; Adams *et al.* 2003, Adams and Muftu 2005). Most of these studies have taken inelastic effects into account using classic plasticity theories.

However, the classical continuum plasticity predicts size-scale independent strength of asperities, while experiments (De Guzman *et al.* 1993, Ma and Clarke 1995, Wang *et al.* 2006) show strong size-scale dependence for asperity contact size smaller than one micrometer. Compression tests of single crystal gold pyramids with $\{114\}$ facets on (001) surface plane (Wang *et al.* 2006) have shown a wide spectrum of contact strength from a few hundred MPa to 3 GPa, depending on the contact edge length ranging from 600 nm to 100 nm. Based on molecular dynamics simulations, it is believed that the size-dependent strength of asperities can reach even higher values (3-10 GPa), when the contact size goes below 100 nm. The asperity strength at the nanometer scale is mostly governed by dislocation nucleation mechanisms, which include homogeneous dislocation nucleation in the bulk and heterogeneous dislocation nucleation at a surface step, surface ledge, contact edge and contact corner, etc. The high contact strength at the small length-scale provides a fundamental basis for the idea of reducing friction by increasing nano-scale roughness. However, there is no convenient model for predicting contact strength of nano-asperities and guiding material selection and geometrical design toward the realization of this idea. The first part of this thesis is devoted to address this issue.

Compared to the surface suspension with asperities of a homogeneous solid, surface suspension with heterogeneous structures is a relatively recent concept and has been less extensively studied. A good illustrative example is the metal matrix composites that are being developed for making tribological components. The light metals in both pure and alloyed form, like aluminum and magnesium, are not considered as

good candidates for tribological applications because of their poor tribological performance. Nevertheless, due to the increasing demand of energy saving and pollution reduction for transportation vehicles, there have been many attempts recently to develop lightweight tribological components with these metals. The key idea here is to include hard reinforcement phases on material surfaces and support the contact and frictional load with these hard phases. Among these composites, Al-Si alloys and Al-Si based composites are the most promising, because of their good castability, excellent heat conductivity and low cost. A near-eutectic Al-Si alloy is now being developed for making liner-less engine blocks at the General Motors R&D center. The silicon particles on the alloy surface are made to protrude above the nominal surface through a chemical surface preparation. In the so-called ultra-mild wear regime, these exposed silicon particles bear the load and prevent adhesion between the counter-surface and the soft aluminum matrix. The friction, wear and scuffing tests on this Al-Si alloy showed that the hard silicon particles were very effective in increasing scuff and wear resistance under moderate load conditions. A heavier load condition induces a transition from the ultra-mild wear regime into the mild wear regime where the silicon particles sink into the matrix. The tribological performance of the alloy is substantially deteriorated due to this sinking-in process. To extend the ultra-mild wear regime to higher loads for wider application, it is highly desirable to improve the suspension capability of the hard particles through microstructure design. The second part of this thesis is focused on studying suspension resistance of hard particles in such surface composites with experiment and finite element simulation.

As solid surfaces are suspended by either rough-surface asperities or surface-composite hard phase particles, friction characteristics of such contact-suspended surfaces must be formulated with suspension kinematics. In traditional homogenization of multiple-asperity contact and friction, much of the interfacial-roughness-layer

(IRL) kinematics has been neglected. Lack of experimental data in IRL kinematics has made it difficult to formulate a comprehensive constitutive relation of friction. In this thesis a new data set is obtained for the normal IRL compliance and the slip precursor displacement of a rough-surface friction process. The measurements were made by an electronic speckle pattern interferometry (ESPI) system for a friction process between two PMMA surfaces.

1.2 Outlines of the present work

A theoretical study on contact strength of nano-asperities is presented in the second chapter. Heterogeneous surface dislocation nucleation due to a wedge stress singularity is proposed and analyzed as an incipient plastic deformation mechanism for an asperity contact size smaller than 100 nm. The proposed mechanism provides a scale-dependence of the contact strength. A quasi-analytical asymptotic solution is obtained employing the 2-D M-integral and stress singularity solution of a wedge. A full numerical simulation is performed to validate the asymptotic solution. A comparison of the model prediction with the MD and experimental results is also provided.

In the third chapter, the suspension capability of a heterogeneous surface structure is studied. The A356 Al/Si alloy is used as a model system. The contact strength of silicon particles embedded in an aluminum matrix is studied with both nanoindentation experiments and FEM simulation. The canonical response of particle indentation is analyzed based on a reduced test configuration. The mechanical properties of Al/Si interface are found to play an important role in controlling the contact strength of silicon particles. A hybrid method of nanoindentation and finite element analysis is used to characterize the silicon particle indentation strength and the mechanical

properties of Al/Si interface. An element-size dependent FEM cohesive-zone law is developed to extract the interface properties.

The last chapter presents an experimental study on macroscopic constitutive law of rough surface suspension and friction. A novel experimental framework is developed to study the contact and friction laws of an interfacial roughness layer for its mechanical response in both the shear and normal directions. The validity of this framework is demonstrated with a benchmark test on rough surface contact of PMMA.

Chapter 2

SCALE DEPENDENT CONTACT STRENGTH OF NANO-ASPERITIES

2.1 Introduction

Research on size-dependent plasticity and strength can be traced back to the early 1950s when Hall and Petch independently published two series of papers on the grain-size dependence of yield strength. For the last two decades, motivated by applications of small-scale electronic devices and mechanical structures, the scale effects in plasticity have attracted increasing interest. Direct evidence of the scale dependence has been acquired through many small-scale experiments, such as torsion (Fleck *et al.* 1994), microbending (Stolken and Evans 1998), nanowire bending (Wu *et al.* 2005), nanoindentation (De Guzman *et al.* 1993, Ma and Clarke 1995), pillar compression (Greer *et al.* 2005) and pyramid indentation (Wang *et al.* 2006). Nearly all of these experiments lead to one observation: in general smaller is stronger or harder.

A number of continuum-based theories (Fleck and Hutchinson 1993, 1997, Gao *et al.* 1999, Huang *et al.* 2000, Acharya and Bassani 2000, Gurtin 2000, 2002) have been

developed to model size-dependent plasticity based on the concept of geometrically necessary dislocations (GNDs)(Ashby 1970). The key idea behind these non-local theories is to incorporate an intrinsic length scale by phenomenologically correlating deformation hardening and strain gradients associated with GNDs. Because of their continuum nature, these theories are applicable to volumes sufficient for dislocation ensembles; length scales from one micron to tens of microns. For sub-micron length scales, continuum theories break down and computational simulations, such as molecular dynamics (MD), discrete dislocation (DD) models, the quasicontinuum (QC) method and the coupled atomistic/discrete dislocation (CADD) method, are preferable and extensively used to study the size effects of plasticity.

The size-dependent contact strength of asperities, which is of fundamental importance in solid-surface contact suspension and friction, has been studied in a novel pyramid compression experiment by Wang *et al.* (2006). In this experiment, self-similar gold nano- and micro-pyramids were fabricated by an electrochemical etching method and compressed using a hard flat punch. The contact strength, p_c , of the pyramids was found to depend on the contact edge length, l , according to $p_c \propto l^{-\lambda}$ with $\lambda = 0.75$. A high contact strength of about 3 GPa was achieved for $l = 100$ nm, which was the smallest attainable contact size in the experiment. Triggered by the work of Wang *et al.* (2006), Ward (2008) performed large-scale molecular dynamics simulations modeling the compression of the same pyramid structure. A similar power law relationship $p_c \propto l^{-\lambda}$ was discovered computationally with a smaller scaling exponent of $\lambda = 0.32$. The largest simulated contact size was limited to 36 nm by the available computational power. Though the projection of the MD result to the experimental length scale seems to fit reasonably well with the experimental data of Wang *et al.* (2006), the length gap between 36-100 nm was yet unexplored. Furthermore, though the MD simulations could reveal many details about plastic deformation, such

as dislocation nucleation and stacking fault formation, the exact mechanism for size dependence of contact strength remained unclear.

For nano-scale contact, the contact size is much smaller than the average spacing of bulk dislocation sources. Therefore the bulk dislocations have a small chance to nucleate and multiply under a contact load, and the plastic deformation is source-limited. To have incipient plasticity, dislocations must be nucleated homogeneously or heterogeneously close to the contact surface (Shenoy *et al.* 2000, Yu *et al.* 2007, Bei *et al.* 2008). The contact strength is thus solely governed by the event of surface dislocation emission. In this chapter, the heterogeneous dislocation nucleation at the contact edges of a nano-asperity contact caused by a wedge stress singularity is analyzed with a dislocation model, and the contact strength is obtained as a function of the contact size. The Rice-Thomson criterion (Rice and Thomson 1974) is used as the condition for dislocation nucleation. The 2-D and 3-D conservation M-integrals are applied to calculate driving forces on the dislocations. The model prediction shows quantitative agreement with the MD and experimental results, and provides new understanding of the plasticity of nano-scale contacts.

The remainder of this chapter is organized as follows. The dislocation model of nano-asperity contact is introduced in Section 2.2. An asymptotic analysis without considering dislocation interaction, which holds for fairly large contact size, is presented in Section 2.3. Section 2.4 describes the full numerical solution obtained by 3-D dislocation simulations, and its comparison with the asymptotic solution. The implications of the model prediction are discussed in Section 2.5. The final section summarizes the concluding remarks of this chapter.

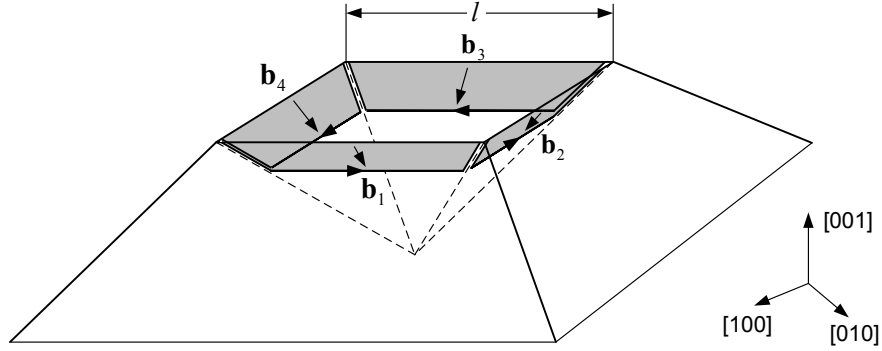


Figure 2.1: A schematic of the dislocation structure in gold pyramids subjected to contact loading.

2.2 Problem definition

The contact strength of a nano-sized gold asperity, as experimentally studied by Wang *et al.* (2006) and atomistically simulated by Ward (2008), is analyzed with a dislocation model. Fig. 2.1 shows a schematic of the asperity geometry. The asperity has a truncated pyramid shape with a (001) square top surface and four {111} side facets. When the top surface is subjected to a contact load, the dislocations are first nucleated at the contact edges due to stress concentration, and are then injected unstably into the bulk. The dislocations are assumed to be nucleated simultaneously at the four contact edges on the four {111} slip planes as shown with dashed lines in Fig. 2.1. The nucleation of partial dislocations with $\frac{a}{6}[112]$ Burgers vectors, as indicated by $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ and $\mathbf{b}_4$ in Fig. 2.1, is considered. Here a denotes the lattice constant of gold. After the nucleation of the partial dislocations, four sessile Lomer locks with $\frac{a}{3}[100]$ Burgers vectors are formed along $[110]$ directions at the intersection of the slip planes. The other slip systems are inactive and therefore are not considered, as suggested by the observation in the atomistic simulations of Ward (2008). The proposed dislocation model is analyzed in the following sections

with anisotropic elasticity. The dislocation lines are approximated by straight line segments for simplicity of analysis. The Rice-Thomson criterion (Rice and Thomson 1974) is used as the dislocation nucleation condition. The driving forces on the dislocations are calculated with 2-D and 3-D conservation M-integrals and various superposition techniques.

2.3 *Asymptotic analysis of contact strength*

When the contact edge length is large compared to the magnitude of Burgers vector b , the dislocation emission is controlled by the leading stress singularity term close to the contact edge. Fig. 2.2(a) shows the configuration of a 2-D wedge containing an edge dislocation under an external load P by a rigid punch. The wedge angle is ϕ , and the angle between the slip plane and the contact surface is denoted by θ . Both conditions of no-slip and frictionless contact between the punch and the wedge top surface are considered in this study. The asymptotic stress field near the edge can be taken as the superposition of two fields, S and Q, as shown in Fig. 2.2(b) and (c). The S field is the stress field of the unloaded wedge with the edge dislocation, while the Q field is the two dimensional leading singularity field of the wedge due to the external load P .

The two-dimensional M-integral conservation law is employed to calculate the configurational self-force on the dislocation in the S field. For an elastic solid, the 2-D M-integral is defined as

$$M \equiv \oint_{\Gamma} (W n_i - t_j u_{j,i}) x_i d\Gamma \quad (2.1)$$

where $W = \frac{1}{2} \sigma_{ij} \epsilon_{ij}$ is the strain energy density, n_i are the components of the unit

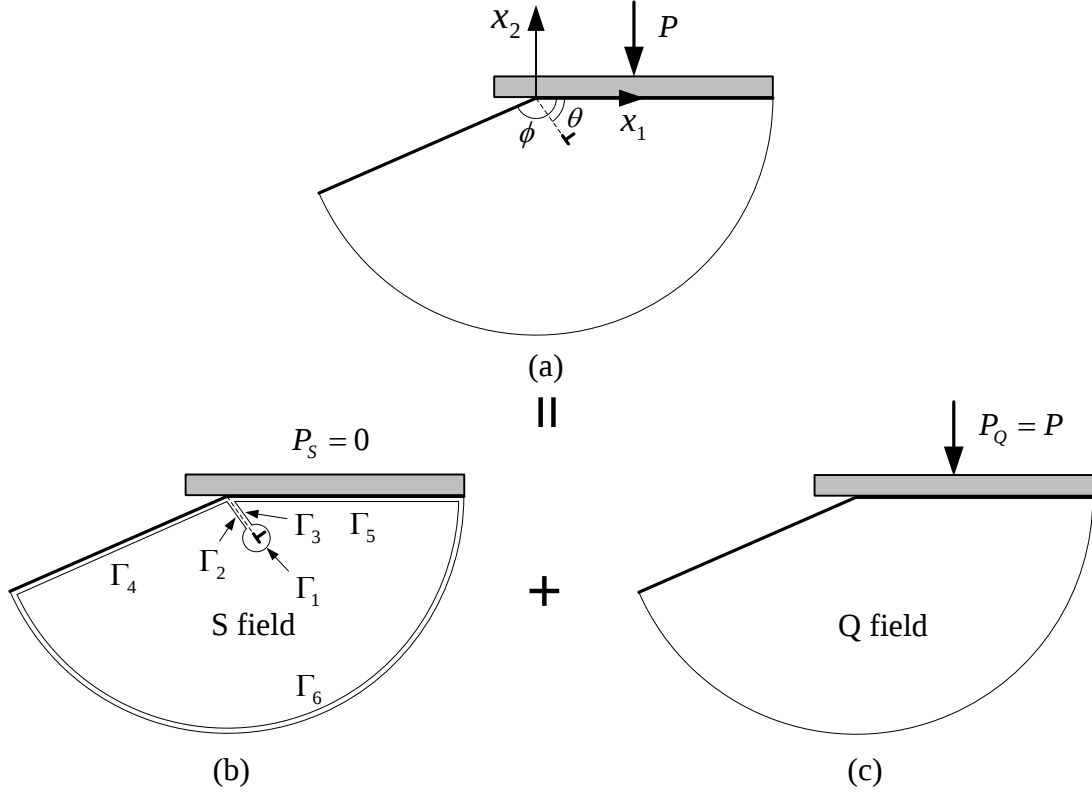


Figure 2.2: The asymptotic stress field (a) near the contact edge is decomposed into two sub-fields: the stress field (b) of a wedge containing an edge dislocation without external load and the stress field (c) of the loaded wedge without a dislocation. The no-slip and frictionless contact conditions between the punch and the wedge top surface are considered.

vector normal to $d\Gamma$, u_j are the components of the displacement field and x_i are the coordinate components. The M-integral conservation law states that $M=0$ for any closed contour Γ enclosing a homogeneous solid. For the calculation of self-force on the dislocation, the origin is taken to be at the wedge corner and the integration contour as shown in Fig. 2.2(b) is considered. The contribution to the M-integral along Γ_2 and Γ_3 cancels each other because of the continuity of the elastic energy density, traction and displacement gradient across the slip plane. The first term $W n_i x_i$ in the integrand of $M(\Gamma_4)$ and $M(\Gamma_5)$ vanishes because n_i is normal to x_i . Obviously, the

second term $t_j u_{j,i} x_i$ in the integrand of $M(\Gamma_4)$ is zero on the traction-free surface Γ_4 . For both no-slip and frictionless contact conditions, $x_2 = 0$ and $t_j u_{j,1} = 0$ hold at Γ_5 . Therefore the contribution of the second term to $M(\Gamma_5)$ also vanishes. As the radius of the circular contour Γ_6 goes to infinity, the far-field stress decays faster than $1/r$ because of zero net force on the two wedge surfaces. Hence, $M(\Gamma_6)$ approaches zero as r goes to infinity. Finally, it can be concluded from the conservation law that the M-integral over the infinitesimal contour Γ_6 around the dislocation core is zero. The configurational self-force J_S on the dislocation can be then calculated as

$$M(\Gamma_1) = -J_S \eta - M_D = 0 \Rightarrow J_S = -\frac{M_D}{\eta} \quad (2.2)$$

where η is the distance between the dislocation and the wedge tip and M_D is the 2-D M-integral around a Volterra dislocation core with the origin located at the core. η can be physically regarded as the process zone size for the dislocation nucleation. It is noticed from Eq. 2.2 that the self-force on the dislocation is only dependent on the dislocation properties and the process zone size η , and is independent of the wedge geometry.

Considering the singularity field Q caused by the external load, of particular interest here is the component of resolved shear stress on the slip plane. Following Chue and Liu (2001), the asymptotic shear stress near the wedge corner can be expressed as

$$\sigma_{r\theta}(r, \theta) = Re \left[\sum_n (Q_n g_n(\theta, \phi) r^{\lambda_n} + \overline{Q_n} h_n(\theta, \phi) r^{\bar{\lambda}_n}) \right] \quad (2.3)$$

where λ_n is a complex eigenvalue of the n-th eigenmode, $[g_n \ h_n]$ is the n-th complex eigenvector and Q_n is the corresponding stress intensity factor. The symmetric form of Eq. 2.3 indicates that the eigenvalues of the wedge solution always appear in conjugate

pairs that correspond to the same eigenmode. Therefore only the eigenvalues with non-negative imaginary parts are considered. For given boundary conditions, the values of λ_n , $g_n(\theta, \phi)$ and $h_n(\theta, \phi)$ are analytically known from the characteristic equations of the wedge solution. The number of the eigenvalues is in general infinite. For the current study, only the eigenvalues with $Re(\lambda_n) < 0$ give stress singularities and are of interest here. The condition of finite elastic strain energy at the corner also limits $Re(\lambda_n) > -1$. The number of the eigenvalues satisfying $-1 < Re(\lambda_n) < 0$ is denoted by N_Q .

The Rice-Thomson nucleation criterion (Rice and Thomson 1974) is adopted as the dislocation nucleation condition at the wedge corner. The criterion is such that, at certain distance $r = \eta$ from the corner, the addition of the self image force J_S and the driving force J_Q due to the applied load must be in balance with the Peierls force J_P and the stacking fault energy γ . In a 3-D asperity contact, the distribution of the driving force along the contact edges is self-similar and nonuniform regardless of contact size. As an approximation, it is assumed that the dislocation is driven by the average driving force $\hat{J}_Q$. Here the hat $\hat{}$ denotes average over the contact edges. The dislocation nucleation criterion can be expressed as

$$\hat{J}_Q = \hat{\sigma}_{r\theta}^{cr}(\eta, \theta)b = M_D/\eta + J_P + \gamma \quad (2.4)$$

The critical average singularity intensity $\hat{Q}_n^{cr}$ can be derived from a dimensional analysis as

$$\hat{Q}_n^{cr} = \frac{\beta_n p^{cr}}{l^{Re(\lambda_n)}} \quad (2.5)$$

where p^{cr} is the critical average punch pressure for dislocation nucleation and l is the contact edge length as shown in Fig. 2.1. The proportionality coefficient β_n is a

function of the wedge angle ϕ and the ratios among the elastic constants C_{ijkl} . For the contact strength of the gold asperity with (114) facets under consideration, β_n is constant. It can be evaluated readily by performing a FEM analysis of the asperity without dislocations, and applying the two-state conservation M-integral (Im and Kim 2000) to the FEM field using an analytic auxiliary field with a complementary eigenvalue of $-\lambda_n$. Then, from Eq. 2.3, 2.4 and 2.5, the contact strength can be written as

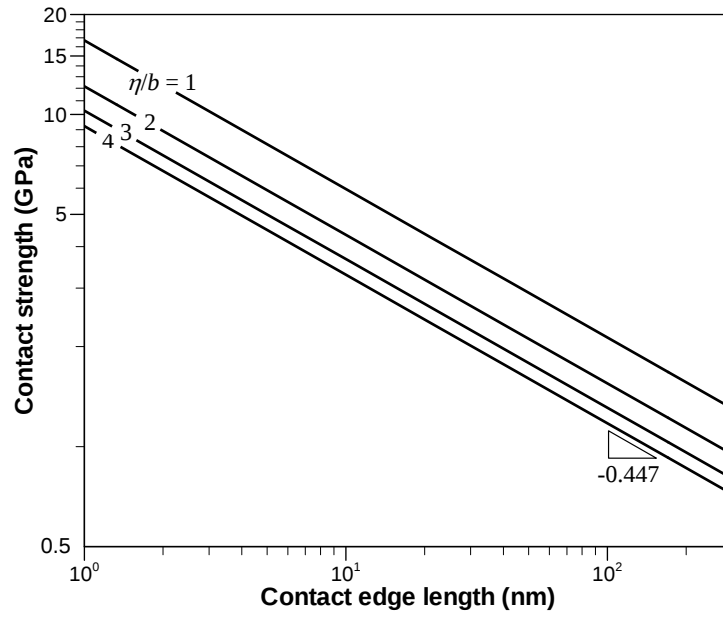
$$p^{\text{cr}} = \frac{\frac{M_D}{\eta} + J_P + \gamma}{\text{Re} \left[\sum_{n=1}^{N_Q} \frac{\beta_n g_n \eta^{\lambda_n} + \bar{\beta}_n h_n \eta^{\bar{\lambda}_n}}{l^{\text{Re}(\lambda_n)}} \right] b} \quad (2.6)$$

The eigenmodes of (114) gold asperity contact for both no-slip and frictionless conditions are studied following the approach by Chue and Liu (2001) and Chue *et al.* (2001). It is found that for both conditions, there is only one singular eigenmode, with $\lambda^{(1)} = -0.447 + 0.025i$ for no-slip contact and $\lambda^{(2)} = -0.497$ for frictionless contact. Eq. 2.6 is then simplified to

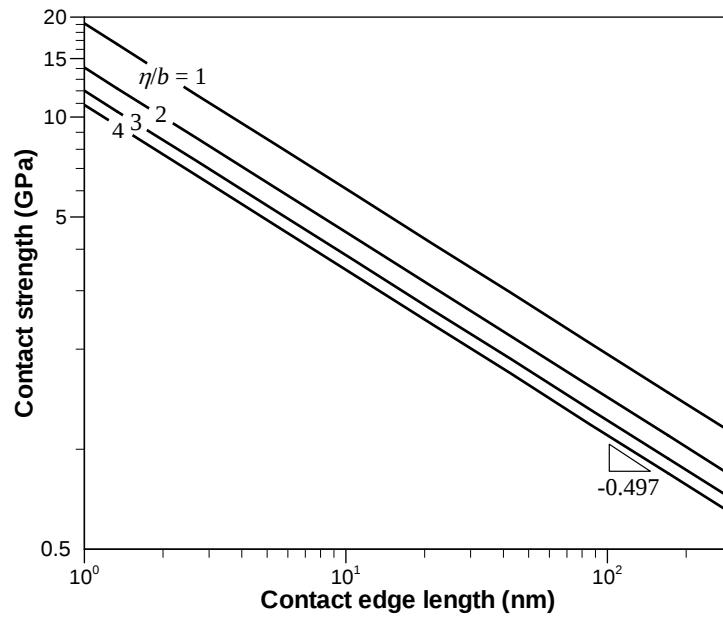
$$p_{(i)}^{\text{cr}} = \left(\frac{M_D}{\eta} + J_P + \gamma \right) \frac{\alpha^{(i)}}{b} \left(\frac{l}{\eta} \right)^{\text{Re}(\lambda^{(i)})} \quad (2.7)$$

where $\alpha^{(i)} = 1/\text{Re}[\beta^{(i)} g^{(i)} \eta^{\text{Im}(\lambda^{(i)})} + \bar{\beta}^{(i)} h^{(i)} \eta^{-\text{Im}(\lambda^{(i)})}]$, and (i) denotes (1) for no-slip contact and (2) for frictionless contact. Eq. 2.7 infers that the asymptotic contact strength $p_{(i)}^{\text{cr}}$ has a power-law dependence on the contact edge length l with a scaling exponent of $\text{Re}(\lambda^{(i)})$.

The contact strength of the gold asperity with (114) facets is calculated and plotted in Fig. 2.3. The following material properties of single crystal gold are used for the calculation, $C_{11} = 186$ GPa, $C_{12} = 157$ GPa, $C_{44} = 42$ GPa, $b = 1.666$ Å, $\tau_P = J_P/b = 10$ MPa and $\gamma = 0.032$ J/m². The 2-D M-integral around the Volterra dislocation,



(a)



(b)

Figure 2.3: Asymptotic solution of size-dependent contact strength for various values of η/b . (a) No slip contact; (b) Frictionless contact.

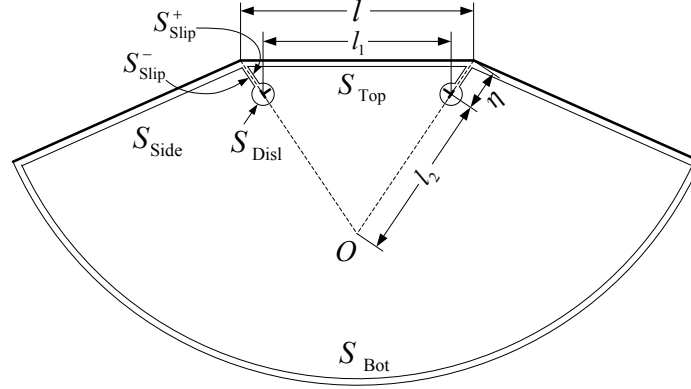


Figure 2.4: The integration surface of 3-D M-integral for the calculation of dislocation configurational force

M_D , in Eq. 2.7 is obtained following Suo (2000) as $M_D = \frac{1}{2\pi} \mathbf{b}^T \mathbf{H}^{-1} \mathbf{b}$, in which $\mathbf{b}$ is the Burgers vector and $\mathbf{H}$ is a positive-definite Hermitian matrix determined by the elastic constants (Suo 1990). In the dislocation model η/b is the only undetermined quantity and can be treated as a fitting parameter. Fig. 2.3 (a) and (b) show the contact strength as a function of contact edge length for the two frictional conditions and different η/b of 1, 2, 3 and 4, which are within the typical range of η/b for single crystals. The contact strength has a power-law decay with increasing contact edge length. The scaling exponents are -0.447 and -0.497, respectively, for the no-slip and frictionless contact. As the process zone size η/b decreases, the contact strength increases rapidly in a nonlinear manner. A comparison with the atomistic result by Ward (2008), which will be presented in detail in Section 2.5, reveals that $\eta/b = 1.25$ gives the best fitting between the model prediction and the atomistic simulation.

2.4 A full numerical solution

For small contact edge length, a deviation from the asymptotic solution is expected due to the effects of dislocation interaction and deterioration of the leading singularity. The analysis of a 3-D dislocation model is carried out to study these effects, and the range of validity of the asymptotic solution. Similar to the asymptotic case, the Rice-Thomson criterion is used, i.e., $J_D = J_P + \gamma b$. For the 3-D configuration as shown in Fig. 2.1, if the displacement and stress fields are known, the average configurational force on the dislocations can be calculated with the 3-D conservation M-integral, which is defined as

$$M \equiv \int_S \{ (W n_i - t_j u_{j,i}) x_i - \frac{1}{2} t_i u_i \} dS. \quad (2.8)$$

Here, S is a closed integration surface surrounding an elastic homogeneous solid. The configurational force is calculated with an integration domain as shown in Fig. 2.4. A 2-D representation of the asperity cross-section is drawn in the figure for clarity. The M-integral surrounding the dislocation segments can be expressed as

$$M^{(\text{Disl})} = 4l_1 l_2 J_D - 4l_1 (M_D - \frac{1}{2} \int_{\Gamma} t_i u_i d\Gamma) - \frac{8\sqrt{3}}{3} \eta (M'_D - \frac{1}{2} \int_{\Gamma'} t_i u_i d\Gamma') \quad (2.9)$$

in which Γ and Γ' are infinitesimal contours around the core lines of the partial and sessile dislocations, respectively, and M_D and M'_D are the corresponding 2-D M-integrals around the dislocation cores. The M-integral contribution from the slip plane is calculated to be

$$M^{(\text{Slip})} = M(S_{\text{Slip}}^+) + M(S_{\text{Slip}}^-) = -\frac{1}{2} \int_{S_{\text{Slip}}^+} \sigma_{ij} n_i^+ b_j dS \quad (2.10)$$

where n_i^+ is the unit normal to S_{Slip}^+ . From the M-integral conservation law, the average configurational force on the partial dislocations can be expressed in terms of the component M-integrals as

$$J_D = \frac{1}{4l_1l_2} \left\{ 4l_1 \left(M_D - \frac{1}{2} \int_{\Gamma} t_i u_i d\Gamma \right) + \frac{8\sqrt{3}}{3} \eta \left(M'_D - \frac{1}{2} \int_{\Gamma'} t_i u_i d\Gamma' \right) \right. \\ \left. - M^{(\text{Slip})} - M^{(\text{Top})} - M^{(\text{Side})} - M^{(\text{Bot})} \right\} \quad (2.11)$$

The term of $M^{(\text{Slip})}$ is divergent as the stress near the core has $1/r$ singularity. Physically, the divergence can be rationalized by the breakdown of linear elasticity near the core structure. Usually a cutoff radius r_0 around the core is used for the integration to overcome the convergence problem. The dislocation core sizes for FCC metals typically range from $b/2$ to $2b$ (Hirth and Lothe 1982). In this study, a cutoff radius of $r_0 = b/2$ is used for evaluating $M^{(\text{Slip})}$.

For the M-integral calculation, the displacement and stress distribution of the 3-D asperity configuration is not analytically available and has to be computed numerically. A finite element analysis (FEA) is performed to obtain the field solution. However, the numerical evaluation of a 3-D M-integral from a FEA solution poses great difficulty. It is well known that stress calculation based on a standard FEA is most accurate at the integration points of finite elements; however, the deformation gradient and stress fields at the boundary surfaces are needed for the M-integral calculation. The regular technique of boundary stress recovery by extrapolation from integration points is found to induce considerable errors. To overcome this problem, a modified scheme of driving force calculation through the field superposition as shown in Fig. 2.5 is proposed. The field solution of the asperity under contact load in Fig. 2.5(a) is decomposed into three sub-fields (b), (c) and (d). The first field (b) is an infinite medium with four dislocation loops extending out of the asperity

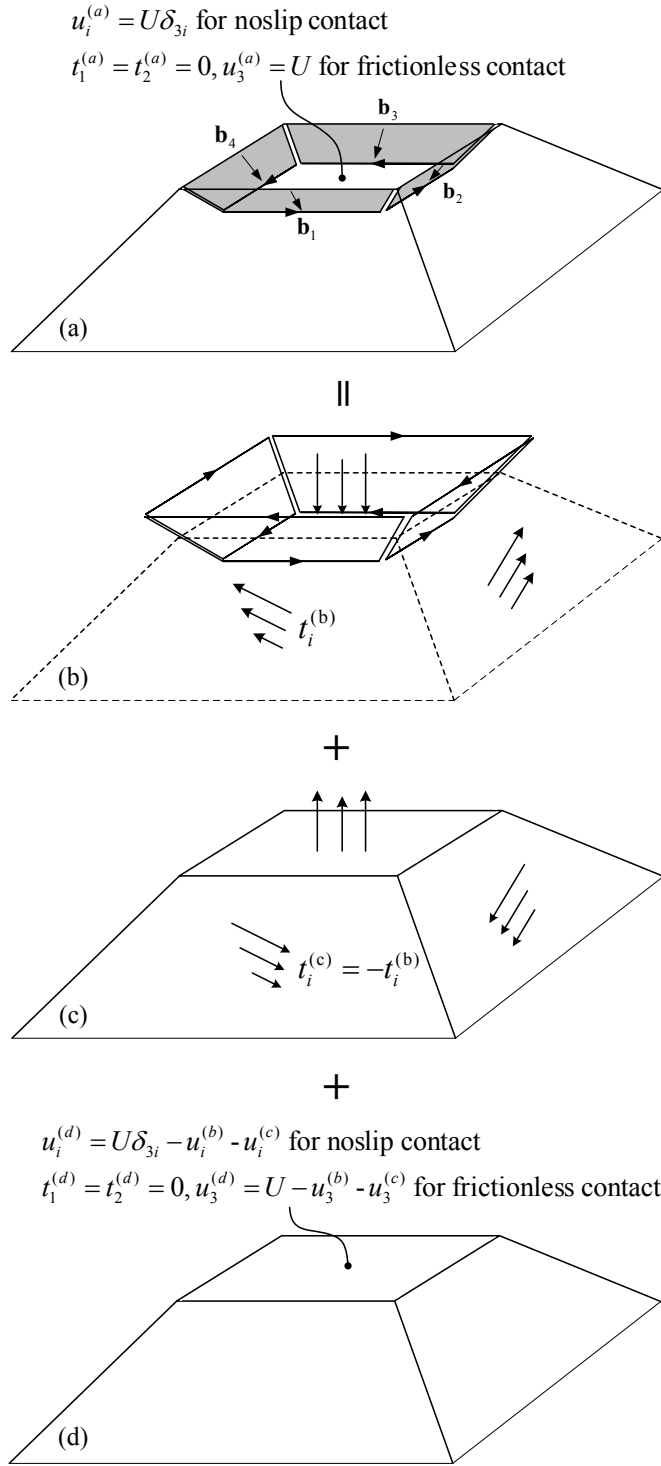
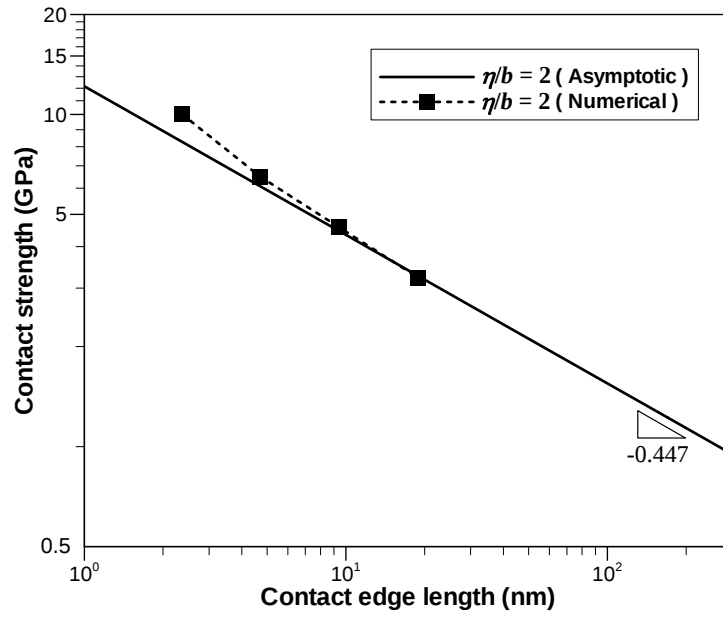


Figure 2.5: The decomposition of the elastostatic field of the 3-D dislocation model

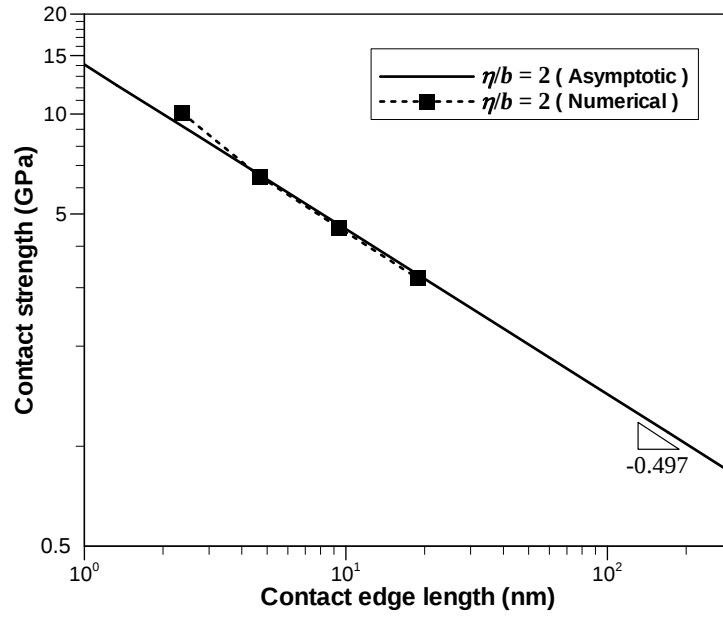
volume. The second field (c) is the elastostatic field of the asperity subjected to a traction boundary condition of $t_i^{(c)} = -t_i^{(b)}$. The third field (d) represents the solution with a displacement boundary condition at the top surface to satisfy the boundary condition of field (a). The superposition of field (b) and (c) gives the elastostatic field of the traction-free asperity containing the dislocations. If Eq. 2.11 is applied to the superposed field, the second and third terms in the 3-D M-integrals vanish due to zero traction boundary condition. The evaluation of strain energy in the first term on the traction-free surface is reduced to a plane stress problem, and can be evaluated accurately with the surface nodal displacements. The additional driving force, J_A , in field (d) can be readily calculated in terms of the average resolved shear stress, τ_A , at the dislocation position by $J_A = \tau_A b$. The total configurational force on the dislocation is then obtained from $J_D = J_S + J_A$.

The elastostatic field (c) and (d) are numerically solved in ABAQUS. The analysis employs 4 symmetry planes and models one-eighth of the volume. 3-D quadrilateral tetrahedral elements are used in the FEM analysis with a refined mesh size of $l_m = b/8$ near the contact edges and dislocation cores. The stress and displacement fields of the dislocation loops in an infinite anisotropic medium are calculated to obtain the boundary conditions of field (c) and (d). The details of the calculation can be found in the appendix of this chapter. The calculated boundary conditions are applied to the finite element model with the DISP and UTRACLOAD subroutines in ABAQUS.

The numerical simulation results are plotted in Fig. 2.6 for an intermediate value of $\eta = 2$, together with the asymptotic solution. It can be seen that, as l decreases, the full numerical simulation predicts higher contact strength due to the stronger effect of dislocation interaction. The frictionless contact shows a slightly quicker convergence to the asymptotic solution than the no-slip contact. In both cases, the differences between the numerical and asymptotic solutions become fairly small and negligible for



(a)



(b)

Figure 2.6: Comparison between the asymptotic and full numerical results for $\eta/b = 2$. (a) No slip contact; (b) Frictionless contact.

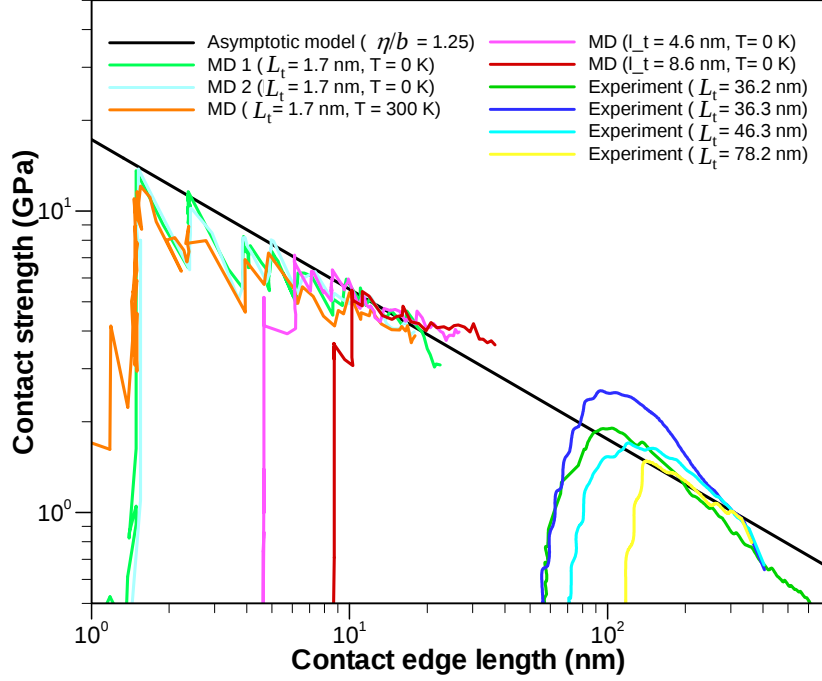


Figure 2.7: Comparison of the model result with the MD (Ward 2008) and experimental (Wang *et al.* 2006) results. Frictionless contact condition and $\eta/b = 1.25$ are used to obtain the asymptotic solution.

a contact edge length larger than 5 nm. Therefore it is concluded that the asymptotic analysis holds for a wide range of contact strength, and can be advantageously used for contact strength evaluation of nano-asperities.

2.5 Discussions

Fig. 2.7 shows the comparison of the model prediction with the MD simulation result by Ward (2008) and the experimental result by Wang *et al.* (2006). The frictionless contact condition is chosen for the comparison, because it is believed to better represent the MD simulation in which only the repulsive force term is used between

the punch and pyramid atoms. The process zone size, η , is the only undetermined quantity in the model and is treated as a fitting parameter. While the MD simulation calculates the contact strength as a function of contact size in a single compression test, the current model predicts the initial contact strength of a truncated pyramid. The value of η/b in the model is calibrated to be 1.25 by fitting the asymptotic solution with the peak strength of the MD simulation curves of two truncated pyramids. The MD curves show zig-zag features due to unstable dislocation emission. Therefore the comparison should be made between the model prediction and the local peaks of the MD curves. The asymptotic solution with $\eta/b = 1.25$ fits well with the MD curves with different initial truncations, although a small difference for $l > 20$ nm is observed due to the hardening effect in the MD simulations. The model curve also passes through the maximum strengths of the experimental curves at $l = 100$ nm. It should be mentioned that the current dislocation model is expected to be valid for the contact size, l , between 5-100 nm. For larger l , the chance of bulk dislocation nucleation and multiplication is believed to become large. Therefore the contact strength may be no longer solely controlled by surface dislocation emission. The model does not apply to $l < 5$ nm either, although the model result appears to fit the MD calculation for a contact size smaller than 5 nm as well. The Volterra dislocation theory used in the model treats the dislocations as line defects. When the distance between dislocation segments is small compared to b , the properties of dislocation core structure changes substantially due to strong dislocation interaction. Therefore the Volterra dislocation theory no longer holds for this small size range. A dislocation model with cohesive dislocation core structure (Rice 1992) can be developed to explore this length scale; but this is beyond the scope of this study.

The model prediction, as expressed in Eq. 2.7, shows some important features of asperity contact strength at the nanometer scale. The strength is found to be

proportional to $(\frac{M_D}{b\eta} + \frac{\gamma}{b} + \frac{J_P}{b})$. The last Peierls force term is usually much smaller than the dislocation core term and the stacking fault energy term. The first term can be expressed as $M_D = \frac{b}{2\pi\eta} \hat{\mathbf{b}}^T \mathbf{H}^{-1} \hat{\mathbf{b}}$, in which $\hat{\mathbf{b}}$ is the unit direction of Burgers vector and $\mathbf{H}^{-1}$ is a positive-definite matrix proportional to the elastic constants. Therefore, for a given geometry, the contact strength at the nanometer scale is primarily governed by the elastic stiffness and the stacking fault energy of the materials. The geometric effects like wedge angle, slip plane orientation and slip direction can be also studied with the current model result given by Eq. 2.6.

The model presented in this study predicts a scaling exponent (~ -0.5) close to the one given by the well-known Nix-Gao relationship of nanoindentation hardness (Nix and Gao 1998). It is worth emphasizing that the physics underlying these two scaling laws are fundamentally different. The scale dependence of Nix-Gao relationship is related to the geometrically necessary dislocations (GNDs) associated with the strain gradient of the deformation field. The contact strength studied in this work is, however, governed by heterogeneous nucleation of surface dislocations at a smaller length scale ($l < 100$ nm) than that of Nix-Gao relationship.

The current focus is only limited to study the initial contact strength of nano-asperities. A potential extension of the model for studying the strength hardening is possible. Four sessile dislocations are formed at the intersection of the slip planes after each partial dislocation emission. A continuous compression on the asperity after first yielding generates four sets of sessile dislocation array with the line directions of $[110]$ and Burgers vectors of $\frac{a}{3}[100]$, which produce image forces for contact strength hardening. The interaction between sessile dislocation arrays and partial dislocation nucleation can be taken into account by replacing the sessile dislocation arrays with a displacement boundary condition. It is also noted that the boundary

element method (BEM) is more appealing than the finite element method (FEM) in the numerical study of asperity strength. When FEM is used, a fine mesh is needed near the contact edges and dislocation cores to resolve the high strain gradient at those locations. The FEM analysis of a 3-D structure with such mesh density is computationally expensive. On the other hand, BEM can provide more accurate distribution of stress and displacement over the interior and boundary at less cost for driving force calculation with the M-integral.

2.6 Chapter summary

A dislocation model has been developed to study the scale-dependent contact strength of nano-asperities. The heterogeneous dislocation nucleation caused by a wedge stress singularity near contact edges is considered in this study. The dislocation nucleation is assumed to obey the Rice-Thomson criterion. The driving forces on dislocations are calculated with the 2-D and 3-D conservation M-integrals. Both the asymptotic analysis and full numerical simulation are performed based on dislocation mechanics and anisotropic elasticity. The contact strength is found to be scaled with the contact size with a scaling exponent close to -0.5. The model predicts that the contact strength at the nanometer scale is largely dependent on the material stiffness and the stacking fault energy. The validity of the model is supported by the comparison with the MD and experimental results. The model results are expected to provide valuable guidance to nano-structure design, e.g., the truncation size and the side surface slope of the nano-asperities, for adhesion and friction reduction.

Appendix A: Numerical calculation of displacement and stress fields of a planar dislocation loop in an infinite anisotropic medium

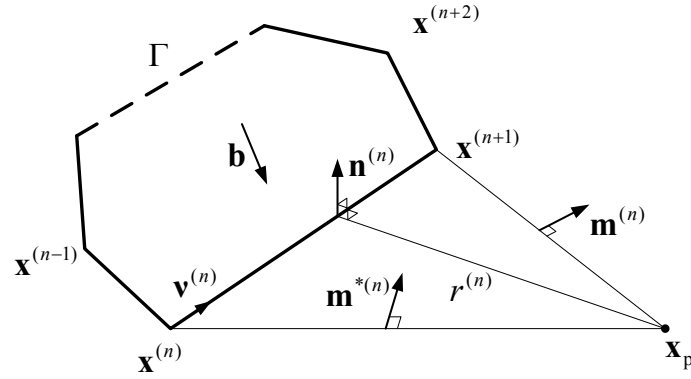


Figure 2.8: A planar dislocation loop.

Fig. 2.8 illustrates a planar dislocation loop that consists of N_s straight segments. The stress components at the point of interest, P , can be constructed by the addition of each segment, $\sigma_{ij}^{(n)}$.

$$\sigma_{ij} = \sum_{n=1}^{N_s} \sigma_{ij}^{(n)} \quad (2.12)$$

The stress field of each dislocation segment can be expressed as (Mura 1982)

$$\sigma_{ij}^{(n)} = \frac{1}{8\pi^2} \epsilon_{qnh} C_{ijpq} C_{lkmn} b_m \nu_h^{(n)} r^{(n)-1} \{I_{lpk}(\mathbf{m}^{*(n)}, \mathbf{n}^{(n)}) - I_{lpk}(\mathbf{m}^{(n)}, \mathbf{n}^{(n)})\} \quad (2.13)$$

in which I_{lpk} is also a function dependent on elastic constants and can be found in Mura (1982). The displacement field of the planar dislocation loop can be written as

the summation of a solid angle term and a line integral as following (Leibfried 1953)

$$u_i = \frac{b_i}{4\pi}\Omega + \epsilon_{lnh}C_{jkmn}b_m \oint_{\Gamma} G_{ijkl}(\mathbf{x}_p - \mathbf{x}')d\Gamma_h(\mathbf{x}') \quad (2.14)$$

where Ω is the solid angle spanned by the dislocation loop, and G_{ijkl} is the Green's function defined as

$$G_{ijkl}(\mathbf{x}) = \frac{1}{8\pi^2x} \oint_{S^1} T_{ij}^{-1}(\xi)\xi_k\xi_l\mathbf{d}\phi \quad (2.15)$$

in which $T_{ij} = C_{ikjl}\xi_k\xi_l$ and S^1 is the unit circle perpendicular to $\mathbf{x}$ on the unit sphere in the ξ -space.

Chapter 3

SUSPENSION RESISTANCE OF REINFORCEMENT PARTICLES IN METAL MATRIX COMPOSITES

3.1 Introduction

The tribological application of metal matrix composites (MMCs) has received great attention due to their superior mechanical properties, e.g., excellent wear and creep resistance, light weight, high stiffness and strength. The performance gain of the MMCs is primarily achieved by distributing the load bearing function more to the reinforcement phases than the matrix. With proper surface treatment and optimal design of the microstructures, such as volume fraction and morphology of the reinforcement phases, the tribological performance of MMCs can be tuned to meet the needs of practical tribological application.

Even though a complete understanding of composite wear mechanisms is still developing, empirically it has been found that for moderate sliding speed, the wear mechanism map can be described by three wear regimes, depending on the magnitude of the contact load (Deuis *et al.* 1997, Wilson and Alpas 1997, Zhang and Alpas

1997, Chen *et al.* 2007). The so called ultra-mild wear regime dominates for very small contact load. In this wear regime the counterface slides against both the metal matrix and the hard particles at the initial stage. The soft metal matrix is worn out much faster than the hard particles, and the entire contact load is finally taken over by the particles. Once this configuration is formed, the contact only takes place between the counterface and the hard particles. The surface is expected to show very good scuff and wear resistance. In practice, the matrix is usually pre-etched to reach this configuration directly without the running-in process (Riahi *et al.* 2003). With the contact load increasing, the wear process shifts to the mild wear regime. In this regime, the particles by themselves can not sustain the large contact load. The matrix surface is continuously worn out due to delamination by subsurface crack nucleation and growth. The severe wear occurs for extremely heavy loads. The matrix of the subsurface undergoes large plastic shear deformation with plastic strain on the order of 1-10. The hard particles in this deformation layer fragment into tiny particles and mix with the matrix to form a hard tribolayer with ultra-fine microstructure beneath the surface.

The key idea of designing MMC-based tribo-components with a low wear rate is to keep the system operating in the ultra-mild wear regime. This requires knowledge of suspension capability of reinforcement particles under contact load. While most of the previous experiments were focused on macroscopic friction/wear testing and microscopic post-observation (Zhang and Alpas 1997, Riahi *et al.* 2003, Chen *et al.* 2007), the micromechanical response of individual reinforcement particles has been generally overlooked. To investigate the dependence of the particle suspension resistance on material properties and particle morphology, it is highly desirable to conduct small-scale experiments and analysis at the single particle level.

The recent development of nano- and micro-mechanical test instruments makes it

possible to mechanically probe nano- and micro- scale systems, and measure the corresponding mechanical responses with fine force and displacement resolutions. Such instruments, e.g., a nanoindenter and an atomic force microscope (AFM), have opened an opportunity to characterize the mechanical properties of small-length-scale structures. In this work, we took a hypoeutectic Al/Si alloy as a model system and used a nanoindenter to study the suspension resistance of silicon particles embedded in an aluminum matrix. The Al/Si alloy is considered as an in-situ composite, since the hard silicon particles in the aluminum matrix are formed during its casting process. The alloy is one of the primary replacements for steel and cast iron in the automotive industry as part of an overall objective towards reducing vehicle weight and increasing fuel efficiency (Rohatgi 1991).

As the medium of load transfer, the interface between the reinforcement particles and the matrix plays a crucial role in determining the suspension resistance of the particles. Therefore, characterization of the mechanical properties of the interfaces is another focal point of this work. The mechanical property characterization of solid interfaces is typically composed of two parts. One is the structural and/or chemical composition characterization. The other is the deformation and failure process characterization, or in other words, strength characterization. While the structural characterization of the interfaces can be made readily with various electron microscopy techniques (Jeong *et al.* 1996, Kloosterman *et al.* 1998, Ferroni *et al.* 2001, Khalid *et al.* 2004), the strength characterization is still a great challenge, especially at a small length scale. It has been widely recognized that the fracture process of an interface is a multi-scale phenomenon covering from the atomistic scale to the macroscopic laboratorial scale (Evans *et al.* 1999, Needleman and Van der Giessen 2001). As a consequence, the strength characterization is highly dependent on the length scale of interest. Typical reinforcement sizes of MMCs are from sub-micron to tens of

microns, and quantitative study of interface strength at this length scale has been difficult, both experimentally and computationally. The experimental measurement of interface strength has been seldom carried out at this length scale. Most of the existing computational continuum modeling (Needleman 1987, Xu and Needleman 1993, Camacho and Ortiz 1996, Moes *et al.* 1999, Xia *et al.* 2007) has been just focused on developing simulation techniques for parametric studies which require experimental validations and verifications. Although atomistic simulations of interface failure (Gall *et al.* 2000, Ward, Curtin and Qi 2006, Ward, Curtin, WA and Qi 2006, Noreyan *et al.* 2008) can imitate the fracture process at a small length scale computationally, the time and length scales which they can handle are so small that scale bridging is needed for the simulation results to be applied to engineering problems in realistic time and length scales.

Interface strength and/or failure processes are often modeled in a framework of a cohesive zone model (CZM) (Needleman 1987, Xu and Needleman 1993, Camacho and Ortiz 1996, Xia *et al.* 2007). CZM is typically used to emulate interfacial slip and decohesion processes in various length scales. CZM assumes that the slip and decohesion processes can be described by the relationship between cohesive traction and separation displacement across the cohesive zone. The relationship is the constitutive relation of the cohesive zone; it depends on the resolution of the deformation kinematics employed in modeling the deformation field which surrounds the cohesive zone. Within the framework of continuum deformation kinematics of linear elasticity, Hong and Kim (2003) developed the field projection method (FPM) to extract crack-tip cohesive zone laws of a homogeneous isotropic elastic solid. The method was then extended by Choi and Kim (2007) to extract the intrinsic nanoscale CZM laws of an interface between two elastic solids which can be either isotropic or anisotropic.

Modeling of the interface failure processes of MMCs, however, typically requires

finite element analysis of the inelastic deformation of the matrix. In this paper, a new framework of a finite element cohesive zone model called the normal-separation induced linear softening cohesive zone model (NILS-CZM), is introduced to simulate the Al/Si interfacial slip and decohesion processes. In the NILS-CZM, the strength of the cohesive zone is scaled from the intrinsic cohesive zone strength to that of the finite element model. The scale bridging is made by enforcing the energy release rate of crack growth to be equivalent to the energy consumption rate of the cohesive zone opening compatible with the admissible finite element deformation; see Appendix for more details. The NILS-CZM enables us to characterize the interface strength with a newly developed hybrid method of nano-indentation and finite element analysis. In addition, the scale-bridging capability of the NILS-CZM allows us to compare the results with the quantities obtained by molecular dynamics simulations of the failure process at the atomistic scale.

The remainder of this paper is organized as follows. In Section 2, the particle nanoindentation problem is defined, and the approach taken to solve the problem is introduced. In Section 3, we describe the experimental procedures and present the experimental results that are processed with a dimensional analysis. Section 4 covers the finite element analysis of particle indentation and the extraction of interface properties through the comparison between the experimental and FEM results. In Section 5, we discuss on the comparison between the values of the interface properties measured experimentally and estimated by atomistic simulations. Concluding remarks are given in the last summary section.

3.2 *Problem definition of particle nanoindentation*

3.2.1 *Generic configuration of particle nanoindentation*

As briefly mentioned in the introduction, the objective of this work is to characterize the nanoindentation response of a hard elastic particle embedded in a ductile matrix, and to construct a general framework of extracting the small-scale material properties of the system from the response characteristics, in particular, the interface properties. Towards this end, the most generic configuration of the particle nanoindentation problem is considered, as shown in Fig. 3.1(a). The geometry of the particle is taken to be a round-bottomed cylinder that is vertically embedded in the matrix. The diameter of the particle cross-section is denoted by D , the buried depth by H , and the radius of the spherical indenter tip by R . The particle is slightly protruding out of the matrix initially before it is subjected to a contact load, P , applied by a rigid spherical indenter. The corresponding indenter displacement caused by the contact load is denoted by h . The elastic modulus and Poissons ratio of the particle are E_p and ν_p , and those of the matrix are E_m and ν_m . The plastic deformation of the matrix is characterized by the J_2 flow theory with isotropic power law hardening. The yield stress and the hardening exponent of the matrix are σ_Y and m , respectively.

The mechanical characteristics of the interface between the particle and the matrix are depicted by the NILS-CZM;

$$\begin{aligned} \begin{bmatrix} \sigma \\ \tau \end{bmatrix} &= \begin{bmatrix} \sigma_0 \\ \tau_0 \text{sgn}(\dot{s}) \end{bmatrix} (1 - \delta/\delta_c), \quad \text{for } 0 < \delta \leq \delta_c \\ \sigma &\leq \sigma_0 \text{ and } \tau = \tau_0 \text{sgn}(\dot{s}), \quad \text{for } \delta = 0 \end{aligned} \quad (3.1)$$

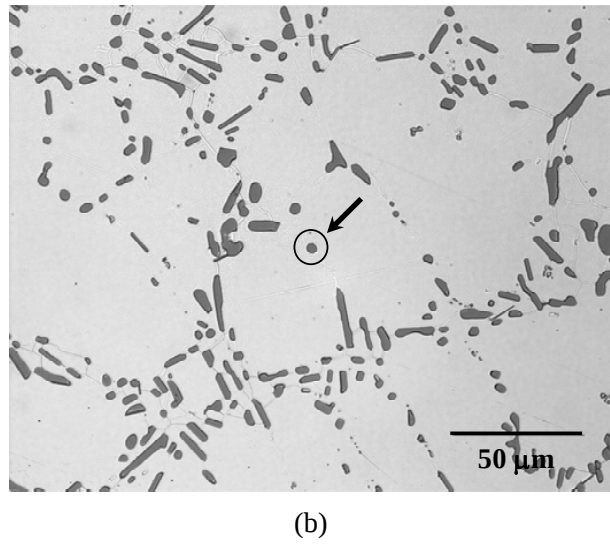
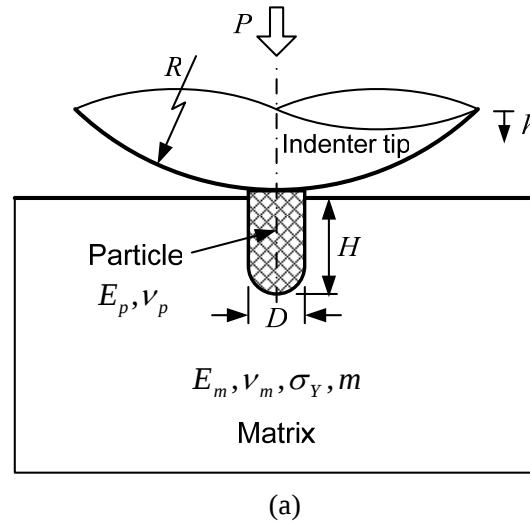


Figure 3.1: (a) A schematic of a nanoindentation test of an elastic particle embedded in a ductile metal matrix; (b) Optical microscope image of the cross-section microstructure of the hypoeutectic Al/Si alloy. A silicon particle selected for a nanoindentation test is shown inside the circle.

with three material parameters, the normal strength, σ_0 , the shear strength, τ_0 , and the critical normal separation, δ_c , of the interface. Eq. 3.1 describes that the normal and shear stresses, σ and τ decrease linearly from σ_0 and τ_0 to zero respectively, as the normal separation, δ , varies from zero to δ_c . The shear resistance, τ , is assumed to be constant with respect to variation of the slip distance, s , for a fixed normal opening. The slip direction is denoted by the sign of the slip rate $\dot{s}$, $\text{sgn}(\dot{s})$.

3.2.2 *Canonical response of particle nanoindentation*

In this sub-section, the response of particle nanoindentation is reduced into a canonical form in a quantitative and systematic way, in order to understand of the particle sinking process caused by nanoindentation and to extract the matrix and interface properties from the indentation response.

In general, the indentation displacement, h , is composed of elastic and plastic parts (see Fig 3.4 (a)),

$$h = h_e + h_p \quad (3.2)$$

The elastic displacement, h_e , is the load times the secant compliance of the indentation system of the displacement measurement. For the generic configuration of particle nanoindentation, h_e , can be decomposed into Hertzian contact displacement and the rest, which is linearly proportional to the load, before the spherical indenter tip makes full contact with the top surface of the particle. Once the tip is in full contact, h_e increases linearly with respect to the load. The elastic displacement is then expressed as

$$h_e = \begin{cases} aP^{\frac{2}{3}} + bP, & \text{for } P < P_c \\ c(P - P_c) + d, & \text{for } P \geq P_c \end{cases} \quad (3.3)$$

where P_c is the indentation load at the onset of full contact. The coefficient a represents the elastic Hertzian contact compliance, b is the rest linear compliance, c is the compliance for the full contact configuration, and d is the elastic displacement when $P = P_c$. The continuity conditions of the elastic displacement and the tangential compliance at $P = P_c$ give the expressions of c and d as $c = \frac{2}{3}aP_c^{-\frac{1}{3}} + b$ and $d = aP_c^{\frac{2}{3}} + bP_c$. The plastic sinking displacement, $h_p = h - h_e$, can be caused by matrix plastic deformation and interfacial slip, accompanied by possible interface decohesion.

Considering a single loading and unloading cycle of the nanoindentation process, the plastic sinking response can be expressed in a dimensionless form as

$$\frac{p}{\sigma_Y} = f_K\left(\frac{h_p}{D}, \frac{H}{D}, \frac{R}{D}, \frac{E_p}{E_m}, \nu_p, \nu_m, \frac{\sigma_Y}{E_m}, m, \frac{\tau_0}{E_m}, \frac{\sigma_0}{E_m}, \frac{\delta_c}{D}\right) \quad (3.4)$$

where $p = \frac{4P}{\pi D^2}$ denotes the particle indentation (PI-) pressure which is the average pressure applied on the top surface of the particle. The subscript K of the function f_K denotes L for loading or U for unloading. For the unloading response, f_K also depends on the PI-pressure at the onset of unloading, p_U ; however, p_U is fixed for all tests in this study, and is not included as a variable in the expression of f_U in Eq. 3.4. Considering that the indenter radius effect on the plastic sinking process is negligible, expression (4) can be further reduced to

$$\bar{p} = \hat{f}_K(\bar{h}_p, \frac{H}{D}, \frac{\sigma_Y}{E_m}, m, \frac{\tau_0}{E_m}, \frac{\sigma_0}{E_m}, \frac{\delta_c}{D}) \quad (3.5)$$

for fixed values of elastic properties, where $\bar{p} = \frac{p}{\sigma_Y}$ and $\bar{h}_p = \frac{h_p}{D}$.

In each particle nanoindentation test, we get an indentation curve of $\bar{p}$ versus $\bar{h}_p$ for the particle aspect ratio (H/D), the matrix properties (σ_Y, m) and the interface

properties $(\tau_0, \sigma_0, \delta_c)$ fixed in Eq. 3.5. If the parameters, $\sigma_Y, m, \tau_0, \sigma_0, \delta_c$, were known a priori, then a finite element simulation model could be used to simulate the experimental relationship between $\bar{p}$ and $\bar{h}_p$ for various H/D . Instead, our objective is to extract the material properties, $\sigma_Y, m, \tau_0, \sigma_0, \delta_c$, using the curves of $\bar{p}$ versus $\bar{h}_p$ for various H/D . Determining the materials properties simultaneously by fitting experiments and FEM simulations is essentially a challenging inverse problem to search for the solution in a large parameter space. However, we found that the complexity of the inverse problem can be resolved by systematically tracking a reduced search path, based on progressive deformation and failure processes of the test. For a strong interface between the particle and the matrix, the yield PI-pressure, $\bar{p}_Y$, near the onset of plastic sinking (see Fig. 3.5 (a); $\bar{h}_p = 0.001$) is primarily dependent on σ_Y and insensitive to other parameters. Therefore, by carrying out many tests for various H/D ratios and plotting $\bar{p}_Y$ against H/D , Eq. 3.5 can be contracted to a relationship of $\bar{p}_Y = \hat{g}(\frac{H}{D}, \frac{\sigma_Y}{E_m})$. Then, the problem is reduced to search for σ_Y/E_m in a single parameter space. After we get σ_Y/E_m , the hardening index m can be determined by matrix nanoindentation tests. The hardening characteristic of the $\bar{p} - \bar{h}_p$ curve reflects the matrix plastic deformation and the interface slip process, which depends on σ_Y, m , and τ_0 . With σ_Y and m being determined, τ_0 can be assessed by fitting the simulated hardening responses with the experimental ones for various H/D . Once τ_0 is determined, the normal decohesion properties can be extracted through comparison between simulated and experimental unloading responses for various H/D . During unloading, the interface can separate in the normal direction because of large strain mismatch across the interface, which is caused by plastic deformation developed during the preceding loading process.

3.3 Experiment

3.3.1 Experimental procedure

A hypoeutectic A356 cast aluminum alloy containing 7 wt.% Si and 0.3 wt.% Mg, provided by General Motors, was used for the particle nanoindentation tests. The alloy was heat treated under a T6 condition, and hot isostatically pressed (HIP) to eliminate the porosity of the aluminum matrix. Fig.3.1(b) shows an optical image of the cross-sectional microstructure of the alloy. The alloy had a dendritic microstructure that consisted of pro-eutectic aluminum dendrites and eutectic walls containing micron-sized silicon particles. Image analysis showed that on the cross section the equivalent circular diameters of the silicon particles varied from 1 to 11 μm , with their mean value at 3.6 μm . Deep etching of the alloy revealed that the majority of the silicon particles in the alloy had a cylindrical fibrous morphology with random orientations. The aspect ratios of the particles were distributed between 1 and 8.

The nanoindentation samples were prepared as described in the following. The test samples were cut into a plate shape of 12 by 12 by 3 mm, approximate size, with a diamond saw, and hot-mounted in a cylindrical thermoplastic substrates. The sample surfaces were ground with 320- and 600-grit sandpapers, and then polished sequentially with 9 μm , 3 μm and 1 μm diamond suspensions. A fine surface finish of 1.0 nm RMS roughness was obtained by the final step of chemical-mechanical polishing with 20 nm colloidal silica. Between consecutive polishing steps, the sample surfaces were wiped clean with wet cotton balls, rinsed thoroughly with distilled water and then blown dry with clean compressed air. The polished sample surfaces were chemically etched with 10% NaOH solution to make the silicon particles on the surface slightly protrude out of the aluminum matrix. The protruding height of the particles was measured as approximately 350 nm with a tapping mode AFM.

The desirable configuration of the particles for nanoindentation, as shown in Fig.3.1(a), envisions that the particles have their axis vertically aligned to the free surface. This configuration has the geometrical constraint that a particle of a circular cylindrical shape will have the circular cross section exposed on the free surface. Accordingly we selected 41 particles of nearly circular exposed area with 2-4 μm diameters for the nanoindentation test. For each selected particle we ensured that there were no other particles in its neighborhood within a 15 μm radius, to avoid multiple contacts of particles with the indenter tip during nanoindentation of the particle.

A Hysitron Triboindenter (Hysitron, Corp) was utilized for the nanoindentation tests. For the indentation tests, the indenter tip was positioned near the center of the particle top surface with a precision of tens of nanometers, to apply relatively uniform indentation pressure on the particle. The existing studies (Bradby *et al.* 2001, Jang *et al.* 2005, Zarudi *et al.* 2005) on silicon indentation have shown that silicon can plastically deform under large hydrostatic and compressive stresses. In order to preclude plastic deformation of the silicon particles, a blunt spherical sapphire tip of 400 μm radius was used to apply an indentation load up to 2.6 GPa. The silicon phase is known to deform elastically at this stress level (Moser *et al.* 2007).

The load function applied to the silicon particles is plotted in Figure 2(a). It consisted of a loading segment accompanied by eight partial unload-reload cycles, and the final unloading segment. The partial unload-reload cycles were used to make an accurate measurement of the elastic compliance of the nanoindentation system under conditions where the load levels of the cycles were within the range in which the indenter had full contact with the top surface of the particle. The peak load on each particle was varied such that the maximum PI-pressure was fixed at 2.6 GPa for all of the particles tested. The loading and unloading rate of the PI-pressure was

held constant to eliminate any rate-dependent effects. The load versus displacement curve was measured and analyzed for each particle.

Prior to each nanoindentation test, the diameter of each particle was measured using tapping-mode AFM topography. After each test, the 3-D morphology of the indented particle was examined by an optical profiler as the sample surface was incrementally etched with 10% NaOH solution until the particle was detached from the matrix. The incremental depth of etching was gradually varied from $0.24\ \mu\text{m}$ to $0.73\ \mu\text{m}$. The buried depth of the tested particle was taken to be the total etching depth at which it was detached from the matrix. If the indented particle showed a complicated 3-D morphology other than a vertical cylindrical shape, it was excluded for the data analysis. In our tests, 17 out of 41 indented silicon particles were useful for the nanoindentation data analysis.

3.3.2 *Experimental results*

Fig. 3.2 shows the PI-pressure versus displacement curves of three particles with different aspect ratios of 2.10 (Particle 1), 0.76 (Particle 2) and 0.45 (Particle3). The indentation responses of the three particles are elastic under small indentation loads, during the loading stage. For higher indentation loads, the partial unload-reload segments of the three curves do not coincide with the monotonic loading portions due to unrecoverable sinking-in of the particles, which indicates plastic deformation of the aluminum matrix and/or Al/Si interface slip. The three curves show different yield PI-pressures and display distinct hardening characteristics for their sinking-in processes. Particle 1 shows a higher yield PI-pressure and steeper hardening compared to the other two particles with shallower aspect ratios. The gentle hardening of the indentation curves of Particles 2 and 3 results in larger plastic sinking-in displacements.

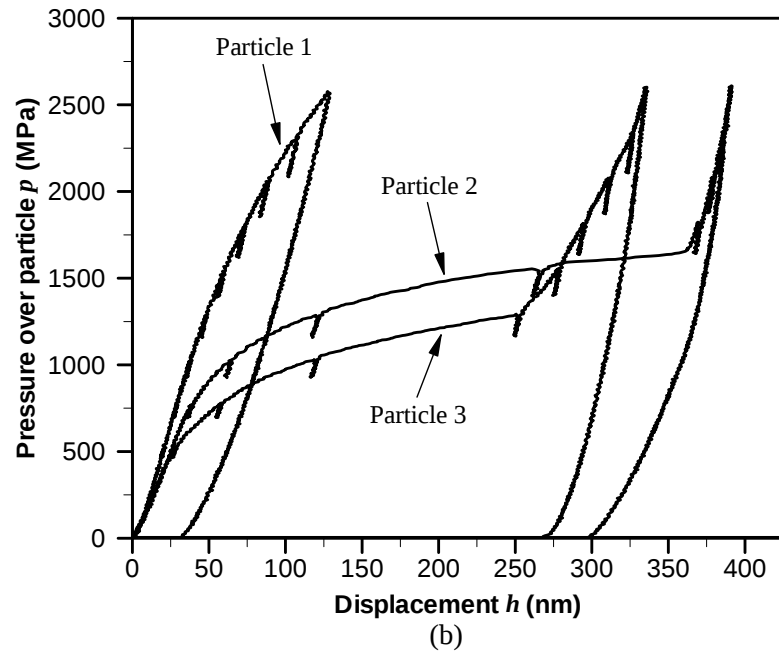
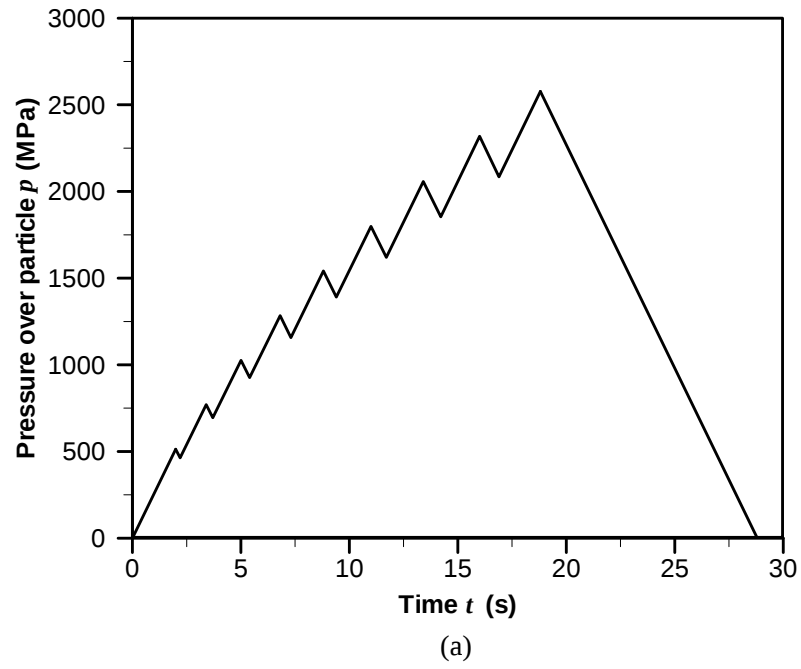


Figure 3.2: (a) The indentation load function applied on the silicon particles; (b) Indentation curves of three particles with different H/D of 2.10 (Particle 1), 0.76 (Particle 2) and 0.45 (Particle 3).

A sharp increase in the indentation stiffness of Particle 2 is found at a PI-pressure of 1.6 GPa. The stiffness increase occurs at a displacement of about 360 nm, which is slightly larger than the original exposed height of the particle. On the other hand, the sudden stiffness increase of Particle 3 occurs at a displacement of 250 nm, which is smaller than the original exposed height of the particle. After the sudden increase, the tangential stiffness of Particle 3 is smaller than that of Particle 2. The sudden stiffness increases are believed to be caused by contacts of the indenter tip with the sunk-in aluminum matrix for the deep particle 2, and the piled-up aluminum matrix for the shallow particle 3. This speculation is verified by the post-indentation AFM topographic images of the particles and the near-by substrate surface elevations.

Fig 3.3 (a)/(b), and (c)/(d) show the AFM topographies of Particles 2 and 3 before and after the test, respectively. In both cases, the surfaces of the particles were above the aluminum surface by about 350 nm before the test. After the nanoindentation test, the particles fully sank into the matrix, with their top surfaces close to the level of the matrix surfaces, as shown in Fig 3.3(b) and (d). Aluminum sinking-in around Particle 2 is evident in Fig 3.3(b); aluminum pile-up caused by indentation is observed for Particle 3 in Fig 3.3(d). Sinking-in of the matrix would delay contact between the tip and the substrate surface for particle 2. Aluminum pile-up around Particle 3 would promote an early-stage contact of the tip with the piled-up region. Consequentially, for a given sinking-in displacement increment, the smaller contact area increase between the tip and the piled-up region would result in a smaller indentation stiffness for Particle 3, than for Particle 2. Among the 17 particles examined, 13 particles fully sank into the matrix, while the other four still protruded out of the matrix by some height after nanoindentation. For the 13 fully sunk particles, we used the portion of the loading below which the tip began to touch the matrix for the load-displacement characterization.

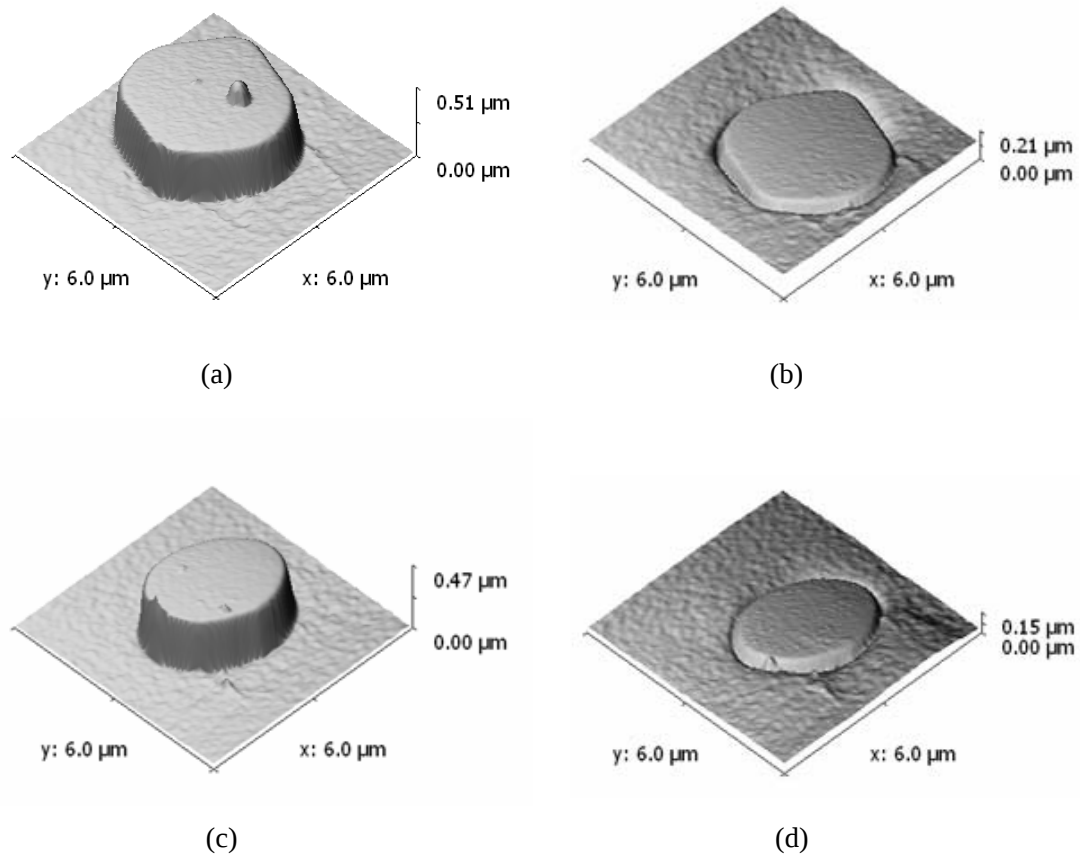


Figure 3.3: AFM images of Particle 2 before (a) and after (b) indentation and Particle 3 before (c) and after (d) indentation. The small bump on the top surface of Particle 2 before indentation was a cluster of colloidal silica particles. It was removed from the top surface before nanoindentation test by rubbing the surface with the indenter tip.

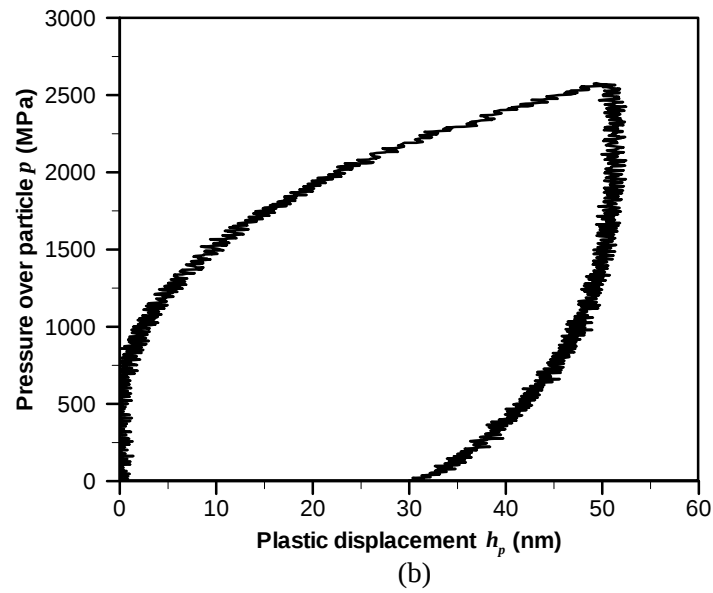
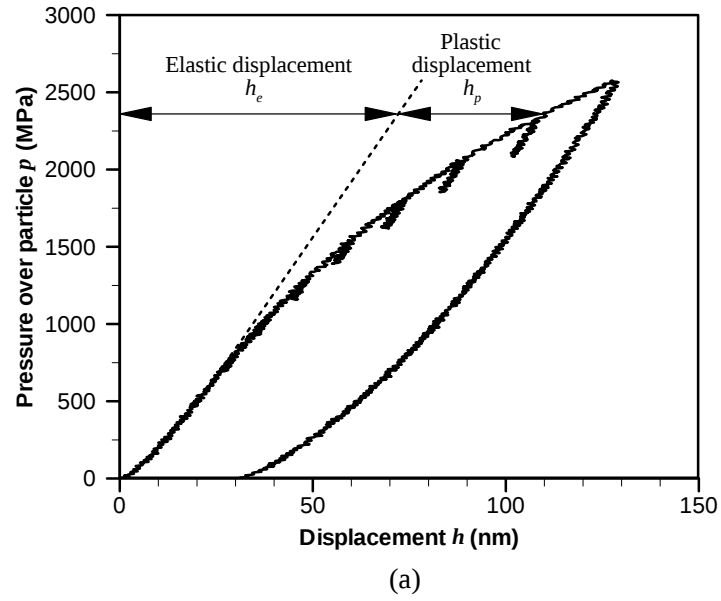


Figure 3.4: (a) Decomposition of the total indentation response of Particle 1 into the elastic and plastic parts; (b) Plastic indentation response of Particle 1 after subtraction of the elastic part.

The indentation curves were analyzed by first removing the elastic response from the raw data, based on Eq. 3.2. To identify the elastic response, the three parameters a , b and P_c in Eq. 3.3 were evaluated by the best fit of Eq. 3.3 with the initial part of the elastic indentation response and the elastic compliance of the partial unload-reload cycles. As an example, the dashed curve in Fig 3.4(a) shows the calculated curve of PI-pressure versus elastic displacement for Particle 1.

The curve of PI-pressure versus plastic displacement, after subtracting the elastic part, is plotted in Fig 3.4(b). The traces of the partial unload-reload cycles were also removed in this plot. Fig 3.4(b) shows that there is no plastic displacement at PI-pressures less than a critical value of 750 MPa. Beyond the critical PI-pressure, plastic sinking occurs with work hardening. The hardening behavior can be approximately represented with three fitting parameters (p_0 , B and n), as a reduced form of Eq. 3.5;

$$p = p_0(\bar{h}_p/B + 1)^n \quad (3.6)$$

Fig 3.4(b) shows that the early part of the unloading response is elastic, and when the PI-pressure drops below 1500 MPa, the plastic displacement reverses as the load decreases. Similar reverse plastic displacements have been observed during unloading for all four particles which partially protruded out of the matrix after unloading. The reverse plastic displacements are considered to be caused by interface separation in opening mode during the unloading process.

As marked on the representative load-displacement trace in Fig 3.5(a), each load-displacement ($p - \bar{h}_p$) curve can be characterized by three quantities, which are the yield PI-pressure $p_Y = p(\bar{h}_p = 0.001)$, the hardening index n , and the reverse-yield PI-pressure drop Δp for $\Delta \bar{h}_p$ at the onset of reverse yielding. These three quantities are plotted as functions of particle aspect ratio H/D in Fig 3.5(b)-(d). Fig 3.5(b)

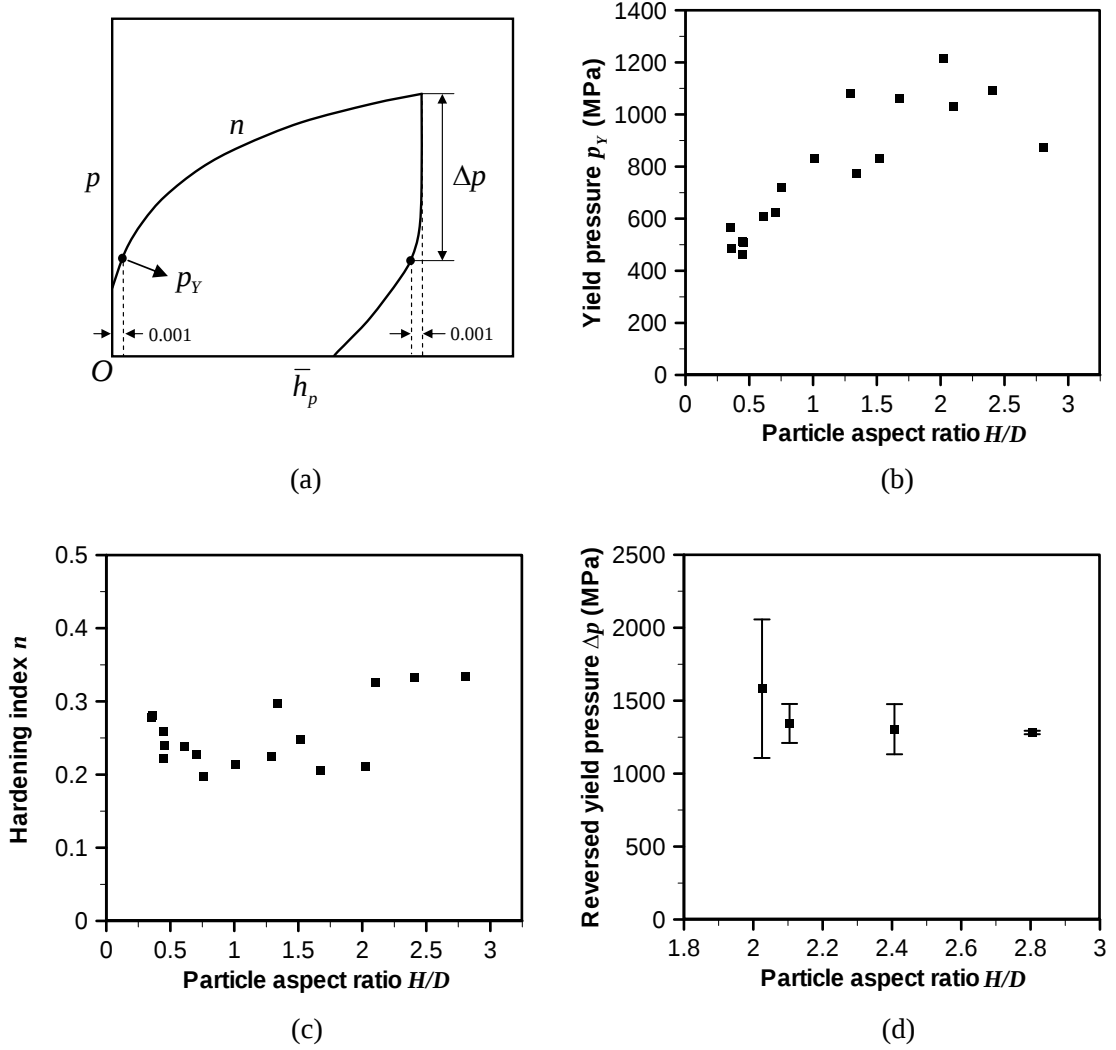


Figure 3.5: (a) Characterization of $p - \bar{h}_p$ curves by three quantities, the yield PI-pressure, p_Y , the hardening index, n , and the reverse-yield PI-pressure drop, Δp . Experimental relationship of (b) yield PI-pressure versus particle aspect ratio; (c) hardening index versus particle aspect ratio; (d) reverse yield PI-pressure versus particle aspect ratio. The error bars in (d) are given by varying the fitting range of the unloading portion for the elastic displacement calculation.

shows that the yield PI-pressure increases as the particle aspect ratio H/D increases. It appears that the yield PI-pressure asymptotically reaches about 1200 MPa for H/D larger than 1.8. Fig 3.5(c) shows that as H/D increases, the hardening index first decreases, and then increases with some scatter. The minimum hardening index occurs around $H/D = 1$. As shown in Fig 3.5(d), the reverse-yield PI-pressure drop is insensitive to H/D and is about 1300 MPa for the four silicon particles partially protruding out of the matrix after nanoindentation.

3.4 *Finite element analysis*

3.4.1 *Finite element model*

Parameteric studies with finite element analyses were carried out to identify underlying micro mechanisms and material properties responsible for the particle indentation characteristics measured experimentally as a function of the particle aspect ratio H/D . As elaborated in Section 3.2, isotropic elasticity and the J_2 flow theory of plasticity with isotropic power-law hardening were employed for the FEM analyses. The Al/Si interface failure processes were simulated with the NILS-CZM as described by Eq. 3.1. While simulation of sub-micron scale plastic deformation could have required modeling based on non-classical theories such as strain gradient plasticity or discrete dislocation algorithms, the length scale of the plastic strain gradient in our particle indentation simulation was sufficiently large so that the classical continuum plasticity could provide ample accuracy in the simulation analyses.

The particle nanoindentation was modeled as an axisymmetric problem with linear quadrilateral elements in ABAQUS. The silicon particle was treated as a round-end cylinder with a fixed diameter of 4 μm and various buried depths of H/D . The

aluminum substrate was also of cylindrical shape of 400 μm diameter and of 300 μm height. The mesh size along the Al/Si interface was 50 nm. The bottom of the substrate was subjected to a fixed displacement boundary condition. The same load function as the one used in the experiment was applied on the particle in the simulation. We used a 400 μm radius indenter in the experiment; however, the silicon particle had approximately 100 μm radius of curvature at the top surface. Therefore, we used the equivalent indenter radius of 80 μm for the flat top silicon model employed in the FEM analysis. The Youngs moduli and Poissons ratios of the materials were 112 GPa and 0.28 for silicon, and 70 GPa and 0.33 for aluminum. The flow stress and the hardening exponent, m , of aluminum were varied and determined through the comparison of the simulation results with the experimental ones.

3.4.2 Finite element analysis with a perfectly bonded interface

As discussed in Section 3.2.2, for a strong interface the relationship between the yield PI-pressure p_Y and the particle aspect ratio H/D is primarily determined by σ_Y . With the assumption that the interface was perfectly bonded, we first performed a series of FEM simulations with different yield stresses σ_Y . Fig. 3.6 shows the simulated relationship between p_Y and H/D for three different yield stresses, together with the experimental data points. The computational curve of versus is best fitted to the experimental data points for a value of $\sigma_Y = 160$ MPa. With the matrix yield stress known, the hardening exponent m was then determined to be 0.3 by carrying out nanoindentation tests of the matrix with a Berkovich tip and comparing the experimental load-displacement curves with a series of FEM simulation curves.

Fig. 3.7 shows contour plots of the Von Mises stress distribution simulated with

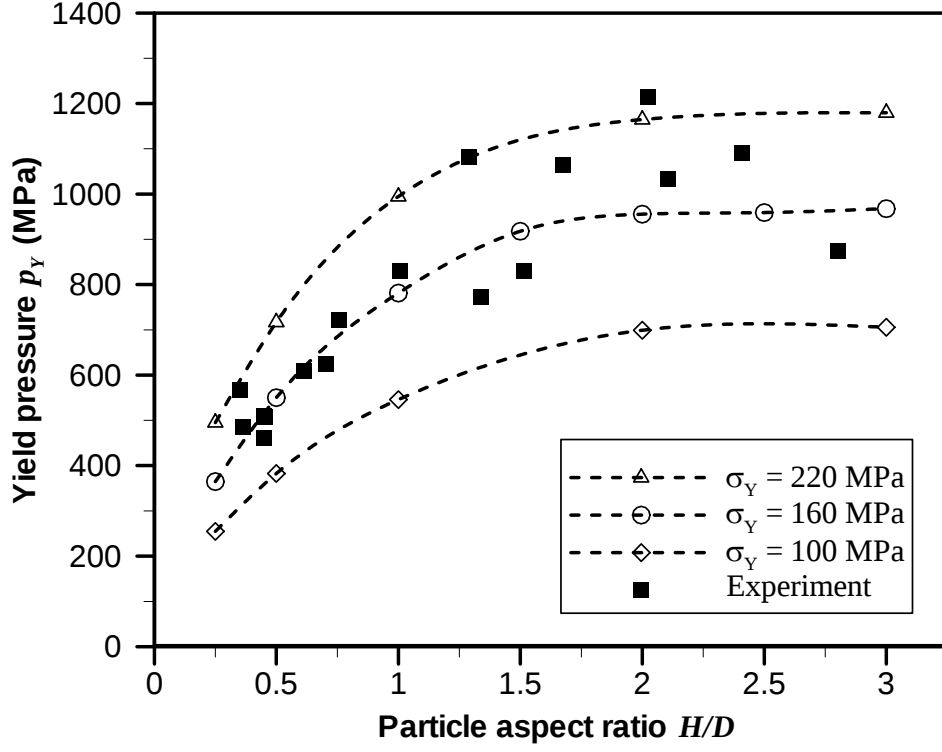


Figure 3.6: Comparison of the yield PI-pressure versus particle aspect ratio between experiment and simulation.

$\sigma_Y = 160$ MPa and $m = 0.30$ for three particle ratios of $H/D = 0.25$, 1.0 , and 3.0 at different indentation stages. For $H/D = 0.25$, the plastic flow initiates near the bottom end of the particle. Then, the boundary of the plastic deformation expands towards the (top) free surface as well as in the direction of the substrate bottom as the load increases. After full unloading, a shallow and widespread zone of residual stresses is observed around the particle. For $H/D = 1$, the zone of plastic deformation develops along the whole interface region simultaneously. After unloading, the residual stress in the aluminum matrix is mostly localized at the intermediate region between the side-wall side and the bottom side of the particle. For $H/D = 3$, the near-interface

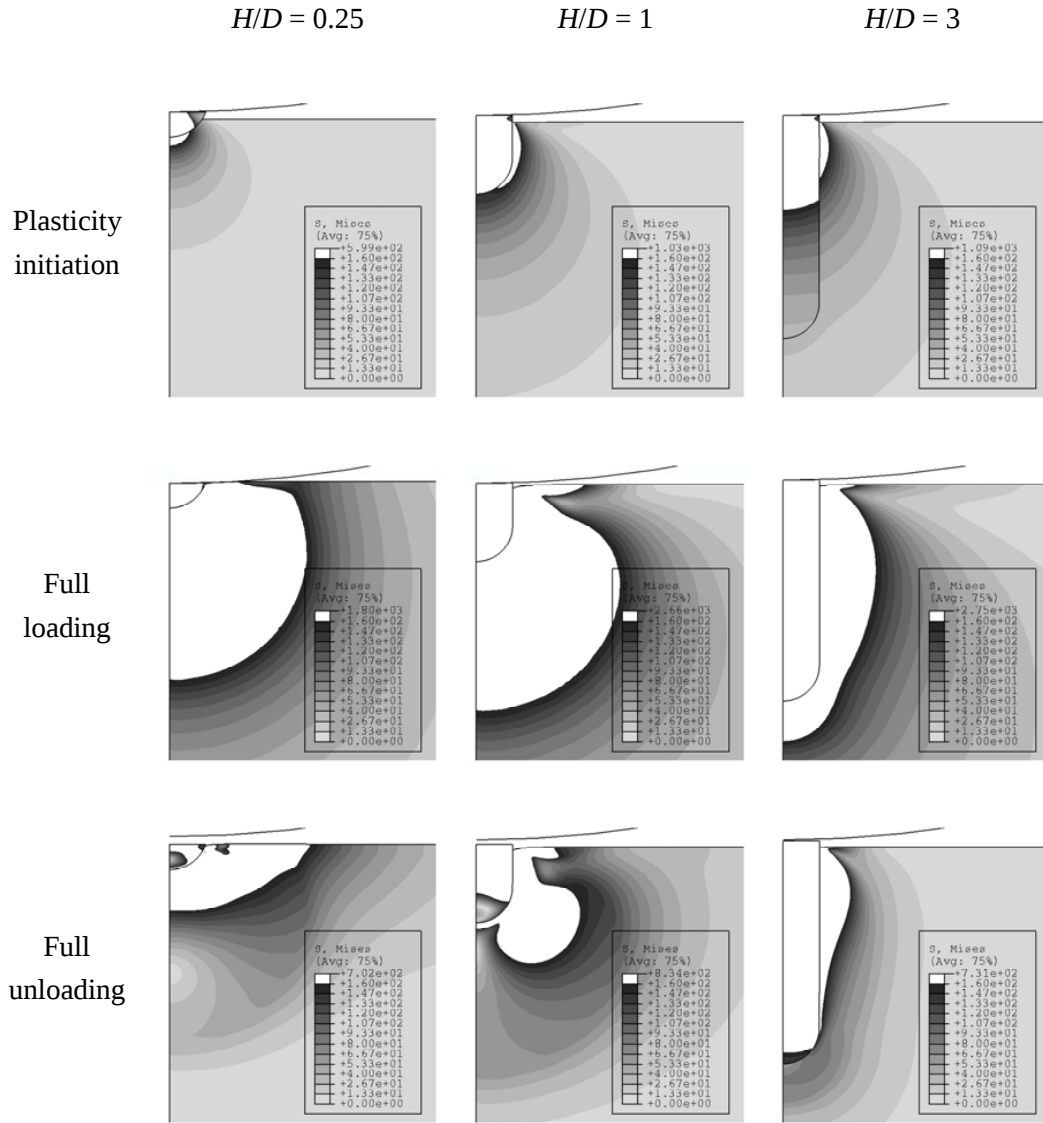


Figure 3.7: Contour plots of the Von Mises stress with a perfectly bonded interface.

zone of the matrix close to the (top) free surface yields first, and then the region of active plastic flow propagates towards the bottom of the particle along the interface. Once it is unloaded, the zone of high residual stress is localized near the interface. The results of the FEM analysis shows that aluminum piles up for the shallow particle of $H/D = 0.25$, but not for the other two particles of larger H/D , which is consistent with the experimental observations in Fig. 3.2(b) and Fig. 3.3.

Using $\sigma_Y = 160$ MPa and $m = 0.3$ for the aluminum matrix, we initially carried out FEM analyses with the assumption of perfect interface bonding to get the indentation hardening index n for various H/D . The computational result, the dashed line with upper triangles in Fig. 3.8, is compared with the experimental data. The comparison shows that the computational hardening indexes are substantially different from the experimental ones over the whole H/D range of interest. The discrepancy is considered to be caused by interface failure, primarily slip, during the loading stage.

3.4.3 *Finite element analysis with interface failure*

The NILS-CZM, as described by Eq. 3.1, was implemented into the FEM to simulate interface slip and decohesion processes. During the loading stage at large indentation loads, both the matrix plastic deformation and the interface slip contribute to the plastic response of particle indentation. Fig. 3.8 shows the simulated curves of n versus H/D for three shear strengths $\tau_0 = 160, 240$, and 320 MPa of the NILS-CZM. The normal strength σ_0 and critical separation δ_c do not play a role for simulating the indentation response during loading stage. For simulation of the response during unloading stage, σ_0 and δ_c are determined by Eq. 3.9 and 3.10 in Appendix B. Compared to the case of a perfectly bonded interface, the particle indentation response with finite shear strength of the interface displays less hardening due to the

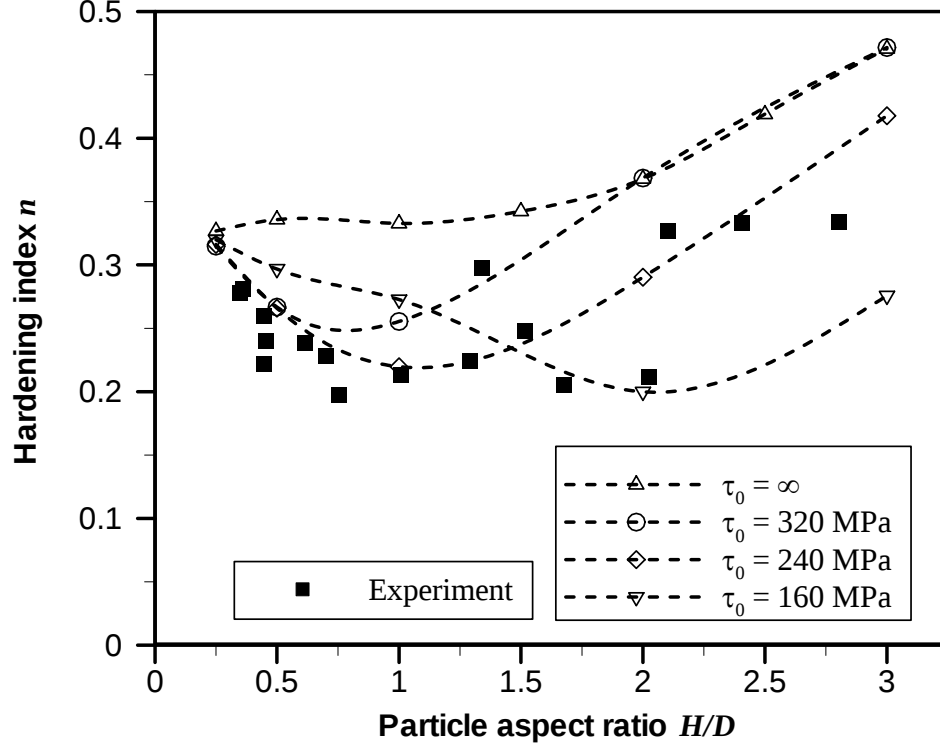


Figure 3.8: Comparison of the hardening index versus particle aspect ratio between experiment and simulation.

interface slip. For small H/D , the indentation plasticity is mostly dominated by the bottom plasticity, and is hardly affected by the interface slip. As H/D increases, the interface slip starts to play an important role in hardening of the indentation response. Interface slip makes the indentation hardening index n drop substantially from the value obtained with the assumption of perfect Al/Si bonding. With the interface shear strength of $\tau_0 = 240$ MPa, the simulated n - H/D curve shows the minimum hardening at the same $H/D \approx 1$ as the experiment, and fits the trend of the experimental data reasonably well. Comparing the n - H/D curves for $\tau_0 = 240$ MPa and perfectly bonded interface, the largest drop of hardening index also occurs

at $H/D \approx 1$. This indicates that the interface slip plays the most significant role in deterioration of indentation hardening for intermediate values of H/D around 1.

During the loading stage, a particle of large aspect ratio (i.e., $H/D > 0.5$) has a Poisson expansion in the lateral direction under the longitudinal compressive load. The Poisson expansion induces extensional plastic strain of the matrix in the hoop direction near the interface. Therefore, during unloading, the elastic radial contraction of the particle results in a tensile stress across the sidewall interface, which can drive the interface decohesion in the opening mode. The decohesion process is also modeled with NILS-CZM of Eq. 3.1.

When NILS-CZM is used, the cohesive zone characteristic sizes are typically different for the opening and shear modes. The FEM model analyses show that during the loading stage the normal stress on the interface is compressive near the stress concentration site, and that a relatively large slipping cohesive zone develops along the interface without formation of an opening cohesive zone. Formation of the slipping cohesive zone represents the interface slip part of the particle sinking. During the unloading stage, both opening and slipping cohesive zones are developed; however, the fracture process is still shear dominated. Since the critical separation of the opening fracture process zone (FPZ) is limited by several atomic bond lengths, the size of the opening cohesive zone is considered to be on the order of 1 nm. On the other hand, the critical slip distance is typically much larger than the critical opening separation for a mixed-mode but shear-dominated interface fracture process, and the slipping zone size is much larger than the opening one. In our indentation simulation, the slipping zone size was larger than the FEM mesh size (50nm) for both loading and unloading stages, while the opening zone size was much smaller than the mesh size.

In finite element simulations, the opening or slipping mechanisms of the finite

element cohesive zone associated with crack growth is limited by the deformation kinematics of the displacement shape function and the element size. If the size of the finite element cohesive zone (FE-CZ) is smaller than the intrinsic cohesive zone size, the finite element simulation can follow the local intrinsic cohesive zone behavior and the FE-CZ constitutive relationship should be the same as the intrinsic cohesive zone law. However, if the FE-CZ size is larger than the intrinsic cohesive zone size, the FE-CZ constitutive relationship should converge to a linear softening cohesive zone law, with the cohesive zone strength scaled by the finite element size. A more detailed description of the scale dependent FE-CZ constitutive relationship, which is based on the equivalent global energy release rate for intrinsic crack growth and the FE-CZ opening process, is presented in the Appendix.

Fig. 3.9 shows the σ_{11} and σ_{12} contour plots for a particle of $H/D = 2.5$ for an opening mode toughness of 0.05 J/m^2 at different PI-pressures during unloading. The plot shows that a mixed-mode interfacial crack is initiated near the free surface at a PI-pressure of $p = 1260 \text{ MPa}$. As the PI-pressure decreases, the crack propagates downwards along the interface, making the top surface of the particle protrude back out. With the normal FE-CZ strength scaled with the mesh size, the FEM simulations show that the reverse yield PI-pressure drop, Δp , is determined by the opening mode fracture toughness, Γ_n . As shown in Fig. 3.10, the pressure drop, Δp , increases as Γ_n increases. The comparison between the simulation and experimental results gives an estimate of the mode I toughness of 0.05 J/m^2 and the total toughness of 0.25 J/m^2 .

3.5 *Discussions*

In this study we have used nanoindentation experiments combined with finite element analyses to measure the matrix and interface properties, such as matrix yield

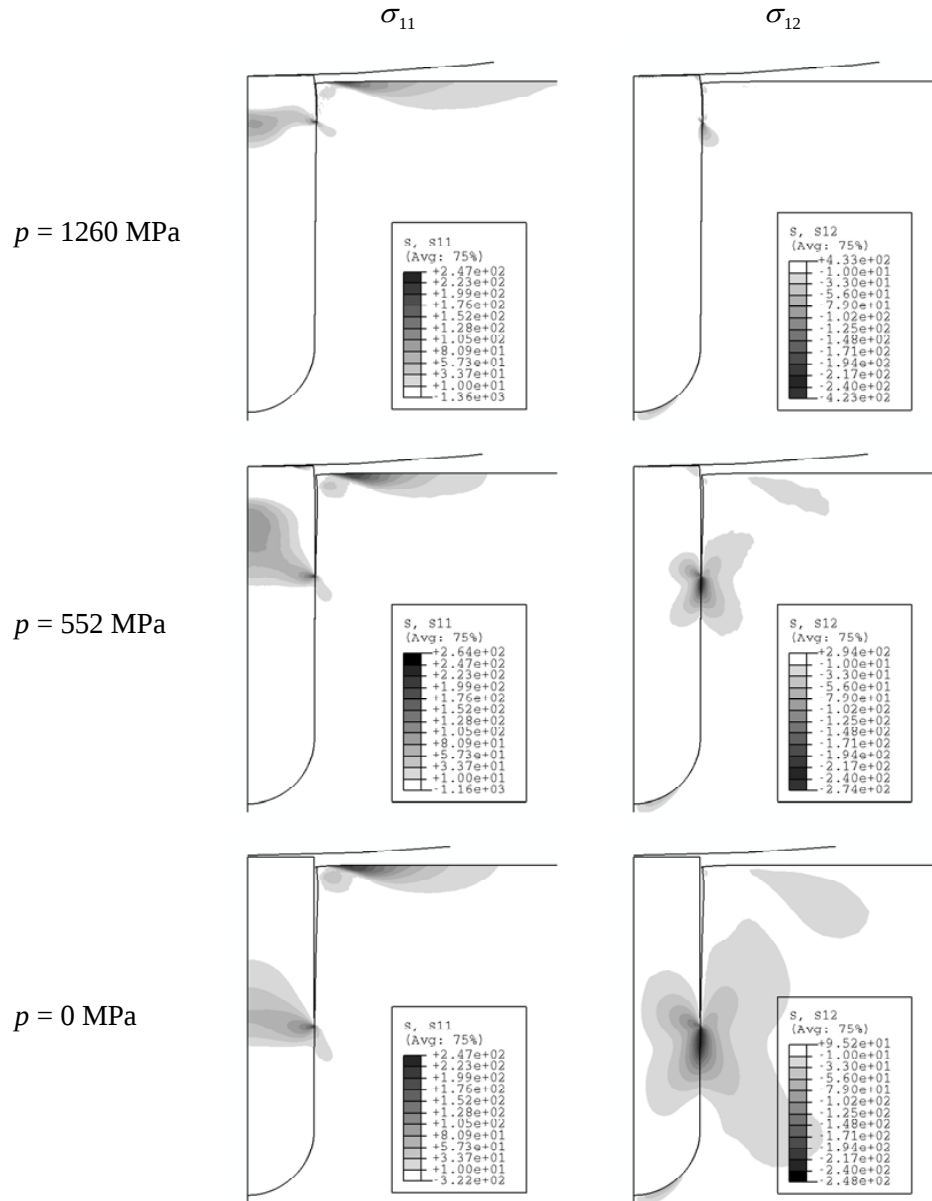


Figure 3.9: Contour plots of σ_{11} and σ_{12} of particle indentation ($H/D = 2.5$) simulated with NILS-CZM during unloading (10x magnification of the displacement in the radial direction).

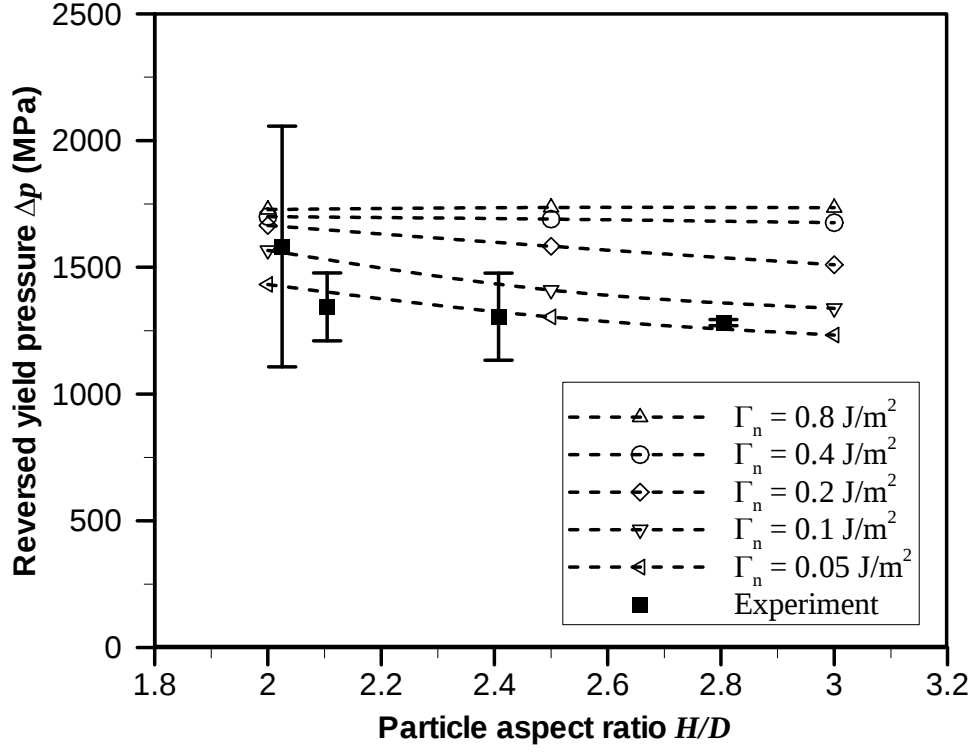


Figure 3.10: Comparison of reverse yield PI-pressure versus particle aspect ratio between experiment and simulation.

stress, hardening index, interface shear strength and toughness, in a metal matrix composite, the cast A356 alloy. For this alloy we have determined the yield stress of the aluminum matrix σ_Y to be about 160 MPa, the Al/Si interface shear strength, τ_0 , to be around 240MPa, and the interface fracture toughness, Γ_0 , to be approximately 0.25 J/m². We have employed isotropic properties of aluminum and the interface toughness in the FEM analyses. Considering that the intrinsic matrix and interface properties are locally anisotropic, the values presented in this work were determined in an average sense. In each nanoindentation test of a single particle, the indentation response fluctuates and gives rise to scatter of the experimental data points,

Table 3.1: Comparison between the material properties measured in the current work and the atomistic estimations

	Current work	Atomistics ^a	Atomistics ^b
Matrix yield stress σ_Y (MPa)	160 ± 6	N/A	N/A
Hardening m	0.3	N/A	N/A
Shear Strength τ_0 (MPa)	240 ± 6	318-1172	N/A
Fracture toughness Γ_0 (J/m ²)	0.25 ± 0.03	0.66-1.73	15
Normal Strength σ_0 (GPa)	0.247 (CZM)	3.9-7.4	22

^aWard, Curtin and Qi (2006), Ward, Curtin, WA and Qi (2006), Noreyan *et al.* (2008)

^bGall *et al.* (2000)

as in Fig. 3.5 (b)-(d), due to the crystal-orientation dependence and other factors like irregular particle geometry. Therefore the estimation of material properties is inaccurate when the response characteristic of only a single particle is considered. However, we took multiple particle responses into account, and the estimation error was believed to be substantially reduced in the isotropic analysis. In Fig. 3.6, Fig. 3.8 and Fig. 3.10, each material property is incrementally varied in the FEM simulations to fit the experimental data points for various aspect ratios, H/D . We estimated the error of each measured property to be 10% of the corresponding increment. The corresponding final values of the measurement with the estimated errors are $\sigma_Y = 160\pm6$ MPa, $\tau_0 = 240\pm6$ MPa and $\Gamma_0 = 0.25\pm0.03$ J/m².

Microscopic material properties were measured at the nanometer scale in the current work. Although the length scale of the current experiment is small, the maximum strain gradient is relatively small due to the relatively weak interface strength, so that the use of strain gradient plasticity theory is not needed. Instead, the use of NILS-CZM together with mode-decoupled scaling provided a relatively accurate assessment of the interface strength at the atomistic length scale. The measured properties are compared with atomistic simulations. Table 3.1 lists the comparison between the measured material properties by this work and the atomistic simulation results given

by Gall et al. (Gall *et al.* 2000) and Qi et al. (Ward, Curtin and Qi 2006, Ward, Curtin, WA and Qi 2006, Noreyan *et al.* 2008). Gall et al. have shown that the tensile strength of the Al(001)||Si(001) interface is 22 GPa and the fracture toughness of the interface is 15 J/m², with a modified embedded atom method (MEAM) potential. With an improved MEAM potential and reduced strain rate, Qi et al. performed atomistic simulations for both test configurations of pure tensile (Ward, Curtin and Qi 2006, Ward, Curtin, WA and Qi 2006) and pure shear (Noreyan *et al.* 2008). They have shown that depending on the crystal orientation the fracture toughness and tensile strength are 0.66-1.73 J/m² and 3.9-7.4 GPa, respectively, and that the shear strength, which is also dependent on the sliding direction, is 0.32-1.17 GPa.

The tensile cohesive zone strength used in the FEM simulations (247 MPa) is one order of magnitude lower than the intrinsic tensile strength of the atomistic estimation (3.9 GPa and up) because the mesh size of the FEM simulations (50 nm) is much larger than that of the intrinsic tensile cohesive zone at the atomistic length scale. The comparison of the tensile strength requires proper scaling as discussed in the Appendix. On the other hand, the measured values of shear strength (240 MPa) and fracture energy (0.25 J/m²), although consistently lower, are of the same order of the mean values of the atomistic calculations by Qi et al. The shear strength estimated by the NILS-CZM is believed to be representative of the atomistic scale shear strength, since the shear cohesive zone size is much larger than the FEM mesh size and thus the FEM analyses could resolve the shear strength of the cohesive zone.

The fracture toughness of 0.25 J/m² is lower than the estimation of the atomistic simulations, and may be explained as follows. The solid Al/Si interface was formed during the solidification process of the cast Al-Si alloy at the eutectic melting point. High resolution TEM observation (Kim *et al.* 2001) reveals that the Al/Si interface in this type of cast Al-Si alloys has an initial atomic structure that is free of defects.

Therefore interface weakening is not likely due to segregation of defects or contamination. Instead, we propose that the weakening is induced by dislocations formed near the interface during the sliding process that were not captured by the atomistic simulations. During the interface slip stage, the interface stress distribution may have been roughened by the attack of bulk dislocations from the aluminum matrix. When the interface opens in the unloading stage, the fracture toughness is reduced due to the effect of partial pre-separations of the interface caused by the dislocation-induced interface stress undulation.

The significance of this work is that it provides insight into designing better composites. In this case the Al-Si alloy is intended for load bearing applications where the alloy surface will come in contact with a counterface; it is desirable to minimize direct contact between the counterface and the aluminum matrix, hence the hard phases, notably the Si particles, are exposed to carry the load. This research shows how the microstructure, i.e., the H/D ratio, influences their ability to carry load. It shows that the yield pressure increases as the H/D ratio approaches 1.5, and that it appears to saturate at higher values. This is understood by examining both the experimental data and the FEM results, which show that particles with substantial buried depths all initiate failure with a similar mechanism, plastic deformation of the supporting matrix initiates at the interface adjacent to the free surface. In application, one would prefer to design alloy processing that leads to oriented high aspect ratio particles at the load bearing surface, perhaps through directional solidification. The data also suggests that the hardening index, n , of the indentation has some dependence on the microstructure. The FEM results suggest that there is a continued gain in hardening at high H/D ratios that the experiment may not support. This might be improved by using a more sophisticated constitutive cohesive law during shearing. The hardening and shear strength of the indentation are closely related to the matrix values.

Using the parameters developed in this work, the modeling can now be extended to more complex microstructural features, notably eutectic Si that is not oriented with respect to the surface, or primary Si.

The measurement method presented in this study can be easily extended to other composite material systems for studying microscopic mechanical properties. It also offers a great opportunity to study the effect of microstructure controls, such as impurity segregation at the interface and chemical modification of the reinforcing inclusions, on the microscopic mechanical properties of the composite material systems.

3.6 Chapter summary

The hard particle sinking in processes of an Al-Si alloy caused by a loading and unloading cycle of normal contact has been investigated. In summary:

(1) A hybrid nanoindentation/FEM method has been developed to study the particle suspension resistance and characterize micromechanical properties of micro-particle reinforced MMCs. The method has been applied to investigate microstructural properties of an A356 aluminum alloy. The method is generic and can be extended to other metal matrix composites.

(2) Innovative data reduction procedures for the hybrid method have been established by identifying a generic configuration of particle nanoindentation and tracing the canonical response of the indentation with FEM simulations. The identification of the generic configuration and dimensional analysis of the canonical response provided a remarkably simple method of measuring microscopic properties of MMCs.

(3) The indentation threshold strength is found to be strongly dependent on the aspect ratio, up to 2, of the buried portion of cylindrically shaped particles. The indentation resistance comes from the plastic-flow strength of the matrix and the slip

strength of the interface. The interface is separated during unloading. An element-size dependent FEM cohesive-zone law is used to extract the interface properties; the results compare well with atomistic estimations.

(4) The NILS cohesive zone law has been introduced for the computational modeling of small-scale interface failure. A scaling law of the mesh-size-dependent cohesive zone strength was developed to bridge the intrinsic and finite element cohesive strengths.

(5) The details of particle sinking-in mechanisms and interface failure processes under contact loading have been simulated by finite element analysis with the NILS-CZM. The finite element simulations revealed that the interface slips during the loading stage and opens up during the unloading stage.

(6) The small-scale Al/Si interface properties have been measured for the first time, through the hybrid nanoindentation/FEM method. The measured interface shear strength and interface toughness were found to be of the same order of magnitude as the MEAM atomistic estimations.

Appendix B: Scaling of the exterior finite-element cohesive zone for a Mode I crack growth at the nanometer scale

In this appendix we describe a finite element cohesive zone formalism to simulate the deformation process, as well as the energy variation, caused by opening crack growth at the atomistic level, with relatively coarse finite elements. In this model we imagine that the near tip deformation associated with a cleavage process is elastic, while the dislocation motion at some distance away from the tip provides the background plasticity. In this formalism we assume that the unloading process of the local finite element deformation kinematics, caused by the crack growth, is elastic and can be represented by an energetically equivalent cohesive zone separation process compatible with the finite element deformation kinematics.

For the elastic unloading process of the local finite element, the normal finite element cohesive stress σ_{coh} is taken as the average normal traction along the element edge of length L ,

$$\sigma_{coh} = \frac{1}{L} \int_0^\xi \sigma_{yy}(x) dx \cong \frac{1}{L} \int_0^\xi \sqrt{\frac{\mu\Gamma_0}{(1-\nu)\pi x}} dx = \frac{2}{L} \sqrt{\frac{\mu\Gamma_0\xi}{(1-\nu)\pi}} \quad (3.7)$$

where $\sigma_{yy}(x)$ is the true normal traction at the element edge, Γ_0 is the opening mode fracture energy and ξ is the distance between the crack tip and the front side corner of the element, as shown in Fig. 3.11(b). For a virtual crack propagation distance of $-d\xi$, the virtual energy release $-\Gamma_0 d\xi$ and the virtual cohesive energy increase

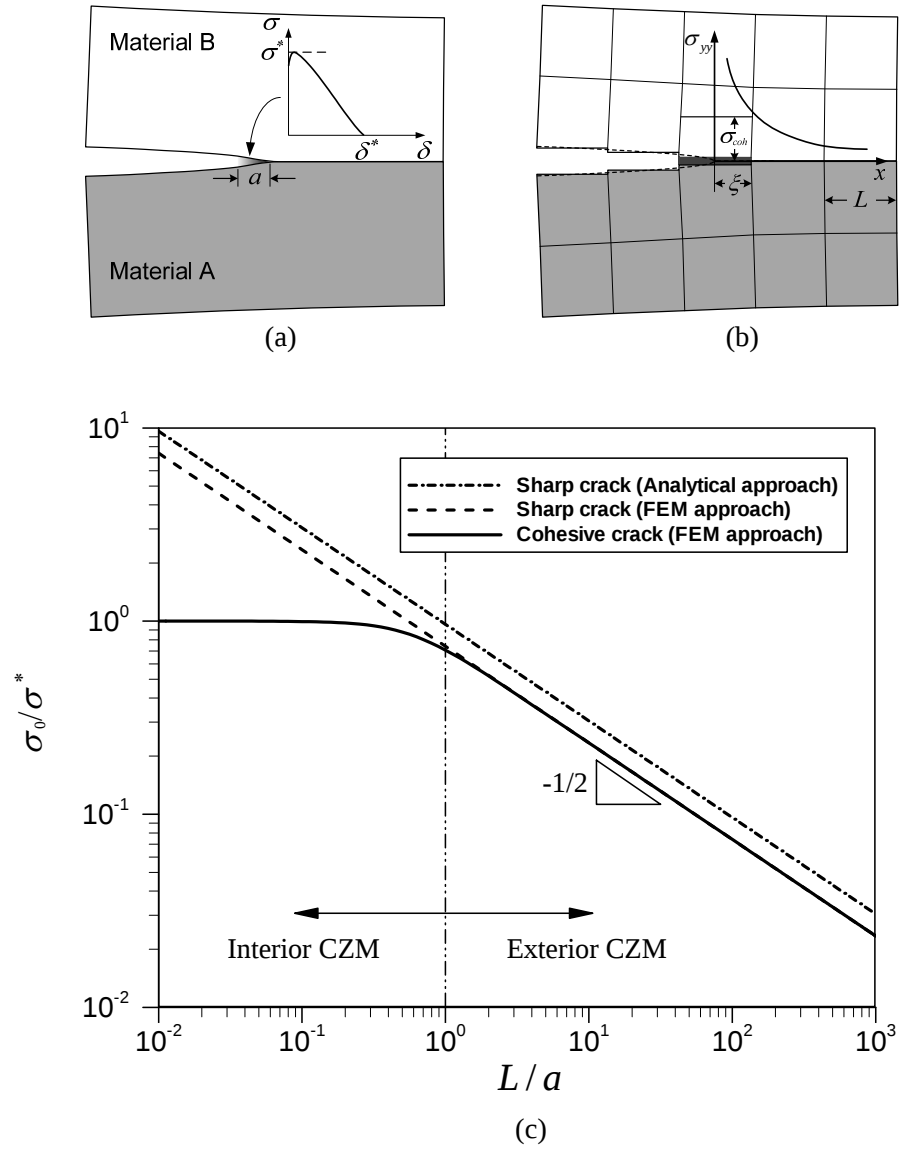


Figure 3.11: (a) A schematic of a Mode I cohesive crack with cohesive length of a ; (b) A model configuration of the exterior cohesive zone model; (c) Scaling law of CZM strength with respect to finite element size.

$L\sigma_{coh}d\delta_{coh}$ must be equivalent. The equivalence provides the relationship

$$\delta_{coh} = \int_L^\xi d\delta_{coh} = - \int_L^\xi \frac{\Gamma_0}{L\sigma_{coh}} d\xi = \sqrt{\frac{\pi(1-\nu)L\Gamma_0}{\mu}} \left(1 - \sqrt{\frac{\xi}{L}}\right) \quad (3.8)$$

Then, by introducing the definitions of

$$\delta_0 = \sqrt{\frac{\pi(1-\nu)L\Gamma_0}{\mu}} \quad (3.9)$$

and

$$\sigma_0 = 2\sqrt{\frac{\mu\Gamma_0}{\pi(1-\nu)L}} \quad (3.10)$$

Eq. 3.8 can be expressed as

$$\sigma_{coh} = \sigma_0 \left(1 - \frac{\delta_{coh}}{\delta_0}\right) \quad (3.11)$$

Eq. 3.11 represents the NILS-CZM for the opening mode. Eq. 3.9 and Eq. 3.10 give the dependence of the critical opening and strength of the NILS-CZM on the finite element size, L . A scaling law similar to Eq. 3.10 was given by Turon *et al.* (2007) by adjusting cohesive strength to allow a minimum number of elements in a cohesive zone. The same form of Eq. 3.11 has been employed by Camacho and Ortiz (1996) to model ceramic fragmentation and by Remmers *et al.* (2008) for the simulation of dynamic crack growth in polymers. However, they have used it as a phenomenological scale-independent cohesive zone constitutive relation for much larger scale fracture processes than the one discussed in this work.

Fig. 3.11(a) shows a continuum representation of a crack growing with an intrinsic cohesive zone of length, a , cohesive strength, σ^* , and critical opening, δ^* . Fig. 3.11(b) shows the finite element kinematics of uniform element separation used to model the crack growth. The finite element size dependent NILS-CZM equations Eq. 3.7 through

Eq. 3.11 were derived for the kinematics of a uniform element separation to make the cohesive zone decohesion process energetically equivalent to the growth of a sharp crack. The dash-dot line in Fig. 3.11(c) shows the element-size dependence of the cohesive zone strength σ_0 . If we employ a linear opening kinematics of the finite element separation, the element-size dependence would follow the dashed line for the growth of a sharp crack and the solid line for the growth of a crack with an intrinsic cohesive zone of length a , as shown in Fig. 3.11(a). When the finite element size, L , is smaller than the intrinsic cohesive zone length, a , the intrinsic cohesive zone constitutive relation is directly used as the finite element cohesive zone law, which is referred to the interior cohesive zone law. On the other hand, if L is larger than a , the finite element cohesive zone strength, σ_0 , and the critical normal separation δ_0 must be scaled by L/a , and the corresponding relationship between σ_{coh} and δ_{coh} is called the exterior cohesive zone law.

The NILS-CZM is strictly applicable to elastic fracture and must be used with caution for elasto-plastic finite element analysis. If the element size is so small that the element-size dependent cohesive zone strength σ_0 becomes larger than the hardening limit, a theory of strain gradient plasticity or a hardening enhancing model must be incorporated to make the analysis meaningful. In our work, the power law hardening index was high enough and σ_0 was within the hardening limit for the element size, so that finite element analysis with the NILS-CZM was believed to provide a sufficiently accurate representation of the crack growth.

Chapter 4

EXPERIMENTAL STUDY ON MICRO-SLIP FRICTION LAWS OF ROUGH SURFACES

4.1 Introduction

The science of friction is sometimes kindly described as a “dirty” field due to its complexity. However it is of great importance in both industry and fundamental research (e.g., earthquake studies), and is drawing increasing attention. A large body of the friction research has been based on empirical studies. The Amontons’ friction law, sometimes called Coulomb’s friction law, is the most well-known constitutive law of friction. This friction law states that the force due to friction is simply proportional to the normal force. Despite widespread acceptance of this classical friction law, there are some important circumstances where the law is not applicable. Dieterich (Dieterich 1978, 1979a) studied experimentally the effect of slip rate on the steady-state behaviors of rock friction. He found that the steady-state friction has a logarithmic dependence on the slip rate. Further, when the slip rate undergoes a sudden change, the friction shows an instantaneous change and evolves to a steady-state value over a characteristic length. This length, which is proportional to surface roughness, is

interpreted as the slip distance required to change the population of asperity contacts. Based on Dieterich's experimental findings, Dieterich (1979b), Rice and Ruina (1983) and Ruina (1983) developed a rate- and state-dependent friction law, which has been widely used in the geological science community to model earthquakes. Prakash and Clifton (Prakash and Clifton 1993, Prakash 1998) investigated the dynamic friction response of a metal plate against a cutting tool material with plate-impact experiments. Their work revealed a pressure history dependent friction law: the frictional stress does not change instantaneously for a sudden change in normal pressure and has a memory of normal pressure history.

More recently it was discovered that, the Amontons' friction law has posed some difficulty in handling certain problems, even based on pure theoretical consideration. It has been shown (Renardy 1992, Adams 1995) that, for two dissimilar elastic half-spaces with Amontons' friction interaction, any small interfacial disturbance can grow unstably for a large combination of material properties and friction coefficients. This non-physical phenomenon arises from the fact that the problem itself is ill-posed. A possible correlation of the ill-posedness with the existence of a generalized Rayleigh wave was proposed by Adams (1995). Following Adams' work, Ranjith and Rice (2001) performed a perturbation analysis and proved the connection between the ill-posedness and the generalized Rayleigh wave. They also showed that the ill-posedness could be regularized by replacing the Amontons' friction law with the one proposed by Prakash and Clifton (Prakash and Clifton 1993, Prakash 1998).

A clear understanding of friction is still lacking in spite of extensive studies. Further experiments and analyses are needed to explore the frictional behaviors and their underlying mechanisms. It is noted that the existing experiments for friction studies have several drawbacks. In these experiments, both the load and displacement are

monitored at a location far from the interface where the actual slip occurs. The displacement measurement at the far field is believed to be quite inaccurate, because the compliance of the system results in an extra displacement which can be on the same order of the characteristic slip distance being examined. Moreover, the typical test configurations used in these experiments, such as pin-on-disk, block-on-block and ring-on-block, impose a spatially inhomogeneous distribution of traction and slip within the contact area. Nevertheless, a uniform distribution is generally assumed for the calculation of normal and frictional stresses and slip distance. The experimental results obtained with such an assumption can be problematic, since the slip characteristics (e.g., instability) can be governed by the actual distribution of traction and displacement.

In this work, a novel experimental framework is developed to address the issues listed above. The frictional behaviors of two contacting rough surfaces are studied with direct optical measurement close to the interface. A localized interface shear zone is formed with a specially designed test configuration. The displacement field around the shear zone is measured using an electronic speckle pattern interferometer (ESPI), owing to its unique features of non-contact, full-field and high-sensitivity measurement. The distributions of traction and displacement along the interface, in both normal and tangential directions, are calculated from the displacement field and combined to yield the friction law of the interface. It is discovered that, the contacting surfaces have an apparent penetration under normal load due to the existence of a compliant roughness layer, and when the interface is subjected to shear load, a slip precursor displacement exists before the frictional stress reaches the value predicted by Amontons' friction law.

The remainder of this chapter is organized as follows. The experimental setup and procedures are described in Section 4.2. The experimental results, including

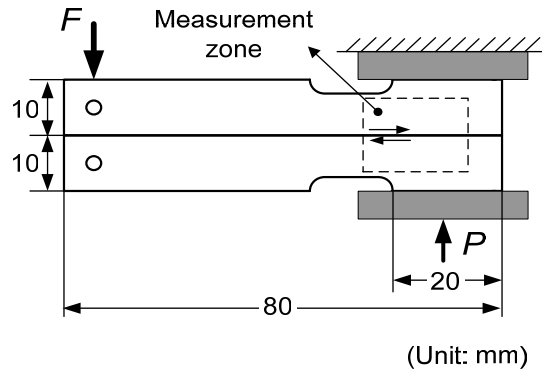
nontrivial data processing procedures, are presented in Section 4.3. The implications of the experimental findings are discussed in Section 4.4. Concluding remarks of this chapter are summarized in the final section.

4.2 *Experimental procedures*

The quasistatic micro-slip friction law of rough surfaces is investigated with direct optical measurement close to the interface. The quasistatic frictional process is usually accompanied with unstable dynamic slip propagation. To overcome this problem, a test configuration as shown in Fig. 4.1(a) is adopted. A portion of the two slender specimen beams are slightly thinned close to one end, at which the beams are clamped together by a grip with a normal load, P . The pressure along the interface is uniformly distributed in the middle of the clamped region, and gradually decays to zero towards the thinned section. When a transverse point force, F , is applied at the other far end, a shear zone is formed at the thinned section by beam bending. As F increases, the slip propagates into the clamped section, but will eventually be suppressed due to the increase of normal pressure. In this manner, the steady state of the slip can be maintained at different load levels. Thus a quasistatic optical measurement is possible.

ESPI, utilizing a four-step phase shifting technique, is used for the measurement of displacement fields. Its principle can be briefly summarized as follows. For a rough surface illuminated with two coherent light beams, the light intensity distribution of the speckle image is

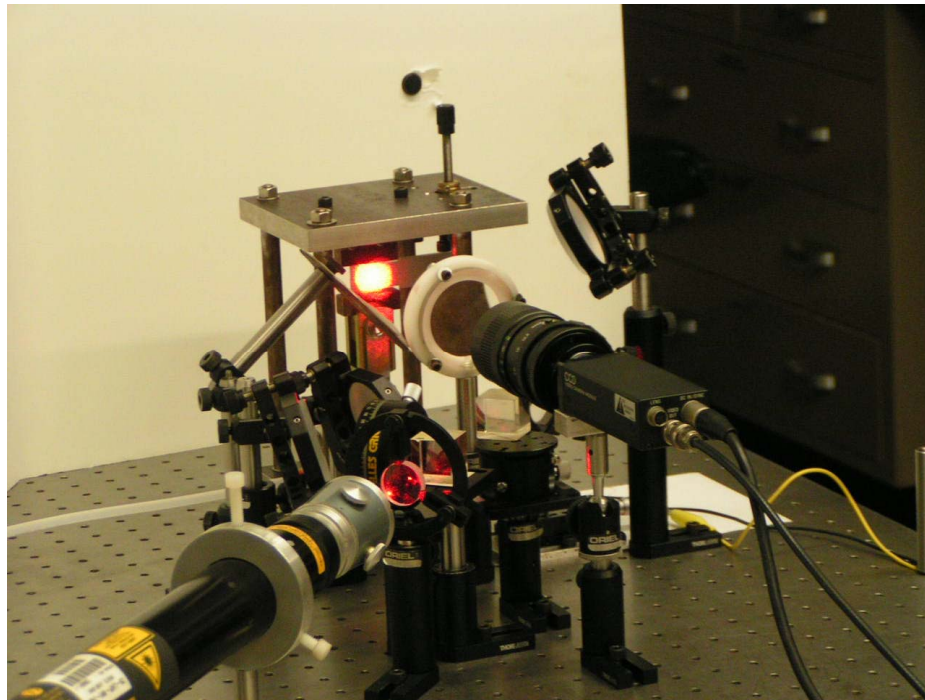
$$I^{(k)}(\mathbf{x}) = I_1(\mathbf{x}) + I_2(\mathbf{x}) + 2\sqrt{I_1(\mathbf{x})I_2(\mathbf{x})} \cos(\phi(\mathbf{x}) + \alpha_k) \quad (4.1)$$



(a)



(b)



(c)

Figure 4.1: (a) A schematic of the test configuration; (b) a close view of the loading device; (c) an experimental ESPI system for 2-D displacement field measurement. The loading device in (c) is switched from left to right for ease of experimental operation. The data presented in Section 4.3 will be consistent with the schematic as shown in (a).

in which $\phi(\mathbf{x})$ is the speckle phase, and $\alpha_k = \{0, \pi/2, \pi, 3\pi/2\}$ is the phase shift at each of the four steps. The speckle phase can be calculated from the speckle images with four-step phase shifting as

$$\phi(\mathbf{x}) = \tan^{-1} \left(\frac{I^{(4)}(\mathbf{x}) - I^{(2)}(\mathbf{x})}{I^{(1)}(\mathbf{x}) - I^{(3)}(\mathbf{x})} \right) \quad (4.2)$$

For small deformation, the displacement field of the rough surface, $\mathbf{u}(\mathbf{x})$, is related to the speckle phase change, $\Delta\phi(\mathbf{x})$, by the formula

$$\Delta\phi(\mathbf{x}) = \phi^*(\mathbf{x}) - \phi(\mathbf{x}) = (\mathbf{k}_2 - \mathbf{k}_1) \cdot \mathbf{u}(\mathbf{x}) \quad (4.3)$$

where $\mathbf{k}_2$ and $\mathbf{k}_1$ are the wave vectors of the two coherent beams, and $\phi(\mathbf{x})$ and $\phi^*(\mathbf{x})$ are the speckle phase distributions of the undeformed and deformed configurations, respectively. By unwrapping the $\Delta\phi(\mathbf{x})$ map, the displacement field can then be obtained with high resolution on the order of a small fraction of the light wavelength.

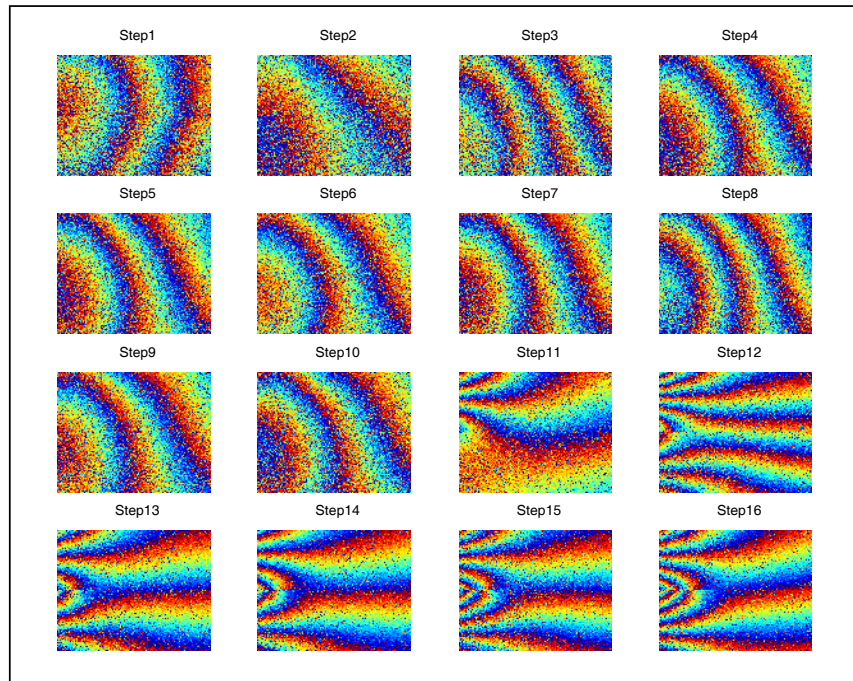
Despite its high resolution, ESPI has some disadvantages associated with the nature of speckles, such as ease of speckle decorrelation and low tolerance to environmental noise. These issues have to be taken into special consideration in the experiment design. Fig. 4.1(b) is a close view of the testing device designed for the friction test. The framework of the device is constructed very compactly with steel to provide adequate rigidity for minimizing speckle decorrelation caused by rigid body motion of the test specimens. An air cylinder driven by compressed air is used for applying the clamping load. The load magnitude is controlled by adjusting the air pressure with a regulator. Compared to other loading options, this method reduces the initiation of vibrations for monitoring and measuring speckle phase images. The transverse point load is applied precisely with displacement control using a micrometer. The

test specimens are made of polymethylmethacrylate (PMMA), and machined into the desired dimensions of 80 mm in length by 10 mm in width by 3 mm in thickness. The two contact surfaces are polished with 300 grid sandpaper. The RMS roughness of the surfaces is measured to be approximately $1\text{ }\mu\text{m}$ with an optical profiler.

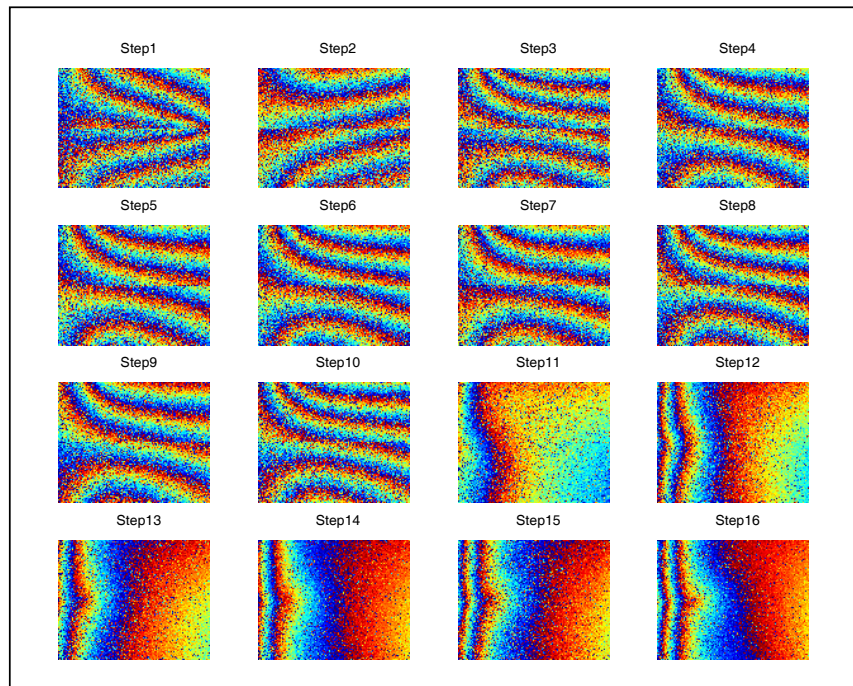
Fig. 4.1(c) shows an experimental ESPI setup for 2-D displacement field measurement around the slip zone. A 30 mW He-Ne laser is used as the light source. The collimated laser beam is split into one reference beam and two illuminating beams for horizontal and vertical displacement measurement. The phase of the reference beam is shifted with a piezoelectric actuator. The sensitivities of the ESPI system are 1.66 and $1.40\text{ }\mu\text{m}$ per fringe for measurement of horizontal and vertical displacements, respectively. To avoid speckle decorrelation, the normal clamping load is first applied up to 1.1 kN by the air cylinder in 10 discrete steps, and the shear load is applied by the micrometer in the following 6 steps. The speckle intensity maps for each step are recorded with a CCD camera, and processed with Eq. 4.2 and 4.3 to get the distributions of phase change and displacement. Knowing the displacement field, the stress field can be calculated if the elastic response of the material is assumed. From the displacement and stress fields, the displacement and traction in the normal and tangential directions along the interface can be extracted and combined to get the quasistatic friction law of the interface.

4.3 Experiment results

Fig. 4.2 shows the measured raw speckle fringes in the horizontal and vertical directions. The discontinuity at the interface is observed for the vertical fringe fields during normal loading and for the horizontal fringe fields during shear loading. The experimental noises in the fringe fields are smoothed out with a moving average filter.

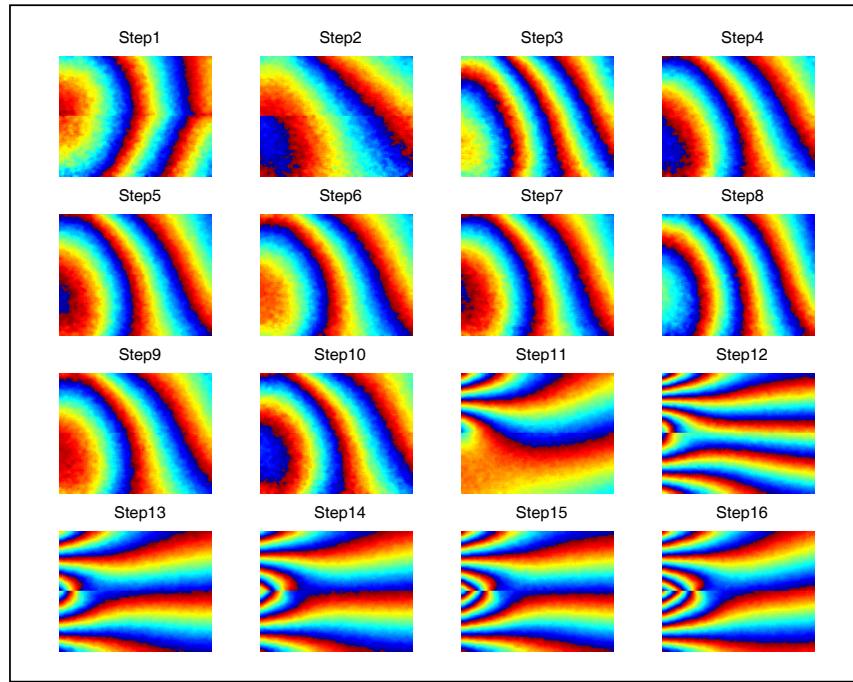


(a)

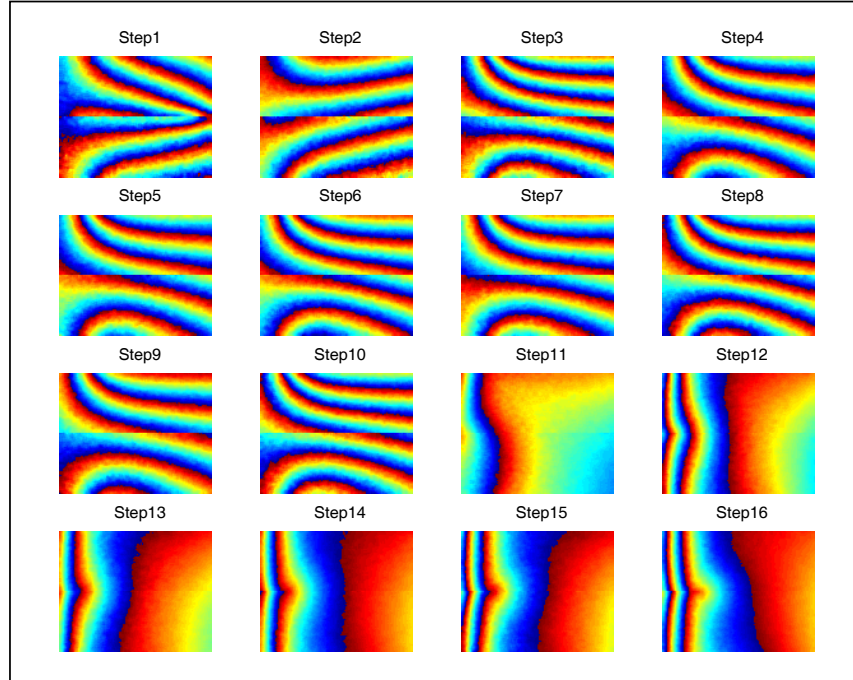


(b)

Figure 4.2: Raw phase fringe maps for each loading step. (a) Horizontal; (b) vertical.



(a)



(b)

Figure 4.3: Smoothed phase fringe maps for each loading step. (a) Horizontal; (b) vertical.

To preserve the discontinuity at the interface, the upper and lower parts of all the fields are smoothed separately, and combined to get the smoothed fringe fields as shown in Fig. 4.3.

By unwrapping the fringe maps in Fig. 4.3, the horizontal and vertical displacement fields are obtained and shown in Fig. 4.4. The horizontal displacement field shows a shear zone formed on the left side of the interface. A striking feature of the vertical displacement field is that, the upper and lower contact surfaces penetrate into each other under normal loading. While some qualitative observations can be made, a direct quantitative calculation based on the raw displacement field is problematic and can lead to erroneous results. The problem arises from two sources. First, though the high-frequency speckle noise is smoothed out with the moving average algorithm, the low-frequency noise still remains and causes large errors in the numerical differentiation of the displacement fields for stress calculation. Second, when the moving average filter is used for smoothing speckle images, the displacement gradient near the boundaries degenerates because a full-size filter can not be applied. To solve these problems, a global smoothing algorithm based on FEM equilibrium (Hong and Kim 2003) is used for data processing. Considering an array of displacement values at pixel positions, $\tilde{\mathbf{u}}$, with experimental noise, the idea of the smoothing algorithm is to determine an equilibrium field, $\mathbf{u}$, that best fits $\tilde{\mathbf{u}}$. Mathematically this is accomplished by minimizing

$$E(\mathbf{u}; \alpha) = \frac{1}{2} \|\mathbf{u} - \tilde{\mathbf{u}}\|^2 + \frac{\alpha}{2} \|\mathbf{C}\mathbf{u}_b\|^2 \quad (4.4)$$

under the equilibrium constraint $\mathbf{f}_i = \mathbf{K}\mathbf{u} = 0$. Here, $\mathbf{f}_i$ are the interior nodal forces and $\mathbf{K}$ is the corresponding partial stiffness matrix. The last term in Eq. 4.4 is included for boundary displacement smoothing, where $\mathbf{u}_b$ are the boundary displacement values, $\mathbf{C}$ is the second derivative operator and α is the weight coefficient. The

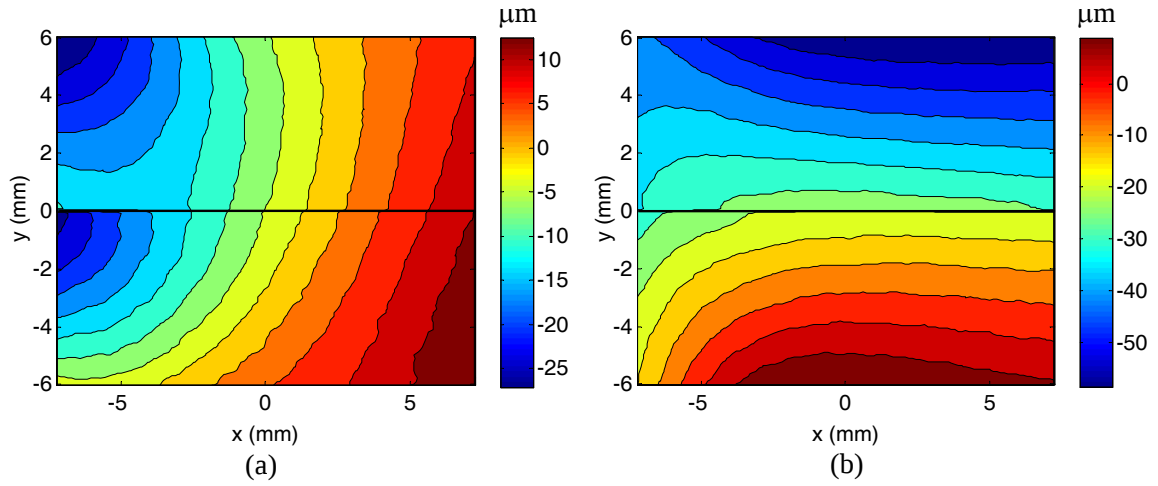


Figure 4.4: Raw displacement fields unwrapped from the smoothed fringe fields. (a) Horizontal displacement field; (b) vertical displacement field.

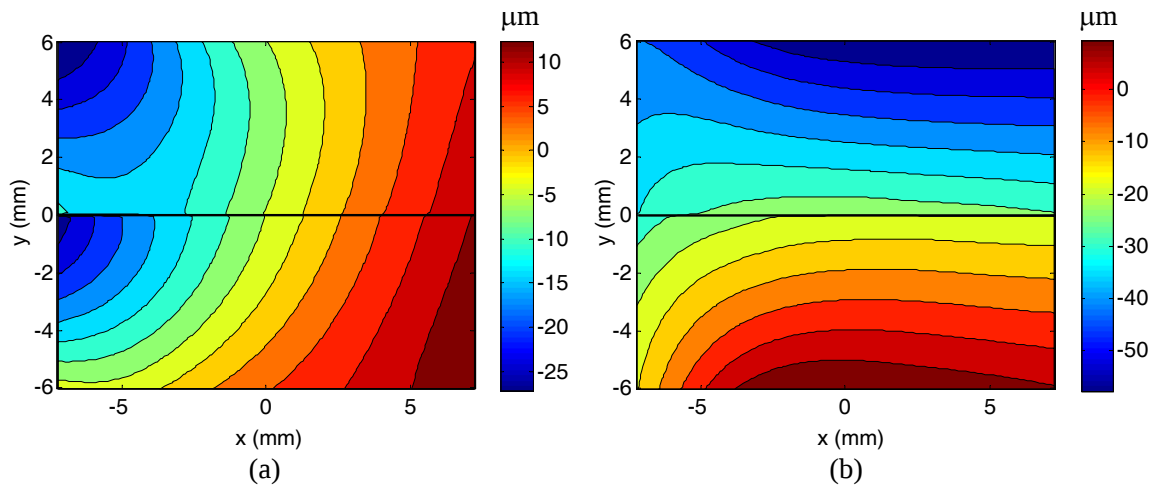


Figure 4.5: Displacement fields smoothed with the FEM equilibrium algorithm. (a) Horizontal displacement field; (b) vertical displacement field.

solution to Eq. 4.4 is obtained with the Lagrange multiplier method as

$$\mathbf{u} = (\mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{K}^T\mathbf{\Delta}^{-1}\mathbf{K}\mathbf{A}^{-1})\tilde{\mathbf{u}} \quad (4.5)$$

in which $\mathbf{\Delta} = -\mathbf{K}\mathbf{A}^{-1}\mathbf{K}^T$ and

$$\mathbf{A} = \begin{pmatrix} \mathbf{I} + \alpha\mathbf{C}^T\mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}.$$

Fig. 4.5 shows the smoothed displacement fields produced with the FEM smoothing technique. The displacement fields of the upper and lower domains are smoothed separately with a boundary smoothing parameter of $\alpha = 1000$. Compared to the raw displacement in Fig. 4.4, the experimental noise is removed while the displacement gradient at the boundaries is recovered. Fig. 4.6 shows the horizontal and vertical displacement profiles of the upper and lower contact surfaces. To completely eliminate the system compliance effect, the displacement profiles and the traction profiles (discussed in detail later) are extrapolated to the interface from the nearest pixels. The displacement discontinuity in Fig. 4.6(a) reveals that a slip zone is formed at $x < -2.5$ mm. Fig. 4.6(b) shows the upper and lower surfaces penetrate into each other for 2 to 5 μm over the interface zone under investigation.

The smoothed displacement fields are differentiated to obtain the strain fields, from which the stress fields are calculated assuming elastic response and a plane stress condition. The material properties of $E = 2.5$ GPa and $\nu = 0.35$ are used for the PMMA specimens tested. Fig. 4.7 shows the calculated distributions of σ_{12} and σ_{22} components. It can be seen from Fig 4.7(a) that a shear stress distribution up to 2.3 MPa is localized within the shear zone. Fig. 4.7(b) shows the compressive stress has a maximum value of about 15 MPa in the clamped region, and decays in

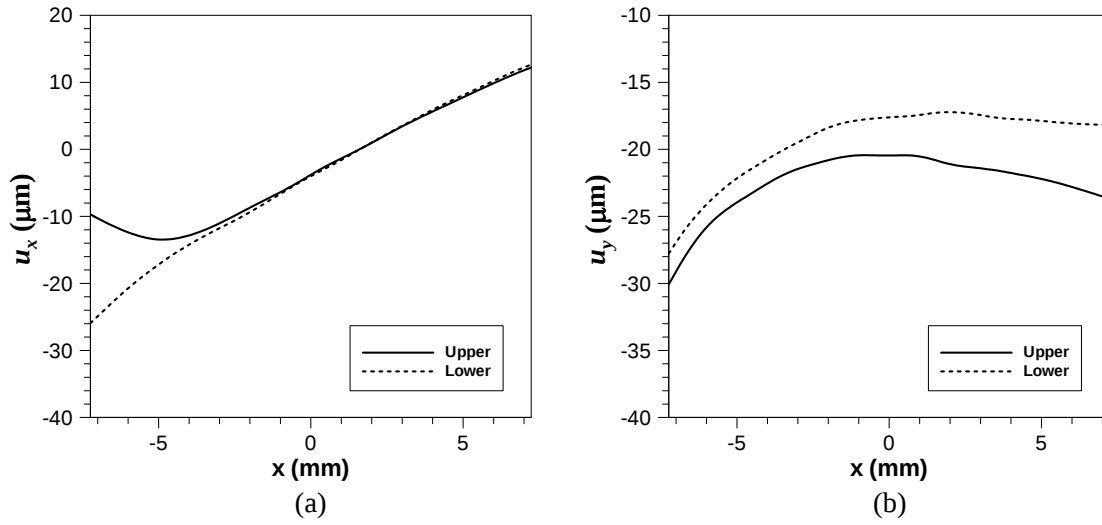


Figure 4.6: Displacement profiles along the interface. (a) Horizontal; (b) vertical.

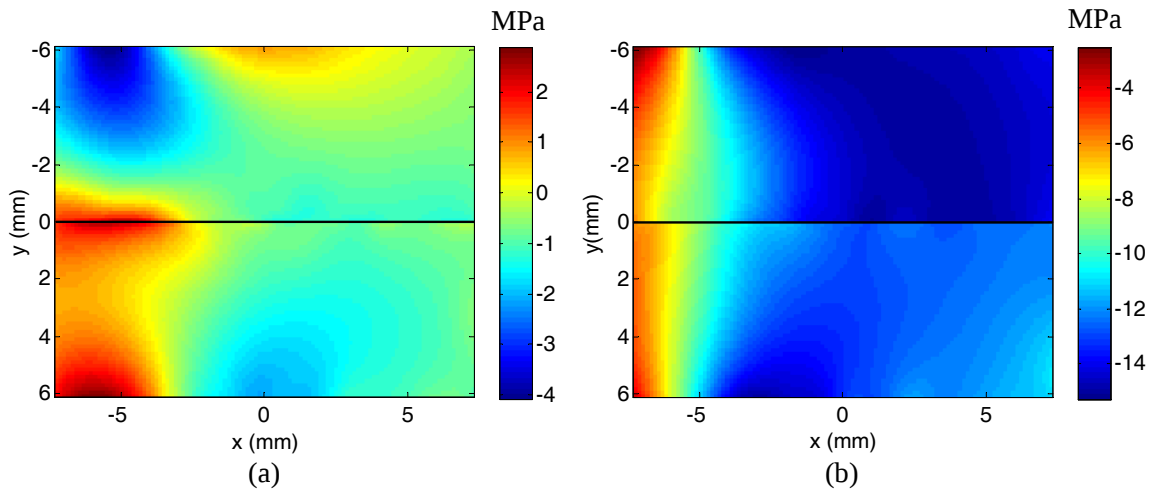


Figure 4.7: Stress fields calculated from the smoothed displacement fields. (a) σ_{12} field; (b) σ_{22} field.

the shear zone. As PMMA has a compressive yield stress above 50MPa (Jasper *et al.* 2002), the elastic response assumption for stress calculation is justified at the current stress state.

From the distributions of traction and relative displacement in the normal and shear directions, a steady state friction law is obtained. Fig. 4.8(a) shows the shear traction and pressure profiles along the interface. As the upper and lower surfaces have slightly different distributions due to experimental errors, they are simply averaged for further data processing. The ratio of average shear stress to normal pressure, τ/p , is plotted in Fig. 4.8 as a function of position. At $x < -5.5\text{mm}$, τ/p reaches a contact value of about 0.28, which is the steady state friction coefficient of PMMA against PMMA. A process zone of 3 mm length ($-5.5\text{ mm} < x < -2.5\text{ mm}$) is required for τ/p to reach the friction coefficient from zero. Fig. 4.8(c) shows the slip distance of the upper surface relative to the lower surface as a function of position. A non-zero slip distance is observed in the process zone. This observation is conflicting with the classic Amonton's law of friction, which predicts that the slip would not occur if the tangential traction is smaller than its limiting value, or in other words, any slip would cause the tangential traction to reach the limit value. The relationship between τ/p and the slip distance, which can be referred as the micro-slip friction law, is plotted in Fig. 4.8(d). It can be clearly seen that the a slip precursor displacement of about $3\text{ }\mu\text{m}$ is required for τ/p to reach the constant friction coefficient of 0.28, despite the fact that the curve does not go through the origin exactly due to experimental error.

Fig. 4.9 shows the normal pressure as a function of the penetration depth. The ten data points are taken at $x = 0\text{ mm}$ during the first ten steps with normal loading. The slope of the curve is relatively small for small penetration depth. As the penetration depth increases, the curve appears to be more linear. A linear least-squares fitting with the five right-most points gives a contact stiffness of $6\text{ MPa}/\mu\text{m}$.

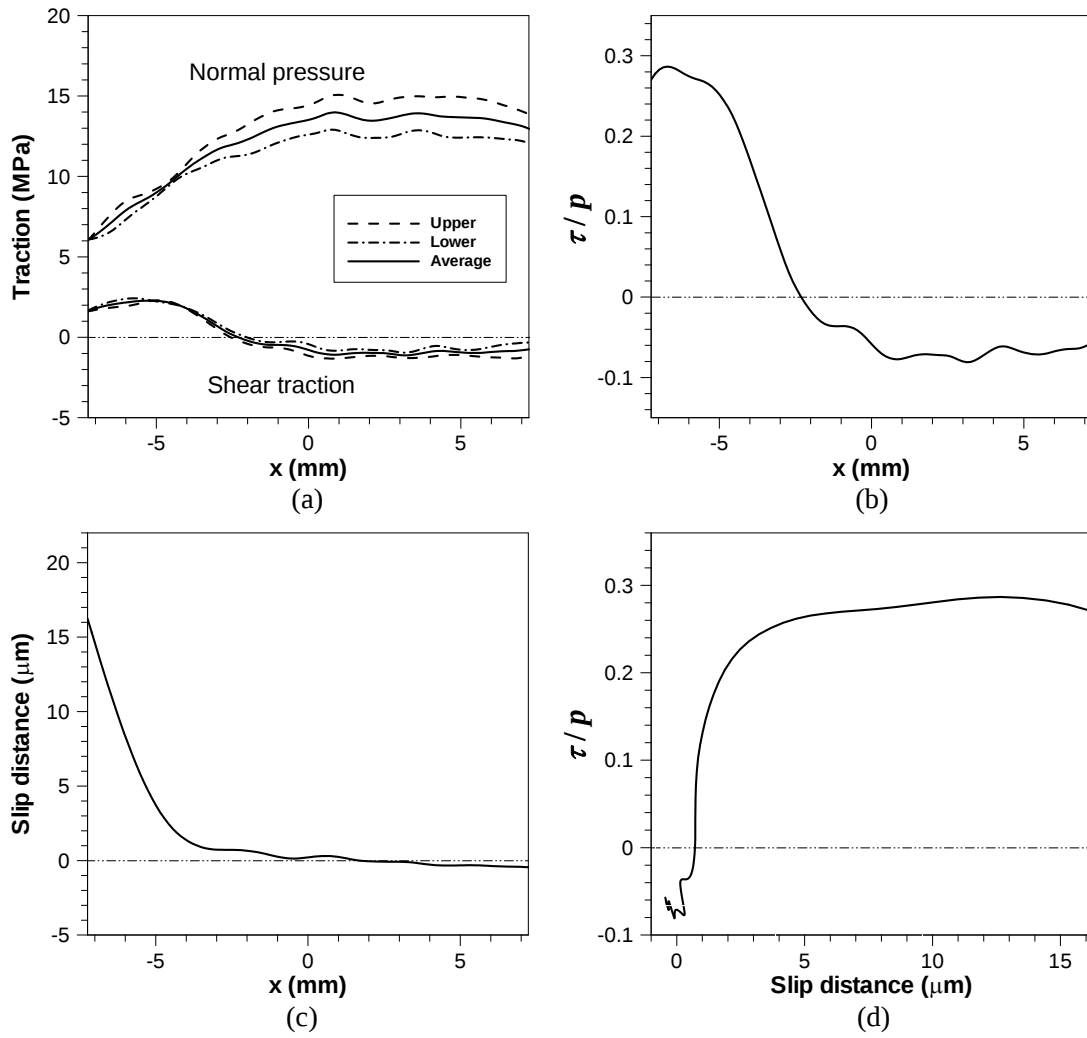


Figure 4.8: (a) Traction distribution along the interface; (b) distribution of ratio of shear stress to pressure along the interface; (c) slip distance profile along the interface; (d) ratio of shear stress to pressure as a function of slip distance.

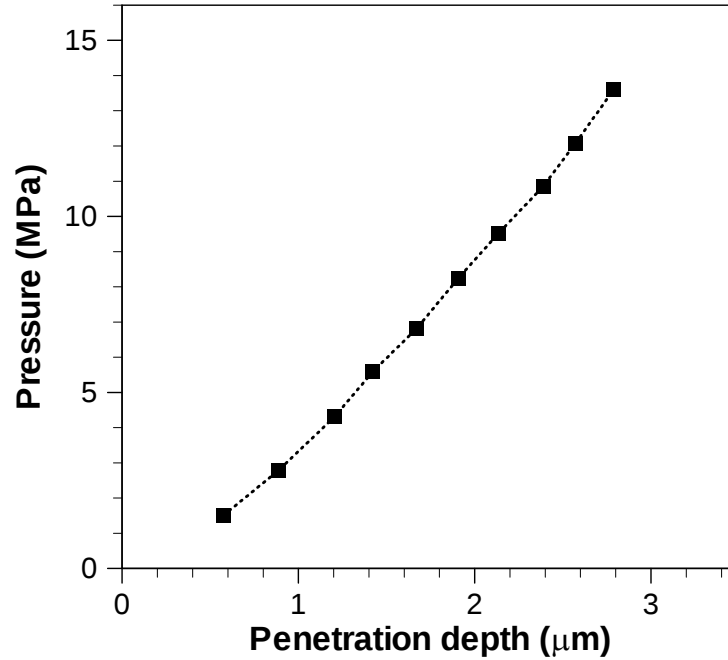


Figure 4.9: The relationship between normal pressure and penetration depth. The data points are obtained at $x = 0$ mm during the first ten steps with normal loading.

4.4 *Discussions*

This work presents a direct quantitative in-situ measurement of the non-rigidity of the rough surface contact in both normal and tangential directions. The experiment reveals an apparent penetration of the contact surfaces into each other under normal pressure. This result appears to contradict a basic physical consideration: solid bodies can never penetrate each other. The contradiction lies in the fact that, the two contact surfaces, even macroscopically flat, are rough at microscopic scales. When the surfaces are brought together, the real contact occurs only at a small number of asperities and the gap between non-contact regions allows a relative displacement. The contact compliance is related to the material properties and surface geometrical

profiles, and can be conceptually regarded as the compliance of an interfacial roughness layer (IRL). The shear compliance can be understood as the effect of IRL in the same manner. The slip precursor displacement before incipient slip is interpreted as the critical sliding distance at which a catastrophic slip is triggered. The current experimental findings provide valuable guidance for further theoretical studies of friction employing statistical mechanics theories, such as mean-field theory and renormalization group approach.

The experimental friction law with contact and shear compliance resembles the one that has been used empirically in computational mechanics. A rigid Amontons' friction law usually causes spurious traction fluctuation in computational simulations. Therefore a moderate compliance is typically implemented in the constitutive law to regularize the solution by trial and error. A physics-based selection criterion for compliance can be provided by this experimental work. Furthermore, in some circumstances, like vibration and fretting wear of fasteners and joints, large-scale slip is not major concern and the slip precursor displacement plays an important role in controlling the system response. The current experimental framework can be readily extended to investigate these phenomena by performing cyclic loading tests.

It is worth mentioning that a non-uniform distribution of normal pressure is applied in the experiment to suppress unstable slip. Therefore the curve of τ/p versus sliding distance as shown in Fig. 4.8(d) is the envelope of a family of curves for different pressures. However, the normal pressure distribution in the slip process zone (8.5 - 12 MPa) is not significantly varied. Therefore the measured friction law is believed to be representative for a pressure around 10 MPa. The ESPI system employed has a limitation on boundary displacement measurements. A FEM smoothing algorithm is currently employed to compensate for the system error. It is expected that, the field projection method (FPM) (Hong and Kim 2003), which can extract the interfacial

law from an interior displacement field, can be used to improve the accuracy of the experimental results.

4.5 Chapter summary

In this work, an experimental framework has been developed, for the first time, for friction test with an electronic speckle pattern interferometer (ESPI). The direct optical measurement close to interface slip zone eliminates the uncertainty of displacement and traction measurements in previous experiments. The validity of the experimental setup is demonstrated by a benchmark test on PMMA friction. An apparent penetration depth is observed with a contact stiffness of $6 \text{ MPa}/\mu\text{m}$ for two contact PMMA surfaces with RMS roughness of $1 \mu\text{m}$. A slip precursor displacement of about $3 \mu\text{m}$ is found before the incipient slip. This experimental framework is expected to facilitate a deeper understanding of friction behaviors of rough surfaces, and has great potential in studies of interface adhesion, cold welding and fretting wear.

Bibliography

Acharya, A. and Bassani, J. (2000), ‘Lattice incompatibility and a gradient theory of crystal plasticity’, *Journal of the Mechanics and Physics of Solids* **48**, 1565–1595.

2.1

Adams, G. (1995), ‘Self-excited oscillations of two elastic half-spaces sliding with a constant coefficient of friction’, *ASME Journal of Applied Mechanics* **62**, 867–872.

4.1

Archard, J. (1957), ‘Elastic deformation and the laws of friction’, *Proceedings of the Royal Society of London Series A* **243**, 190–205. 1.1

Ashby, M. (1970), ‘The deformation of plastically non-homogeneous materials’, *Philosophical Magazine* **21**, 399–424. 2.1

Bei, H., Gao, Y., Shim, S., George, E. and Pharr, G. (2008), ‘Strength differences arising from homogeneous versus heterogeneous dislocation nucleation’, *Physical Review B*. 2.1

Bowden, F. and Tabor, D. (1950), *The Friction and Lubrication of Solids*, Clarendon Press, Oxford. 1.1

- Bradby, J., Williams, J., Wong-Leung, J., Swain, M. and Munroe, P. (2001), ‘Mechanical deformation in silicon by micro-indentation’, *Journal of Materials Research* **16**, 1500–1507. 3.3.1
- Camacho, G. and Ortiz, M. (1996), ‘Computational modelling of impact damage in brittle materials’, *International Journal of Solids and Structures* **33**, 2899–2938. 3.1, 3.6
- Chen, M., Perry, T. and Alpas, A. T. (2007), ‘Ultra-mild wear in eutectic Al-Si alloys’, *Wear* **263**(Part 1 Sp. Iss. SI), 552–561. 3.1
- Choi, S. and Kim, K. (2007), ‘Nanoscale planar field projections of atomic decohesion and slip in crystalline solids. Part I. A crack-tip cohesive zone’, *Philosophical Magazine* **87**, 1889–1919. 3.1
- Chue, C. and Liu, C. (2001), ‘A general solution on stress singularities in an anisotropic wedge’, *International Journal of Solids and Structure* **38**, 6889–6906. 2.3, 2.3
- Chue, C., Tseng, C. and Liu, C. (2001), ‘On stress singularities in an anisotropic wedge for various boundary conditions’, *Composite Structures* **54**, 87–102. 2.3
- De Guzman, M. S., Neubauer, G., Flinn, P. and Nix, W. D. (1993), ‘The role of indentation depth on the measured hardness of materials’, *Materials Research Symposium Proceedings* **308**, 613–618. 1.1, 2.1
- Deuis, R., Subramanian, C. and Yellup, J. (1997), ‘Dry sliding wear of aluminium composites - A review’, *Composites Science and Technology* **57**(4), 415–435. 3.1
- Dieterich, J. (1978), ‘Time-dependent friction and the mechanics of stick-slip’, *Pure and Applied Geophysics* **116**, 790–806. 4.1

- Dieterich, J. (1979a), ‘Modeling of rock friction 1. experimental results and constitutive equations’, *Journal of Geophysical Research* **84**, 2161–2168. 4.1
- Dieterich, J. (1979b), ‘Modeling of rock friction 2. simulation of preseismic slip’, *Journal of Geophysical Research* **84**, 2169–2175. 4.1
- Evans, A., Hutchinson, J. and Wei, Y. (1999), ‘Interface adhesion: Effects of plasticity and segregation’, *Acta Materialia* **47**, 4093–4113. 3.1
- Ferroni, L., Pezzotti, G., Isshiki, T. and Kleebe, H. (2001), ‘Determination of amorphous interfacial phases in Al₂O₃/SiC nanocomposites by computer-aided high resolution electron microscopy’, *Acta Materialia* **49**, 2109–2113. 3.1
- Fleck, N. and Hutchinson, J. (1993), ‘A phenomenological theory for strain gradient effects in plasticity’, *Journal of the Mechanics and Physics of Solids* **41**, 1825–1857. 2.1
- Fleck, N. and Hutchinson, J. (1997), ‘Strain gradient plasticity’, *Advances in Applied Mechanics* **33**, 295C361. 2.1
- Fleck, N., Muller, G., Ashby, M. and Hutchinson, J. (1994), ‘Strain gradient plasticity - theory and experiment’, *Acta Metallurgica et Materialia* **42**, 475–487. 2.1
- Gall, K., Horstemeyer, M., Van Schilfgaarde, M. and Baskes, M. (2000), ‘Atomistic simulations on the tensile debonding of an aluminum-silicon interface’, *Journal of the Mechanics and Physics of Solids* **48**, 2183–2212. 3.1, b, 3.5
- Gao, H., Huang, Y., Nix, W. and Hutchinson, J. (1999), ‘Mechanism-based strain gradient plasticity - I. Theory’, *Journal of the Mechanics and Physics of Solids* **47**, 1239–1263. 2.1

- Greenwood, J. and Williamson, J. (1966), ‘Contact of nominally flat surfaces’, *Proceedings of the Royal Society of London Series A* **295**, 300–319. 1.1
- Greer, J., Oliver, W. and Nix, W. (2005), ‘Size dependence of mechanical properties of gold at the micron scale in the absence of strain gradients’, *Acta Materialia* **53**, 1821–1830. 2.1
- Gurtin, M. (2000), ‘On the plasticity of single crystals: free energy, microforces, plastic-strain gradients’, *Journal of the Mechanics and Physics of Solids* **48**, 989–1036. 2.1
- Gurtin, M. (2002), ‘A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations’, *Journal of the Mechanics and Physics of Solids* **50**, 5–32. 2.1
- Hirth, J. and Lothe, J. (1982), *Theory of dislocations*, 2 edn, New York: Wiley. 2.4
- Hong, S. and Kim, K. (2003), ‘Extraction of cohesive-zone laws from elastic far-fields of a cohesive crack tip: a field projection method’, *Journal of the Mechanics and Physics of Solids* **51**, 1267–1286. 3.1, 4.3, 4.4
- Huang, Y., Gao, H., Nix, W. and Hutchinson, J. (2000), ‘Mechanism-based strain gradient plasticity - II. Analysis’, *Journal of the Mechanics and Physics of Solids* **48**, 99–128. 2.1
- Im, S. and Kim, K.-S. (2000), ‘An application of two-state M-integral for computing the intensity of the singular tip field for a generic wedge’, *Journal of the Mechanics and Physics of Solids* **48**, 129–151. 2.3
- Jang, J., Lance, M., Wen, S., Tsui, T. and Pharr, G. (2005), ‘Indentation-induced

- phase transformations in silicon: influences of load, rate and indenter angle on the transformation behavior', *Acta Materialia* **53**, 1759–1770. 3.3.1
- Jasper, L., Deramond, H., Mathis, J. and Belkoff, S. (2002), 'Material properties of various cements for use with vertebroplasty', *Journal of Materials Science: Materials in Medicine* **13**, 1–5. 4.3
- Jay, G. D., Torres, J. R., Rhee, D. K., Helminen, H. J., Hytinen, M. M., Cha, C.-J., Elsaid, K., Kim, K.-S., Cui, Y. and Warman, M. L. (2007), 'Association between friction and wear in diarthrodial joints lacking lubricin', *Arthritis and Rheumatism* **56**, 3662–3669. 1.1
- Jeong, H., Hiraga, K., Mabuchi, M. and K, H. (1996), 'Interface structure of Si₃N₄-whisker-reinforced Al-Mg-Si alloy (Al alloy 6061) composites studied by high-resolution electron microscopy', *Philosophical Magazine Letters* **74**, 73–80. 3.1
- Khalid, F., Beffort, O., Klotz, U., Keller, B. and Gasser, P. (2004), 'Microstructure and interfacial characteristics of aluminium-diamond composite materials', *Diamond and Related Materials* **13**, 393–400. 3.1
- Kim, T., Lee, B., Lee, C. and Chun, B. (2001), 'Microstructure of rapidly solidified Al-20Si alloy powders', *Materials Science and Engineering A* **304**, 617–620. 3.5
- Kloosterman, A., Kooi, B. and De Hosson, J. (1998), 'Electron microscopy of reaction layers between SiC and Ti-6Al-4V after laser embedding', *Acta Materialia* **46**, 6205–6217. 3.1
- Leibfried, G. (1953), 'Versetzungen in anisotropem material', *Zeitschrift fur Physik* **135**, 23–43. 2.6

- Li, Q. (2008), Micromechanics of Pseudo-Single-Asperity Friction: Effects of Nanometer-Scale Roughness, PhD thesis, Brown University. 1.1
- Ma, Q. and Clarke, D. (1995), ‘Size-dependent hardness of silver single-crystals’, *Journal of Materials Research* **10**, 853–863. 1.1, 2.1
- Moes, N., Dolbow, J. and Belytschko, T. (1999), ‘A finite element method for crack growth without remeshing’, *International Journal for Numerical Methods in Engineering* **46**, 131–150. 3.1
- Moser, B., Wasmer, K., Barbieri, L. and Michler, J. (2007), ‘Strength and fracture of Si micropillars: A new scanning electron microscopy-based micro-compression test’, *Journal of Materials Research* **22**, 1004–1011. 3.3.1
- Mura, T. (1982), *Micromechanics of defects in solids*, 1 edn, Martinus Nijhoff Publishers. 2.6, 2.6
- Needleman, A. (1987), ‘A continuum model for void nucleation by inclusion debonding’, *Journal of Applied Mechanics-Transactions of the ASME* **54**, 525–531. 3.1
- Needleman, A. and Van der Giessen, E. (2001), ‘Micromechanics of fracture: Connecting physics to engineering’, *MRS Bulletin* **26**, 211–214. 3.1
- Nix, W. and Gao, H. (1998), ‘Indentation size effects in crystalline materials: A law for strain gradient plasticity’, *Journal of the Mechanics and Physics of Solids* **46**, 411–425. 2.5
- Noreyan, A., Qi, Y. and Stoilov, A. (2008), ‘Critical shear stresses at aluminum-silicon interfaces’, *Acta Materialia*. 3.1, a, 3.5
- Prakash, V. (1998), ‘Frictional response of sliding interfaces subjected to time varying normal pressures’, *Journal of Tribology ASME* **120**, 97–102. 4.1

- Prakash, V. and Clifton, R. (1993), ‘Time resolved dynamic friction measurements in pressure-shear’, *Experimental Techniques in the Dynamics of Deformable Bodies*, Editor: K.T. Ramesh, New York, ASME **165**, 33–48. 4.1
- Ranjith, K. and Rice, J. (2001), ‘Slip dynamics at an interface between dissimilar materials’, *Journal of the Mechanics and Physics of Solids* **49**, 341–361. 4.1
- Remmers, J., de Borst, R. and Needleman, A. (2008), ‘The simulation of dynamic crack propagation using the cohesive segments method’, *Journal of the Mechanics and Physics of Solids* **56**, 70–92. 3.6
- Renardy, M. (1992), ‘Ill-posedness at the boundary for elastic solids sliding under Coulomb friction’, *Journal of Elasticity* **27**, 281–287. 4.1
- Riahi, A., Perry, T. and Alpas, A. (2003), ‘Scuffing resistances of Al-Si alloys: effects of etching condition, surface roughness and particle morphology’, *Materials Science and Engineering A-Structural Materials Properties Microstructure and Processing* **343**(1-2), 76–81. 3.1
- Rice, J. (1992), ‘Dislocation nucleation from a crack tip - an analysis based on the peierls concept’, *Journal of the Mechanics and Physics of Solids* **40**, 239–271. 2.5
- Rice, J. and Ruina, A. (1983), ‘Stability of steady frictional slipping’, *ASME Journal of Applied Mechanics* **50**, 343–349. 4.1
- Rice, J. and Thomson, R. (1974), ‘Ductile versus brittle behavior of crystals’, *Philosophical Magazine* **29**, 73–97. 2.1, 2.2, 2.3
- Rohatgi, P. (1991), ‘Cast aluminum-matrix composites for automotive applications’, *JOM-Journal of the Minerals Metals and Materials Society* **43**, 10–15. 3.1

- Ruina, A. (1983), ‘Modeling of rock friction 2. simulation of preseismic slip’, *Journal of Geophysical Research* **88**, 10359–10370. 4.1
- Shenoy, V., Phillips, R. and Tadmor, E. (2000), ‘Nucleation of dislocations beneath a plane strain indenter’, *Journal of the Mechanics and Physics of Solids* **48**, 649–673. 2.1
- Stolken, J. and Evans, A. (1998), ‘A microbend test method for measuring the plasticity length scale’, *Acta Materialia* **46**, 5109–5115. 2.1
- Suo, Z. (1990), ‘Singularities, interfaces and cracks in dissimilar anisotropic media’, *Proceedings of the Royal Society of London Series A-Mathematical Physical and Engineering Sciences* **427**, 331–358. 2.3
- Suo, Z. (2000), ‘Zener’s crack and the M-integral’, *ASME Journal of Applied Mechanics* **67**, 417–418. 2.3
- Turon, A., Davila, C., Camanho, P. and Costa, J. (2007), ‘An engineering solution for mesh size effects in the simulation of delamination using cohesive zone models’, *Engineering Fracture Mechanics* **74**, 1665–1682. 3.6
- Wang, J., Lian, J., Greer, J., Nix, W. and Kim, K. (2006), ‘Size effect in contact compression of nano- and microscale pyramid structures’, *Acta Materialia* **54**, 3973–3982. 1.1, 2.1, 2.2, 2.7, 2.5
- Ward, D. (2008), Nanocomposite and nanoasperity plasticity: a molecular dynamics and energetics study, PhD thesis, Brown University. 2.1, 2.2, 2.3, 2.7, 2.5
- Ward, D., Curtin, W. and Qi, Y. (2006), ‘Aluminum-silicon interfaces and nanocomposites: A molecular dynamics study’, *Composites Science and Technology* **66**, 1151–1161. 3.1, a, 3.5

- Ward, D., Curtin, WA and Qi, Y. (2006), ‘Mechanical behavior of aluminum-silicon nanocomposites: A molecular dynamics study’, *Acta Materialia* **54**, 4441–4451. 3.1, a, 3.5
- Wilson, S. and Alpas, A. (1997), ‘Wear mechanism maps for metal matrix composites’, *Wear* **212**(1), 41–49. 3.1
- Wu, B., Heidelberg, A. and Boland, J. (2005), ‘Mechanical properties of ultrahigh-strength gold nanowires’, *Nature Materials* **4**, 525–529. 2.1
- Xia, S., Gao, Y., Bower, A., Lev, L. and Cheng, Y. (2007), ‘Delamination mechanism maps for a strong elastic coating on an elastic-plastic substrate subjected to contact loading’, *International Journal of Solids and Structures* **44**, 3685–3699. 3.1
- Xu, X. and Needleman, A. (1993), ‘Void nucleation by inclusion debonding in a crystal matrix’, *Modelling and Simulation in Materials Science and Engineering* **1**, 111–132. 3.1
- Yu, H., Shrotriya, P., Gao, Y. and Kim, K. (2007), ‘Micro-plasticity of surface steps under adhesive contact: Part I - Surface yielding controlled by single-dislocation nucleation’, *Journal of the Mechanics and Physics of Solids* **55**, 489–516. 2.1
- Zarudi, I., Zhang, L., Cheong, W. and Yu, T. (2005), ‘The difference of phase distributions in silicon after indentation with Berkovich and spherical indenters’, *Acta Materialia* **53**, 4795–4800. 3.3.1
- Zhang, J. and Alpas, A. (1997), ‘Transition between mild and severe wear in aluminium alloys’, *ACTA Materialia* **45**(2), 513–528. 3.1