RICE UNIVERSITY

Study of Fault Gouge Influences on Mechanical and Frictional Behavior of Granular Shear Zones Using the Distinct Element Method

by

Yonggui Guo

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APPROVED, THESIS COMMITTEE:

Julia K. Morgan, Assistant Professor, Chair
Earth Science

Hans G Ave Lallemant, Professor
Earth Science

Adrian Lenardic, Assistant Professor
Earth Science

William Symes, Noah Harding Professor
Computational and Applied Mathematics

HOUSTON, TEXAS

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ABSTRACT

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Studies of fault gouge and its role in shear zone deformation are the key to understanding the mechanics of earthquakes and fault zone evolution. With the advantage of exploring the micromechanical process of gouge deformation in “real time”, the combination of the Distinct Element Method (DEM) and linear elastic contact bonds provides an opportunity to deform complex, heterogeneous granular assemblages that approximate natural shear zones in a more realistic way, and to study gouge deformation processes that are responsible for unstable sliding of fault zones.

Granular assemblages of multiple shaped grains were sheared over a range of normal stresses, $\sigma_n$, in order to examine the influences of $\sigma_n$, gouge grain shape, grain comminution, and associated dynamic changes in grain characteristics on the frictional behavior of granular shear zones. The results show an inverse power law relationship between $\sigma_n$ and maximum sliding friction, where both its coefficient and exponent are dependent on gouge angularity. Enhanced grain rolling alone does not explain the low frictional strengths of simulated granular assemblages. Shear zone strength is dependent on the competition between strength reduction by fracturing and strength variation by changes in grain characteristics that are related to the partitioning of different deformation mechanisms.
DEM experiments were also conducted to simulate the growth of fault gouge zones, for the purposes of studying the processes of gouge zone evolution, and its dependence on $\sigma_n$ and uniaxial compressive strength, $\sigma_{uc3}$. The simulated fault gouge zones exhibit two distinct stages of evolution, i.e., fast growth and slow growth, distinguished by a switch in deformation mechanism from dominantly wear of the fault blocks to dominantly shearing of existing fault gouge. During the fast growth stage, the rates of gouge thickening and bond breakage decrease exponentially and are proportional to $\sigma_n$ and inversely proportional to $\sigma_{uc3}$, but the rates become relatively constant and the dependency reverses during the slow growth stage. Gouge properties show complex correlations and dependences on shear displacement, $\sigma_n$ and $\sigma_{uc3}$, demonstrating the important effects of depth, mechanical properties of fault rocks, and gouge properties on the evolution and stability of natural faults.
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Chapter 1

Introduction

During faulting at shallow depths, frictional sliding of brittle shear zones is accompanied by surface wear that produces angular rock detritus, called fault gouge. The presence of gouge allows strain to be accommodated within gouge zones, and therefore significantly affects the mechanical and seismic behavior of faults [Byerlee, 1967; Scholz et al., 1969, 1972; Byerlee and Summers, 1976; Marone and Scholz, 1988]. In natural fault zones, gouge physical and structural properties evolve over time as a result of continued accumulation of wear products, gouge grain comminution, and reorganization, dependent on deformation conditions such as normal stress, strain rate, and rock strength. The evolving gouge properties, therefore, lead to complex frictional responses of natural faults that form from a variety of source rocks under a wide range of loading conditions.

The wealth of data coming out of field observations and laboratory experiments has yielded significant insights into the complexity of frictional and mechanical behavior during fault zone deformation in the presence of fault gouge. Although previous studies have demonstrated the effects of gouge on fault zone evolution, the underlying micromechanical processes responsible for these effects remain elusive. With field observations and laboratory experiments, it is difficult to directly correlate variations in gouge frictional properties to their physical and structural properties in real time, and to isolate the corresponding deformation mechanisms. Therefore, many important problems related to gouge deformation, such as which deformation mechanisms are active, when and how these influence the frictional strength of fault zones, cannot be fully addressed.
Key factors in gouge evolution include gouge thickness, grain shape, size, size
distribution, organization, and microstructure.

Particle-based numerical simulations, such as the Distinct Element Method
(DEM) [Cundall and Strack, 1979], have the capability of exploring the micromechanics
of particle interactions and relating them to characteristic deformation processes and
variation of frictional strength in "real time" [Mora and Place, 1998, 1999; Morgan and
Boettcher, 1999; Morgan, 1999; Place and Mora, 2000]. However, many of the early
simulations have been very simple, for example, using idealized spherical particles,
maintaining constant particle shapes and sizes, and preventing fracture and comminution
during shear [Mora and Place, 1998, 1999; Morgan and Boettcher, 1999; Morgan, 1999;
Place and Mora, 2000]. Natural gouge grains, in contrast, are highly irregular in shape
and undergo pervasive fracture and comminution during shear zone deformation [Sammis
et al., 1987; Marone and Scholz, 1989; Mair et al., 2002]. The simplicity of previous
numerical models, therefore, limits their applicability to natural granular shear zones.

In order to explore the consequences of evolving shear zones and gouge
properties and to identify their effects on the frictional strength of fault zones,
interparticle bonding and fracture mechanisms were introduced in the DEM models. By
adding breakable bonds between adjacent particles, rocks and grains can be approximated
by assemblages of closely packed, circular particles of various sizes. In this way,
arbitrarily shaped grains can be generated and tracked during shear deformation. Fracture
and comminution can be simulated by bond breakage. The resulting simulations are much
more realistic approximations of the deformation processes of natural shear zones.
The results of three suites of DEM experiments in two dimensions are presented here, in order of increasing complexity of grain and fault surface properties. In the first suite of experiments, simulated fault gouges are constructed directly using mixes of unbreakable rounded and triangular grains. They were deformed over a range of normal stresses. In this way, we can study the effects of grain shape and normal stress on frictional properties of granular shear zones. Frictional strength was observed to decrease with increasing normal stress, according to a power law relationship. Grain shape controls the normal stress dependence of friction by influencing both the coefficient and exponent of the power law relationship. This study (Chapter 2) has been published in Journal of Geophysical Research [Guo and Morgan, 2004].

The second suite of experiments uses similar initial configuration to the first suite of experiments, but allows for gouge grain breakage, according to predefined interparticle bond strengths. Therefore, simulated gouges can undergo grain comminution, causing dynamic changes in grain characteristics during shear zone deformation. The results show that grain comminution changes the partitioning of different deformation mechanisms. Simulated shear zone strengths are strongly dependent on the direction and degree of change in grain shape due to grain comminution. This study (Chapter 3) has been resubmitted to the Journal of Geophysical Research, following revision [Guo and Morgan, resubmitted].

The last suite of experiments takes one step further, allowing fault blocks to fracture and break down and naturally form fault gouge. This results in progressive changes in gouge thickness, grain shape, size, and size distribution. These dynamic variations depend strongly on loading conditions and material properties, i.e., shear
displacement, normal stress, and rock uniaxial compressive strength. The simulated shear zones experience two distinct stages of gouge zone development with the transition, marked by a significant decrease in wear rate. The frictional and mechanical properties of the evolving shear zones show complex correlations with gouge properties during each evolutionary stage, and also dependent on normal stress and rock strength. This study presented as two separate papers (Chapters 4 and 5), and will be submitted to Journal of Geophysical Research.

The numerical simulations successfully reproduce many observations in the field and laboratory, such as the development of characteristic shear fractures in the deforming gouge, and normal stress and grain shape dependence of shear zone strength. The simulations also yield interesting findings that have not been reported in previous gouge zone studies, such as multiple stages of gouge zone development and their distinct dependences on shear displacement, normal stress, and rock strength. These encouraging results suggest the feasibility, necessity, and importance of improving numerical models and extending the current studies into the future.
Chapter 2

Influence of Normal Stress and Grain Shape on Granular Friction:

Results of Discrete Element Simulations

2.1. Abstract

Laboratory experiments of granular shear deformation demonstrate that loading conditions and grain characteristics can significantly affect the macroscopic friction of a granular material under shear. We have examined the variation of maximum sliding friction with normal stress and grain shape using a version of the Distinct Element Method (DEM) that includes bonds between adjacent particles. In this way, irregularly shaped grains can be generated to reproduce more realistic fault gouge with a range of grain sizes and shapes. Two types of grains were designed to represent quartz gouge: rounded grains composed of 7 close-packed particles, and triangular grains composed of 6 close-packed particles. DEM experiments were conducted by shearing granular assemblages with different grain shape distributions using identical boundary configurations (i.e., wall surface roughness) over a range of normal stresses from 5 to 100 MPa, and compared to equivalent experiments using reference circular particle assemblages. The results show an inverse power law relationship between normal stress and maximum sliding friction in all cases, where both its coefficient and exponent are dependent on gouge angularity. Under normal stress over 20 MPa, triangular grain assemblages exhibit the highest frictional strength, and also the highest abundance of rotating grains, demonstrating that enhanced grain rolling alone does not explain the low frictional strength of simulated granular assemblages.
2.2. Introduction

Frictional sliding of brittle shear zones at shallow depth is commonly accompanied by production, accumulation, and evolution of non-cohesive wear detritus with angular forms called fault gouge. It has long been recognized that the presence of fault gouge has significant effects on the mechanical behavior of fault zones [Byerlee, 1967; Byerlee and Summers, 1976; Scholz et al, 1972], and the stability of natural faults [Scholz et al., 1969; Marone and Scholz, 1988]. Therefore, a full understanding of fault strength, dynamic behavior, and earthquake mechanisms requires a complete knowledge of the frictional properties of fault gouge under a wide range of conditions.

A considerable body of experimental work has been carried out to identify the effects of a variety of gouge materials on frictional behavior of fault zones under various experimental conditions. Early work was focused on the effects of gouge on base level rock friction, as the production of gouge during slip of initially bare rock surfaces was found to result in a decrease in frictional resistance [e.g., Byerlee, 1967; Scholz et al, 1972]. Studies of gouge rock friction [Engelder et al., 1975; Byerlee et al., 1978; Logan et al., 1979; Moore et al., 1988; Tullis et al., 1989] indicated that the accumulation of gouge, and development of shear localization features within gouge, may influence fault constitutive behavior and stability of sliding. Further studies [Dieterich, 1979; Ruina, 1983; Rice and Ruina, 1983; Chester and Higgs, 1992; Reinen et al., 1994; Perrin et al., 1995] demonstrated that second-order variations in friction of simulated fault zones can be described by several constitutive laws in terms of slip rate and state of the frictional shear zone. The Dieterich-Ruina rate/state constitutive law, currently in best agreement with experimental results [Beeler et al., 1994; Nakatani, 2001], provides the basis for
predicting the frictional response to a change in slip rate (i.e., velocity strengthening and velocity weakening).

To validate and constrain the constitutive laws for frictional evolution under a wide range of conditions, laboratory experiments investigating the effects of variations in extrinsic factors on the frictional strength of simulated fault gouge have been carried out. These factors include normal load [Linker and Dieterich, 1992; Richardson and Marone, 1999], shear load [Nakatani and Mochizuki, 1996; Nakatani, 1998; Karner and Marone, 1998; Olsen et al., 1998], loading velocity [Mair and Marone, 1999], normal stress ($\sigma_n$) vibrations [Richardson and Marone, 1999], shear load perturbations [Karner and Marone, 2001], shear displacement [Beeler et al., 1996], and hydrothermal conditions [Karner et al., 1997]. These studies have led to empirical descriptions of friction in terms of the various extrinsic factors. Nonetheless, none of the existing friction laws can completely describe the observed frictional behavior of fault gouge, due in part to the complexity and evolution of the topography of the contacting surfaces [e.g., Karner and Marone, 1998; Richardson and Marone, 1999, Karner and Marone, 2001]. Recently, attention has been focused on the influences of various intrinsic factors, such as mineralogy [Olsen et al., 1998; Saffer, 2001], grain shape, size, size distribution, and surface roughness [Mair and Marone, 2000; Frye and Marone, 2002; Mair et al., 2002], on shear zone strength and sliding behavior. As an example of these influences, recent investigations have demonstrated that the coefficient of sliding friction for gouge made of spherical glass beads is markedly lower than for angular quartz sand [Mair et al., 2002].

Laboratory experiments have made significant advances in understanding the effects of gouge on rock friction, but as shown above, the underlying micromechanical
processes of these effects remain elusive. Poor understanding of the micromechanics of
gouge deformation has obviously impeded the development of the next generation of
constitutive laws built upon a micromechanical framework to quantitatively interpret
friction data. With laboratory experiments, it is difficult to set up experiments under
identical boundary conditions in order to directly correlate variations in gouge friction to
variations of extrinsic factors, intrinsic factors, and corresponding deformation
mechanisms during simulated gouge deformation. Therefore, many important problems
related to micromechanics of gouge cannot be fully addressed by current laboratory
experiments. For example, outstanding questions include how deformation is partitioned
among mechanisms such as grain rolling, sliding, and fracturing, and how deformation
mechanisms affect both base level and second order frictional strength of fault gouge, and
evolve with grain size, shape, size distribution, configuration, and microstructure.

Numerical simulations of the frictional behavior of fault zones represent an
alternative approach for exploring micromechanisms of shear zone deformation, and
offer an outstanding opportunity to extend our knowledge of fault mechanics beyond the
domain accessible to laboratory observations [Mora and Place, 1998, 1999; Morgan and
Boettcher, 1999; Morgan, 1999; Place and Mora, 2000]. Unlike many continuum
numerical models based on the macroscopic and continuous media in which rheology is
assumed in advance (i.e., intrinsic properties are averaged) [Day, 1982; Fukuyama and
Madariaga, 1995; Madariaga et al., 1997; Tang, 1997], the distinct element method
(DEM) [Cundall and Strack, 1979] provides a way to study the dynamic behavior of
discontinuous granular materials, and therefore fault gouge, as a function of intrinsic
variables and contact physics. This technique has been successfully employed to
reproduce characteristic shear fracture arrays commonly observed in naturally and experimentally deformed gouges [Morgan and Boettcher, 1999].

One limitation in many of the recent DEM simulations, however, has been the use of circular gouge grains. Base friction values obtained from 2-D DEM simulations are about 0.3 [e.g., Morgan, 1999], significantly lower than the base level friction predicted by Byerlee’s law, raising concerns that the simulations represent non-physical results. Laboratory experiments carried out on real materials with equally simple 2-D geometries, e.g., quartz rods and even pasta, however, have yielded remarkably similar friction data to numerical simulations of 2-D circular particles, thereby confirming the first order DEM friction values [Frye and Marone, 2002]. Further idealized laboratory studies of 3-D spherical particles have demonstrated slightly higher friction values, approaching 0.45, but also show that friction increases with particle angularity [Mair et al., 2002]. These lab results serve to validate the DEM simulations, but show that circular particles are too simple to represent real fault gouge. Natural fault gouge is usually composed of angular-shaped grains that are thought to exhibit significantly less grain rolling and more grain interlocking than particle dynamics simulations [Mora and Place, 1998, 1999; Morgan and Boettcher, 1999; Mair et al., 2002]. Here, we further our understanding of the role of particle angularity on the first order friction value by considering irregularly shaped grains with different abundances within simulated fault gouge.

Laboratory experiments on angular sand also show that $\sigma_n$ plays an important role in the development of microstructures in fault gouge by controlling the active deformation mechanisms, i.e., rolling and sliding dominate in the non-fracturing regime, and fracture and grain size reduction are more active at higher normal stresses [Mair et
al., 2002]. The results suggest that active deformation mechanisms are not only dependent on grain shape, but also on $\sigma_n$. Therefore $\sigma_n$ may also lead to additional variations of friction. In fact, second order effects on friction associated with variations in $\sigma_n$ have been shown to produce a decreasing trend in friction observed in many laboratory experiments [e.g., Maurer, 1965; Murrell, 1965; Byerlee, 1967, 1968; Handin, 1969; Jaeger, 1970; Edmond and Murrell, 1971; Saffer et al., 2001; Saffer and Marone, 2003], but the dependency of friction on $\sigma_n$ has not been well studied in previous numerical simulations on rock friction. As it is often difficult to conduct laboratory experiments under exactly the same conditions to examine the effect of a single variable on the variation of rock friction, numerical experiments can provide a better understanding of effect of $\sigma_n$ on active deformation mechanisms and friction.

In order to study the variation of frictional strength and dynamic behavior of fault zones as a result of changing grain shape and $\sigma_n$, we carry out DEM simulations using grains constituted of bonded circular particles under a range of normal stresses from 5 to 100 MPa. In this way, irregularly shaped grains can be generated to reproduce more realistic fault gouge morphology, and we can quantify the effects of gouge grain shape and $\sigma_n$ on the friction of simulated granular assemblages. Simulations are carried out in 2-D for comparison with previous modeling studies. The results show that angular grain assemblages are stronger than rounded grain assemblages, as observed in laboratory experiments of 3-D materials [Mair et al., 2002]. Frictional strength of simulated granular assemblages increases nonlinearily with decreasing $\sigma_n$, and follows an inverse power law that is identical in form to a theoretical friction law based on Hertzian contact model [Bowden and Tabor, 1964; Jaeger and Cook, 1976; Villaggio, 1979]. The
decreasing trend of sliding friction with increasing $\sigma_n$ is comparable to recent lab observations [Saffer et al., 2001; Saffer and Marone, 2003]. Grain shape irregularity is also observed to affect the strength of granular assemblages. It determines the rate of change in friction by increasing both the coefficient and exponent of the friction law. Our results demonstrate that DEM simulations can appropriately represent the characteristic mechanical behavior of irregular granular gouge, bringing us one step closer to understanding the micromechanics of fault slip and friction.

2.3. Experimental Method

2.3.1. DEM

The distinct element method (DEM) [Cundall and Strack, 1979] is a numerical technique that was initially proposed as a new tool to investigate the mechanical behavior of assemblies of discs and spheres as analogs of soil, rock, or industrial materials. The principles on which DEM is based have been described very well by others [Cundall and Strack, 1979; Antonellini and Pollard, 1995; Morgan and Boettcher, 1999; Burbidge and Braun, 2002]. It has been shown that this technique is a suitable tool for modeling real granular materials, such as sand and fault gouge [Cundall and Hart, 1989; Morgan and Boettcher, 1999; Morgan, 1999]. Although most DEM simulations were carried out in 2-D, the technique can be also used to simulate 3-D assemblages at higher computational expense [e.g., Hazzard and Mair, 2003]. Previous DEM simulations have been limited in several ways: lack of grain fracture; use of circular or spherical particles; and lack of evolution of grain shape and size during the simulations. In contrast, in natural systems, highly angular particles undergo pervasive fracture and comminution during faulting and
shearing [Sammis et al., 1987; Marone and Scholz, 1989; Mair et al., 2002]. Ultimately, these limitations need to be overcome in order to simulate the shear zone deformation in a more realistic way.

As a first step, we examine the role of grain shape on base level friction of granular shear zones, maintaining a 2-D geometry for computational efficiency. In order to build angular grains, we introduce interparticle bonds. Various numerical models [Zubelwicz, 1987; Plesha and Aifantis, 1983; Trent, 1987; Iwashita and Hakuno, 1990; Bruno and Nelson, 1991; Bojtár and Bagi, 1993; Donzé and Magnier, 1995; Jirásek et al.; 1995] have been proposed to simulate breakable interparticle bonds and grain fracture. Here, we have incorporated a similar linear elastic particle bond model (Figure

![Diagram](image)

Figure 1. Schematic diagram of interparticle bond and its mechanical analogs. The bond between particles behaves as two elastic springs (a and b) that generate and transmit normal and shear forces, respectively, and an elastic beam (c) that transmits moment.
1) into DEM for the purpose of generating arbitrary-shaped grains, and eventually, for simulating fracture during granular shear [Chapter 3; Guo and Morgan, resubmitted]. The method builds on a bond model used in the Particle Flow Code in 2 Dimensions [Itasca Consulting Group, 1999] with some necessary modifications as described below.

In our model, two bonded particles are assigned a zero separation when the bond is formed, defining a zero force configuration. Dynamically, the bond between particles behaves as two elastic springs (normal and shear) (Figure 1a) and an elastic beam (Figure 1b). The normal spring, with normal stiffness \( k_n \), produces and transmits a restoring normal force (both tensile and compressive). The shear spring, with shear stiffness \( k_s \), produces and transmits a restoring shear force. The beam transmits a moment if a relative rotation occurs between the two bonded particles. The interparticle bonds are assumed to deform in a linear elastic manner within a predefined failure criterion for each mode, as the bonded particles are displaced and rotated from their equilibrium positions. Forces and moment within the elastic bond are proportional to bond stiffness and bond cross-sectional area, and therefore can be calculated from the known displacements by

\[
F_n = k_n \cdot A \cdot \delta_n \tag{1}
\]

\[
F_s = k_s \cdot A \cdot \delta_s \tag{2}
\]

\[
M = k_n \cdot I \cdot \theta \tag{3}
\]

where \( F_n, F_s, \) and \( M \) are the normal force, shear force, and moment within the bond, respectively. \( \delta_n, \delta_s, \) and \( \theta \) are the relative normal, shear, and angular displacements at the particle contact, respectively. Both the cross-sectional area of the bond \( A \) defined at
bond formation, and the moment of inertia of the bond cross-section \( I \), are a function of the effective radius of the bond cross-section \( R \), and defined as

\[ A = \pi \cdot R^2 \]  
(4)

\[ I = \frac{1}{4} \cdot A \cdot R^2 \]  
(5)

\( R \) is determined by the radius of two contact particles \( R_1 \) and \( R_2 \), and given by

\[ R = \frac{2 \cdot R_1 \cdot R_2}{R_1 + R_2} \]  
(6)

By assuming that tensile normal force is positive, the normal stress (both tensile and compressive) and shear stress acting on the bond can be defined as

\[ \sigma = \frac{F_n}{A} + \frac{|M|}{I} \cdot R \]  
(7)

\[ \tau = \frac{|F_s|}{A} \]  
(8)

For the case of unbonded particles in contact, contact force is described using the non-linear Hertz-Mindlin contact model [Mindlin and Deresiewicz, 1953; Johnson, 1985]

\[ F_n = \left( \frac{2G\sqrt{2R}}{3(1-v)} \right) \delta_n^{3/2} \]  
(9)

\[ F_s = \left( \frac{2(3R^2G^2(1-v))^{1/3}}{(2-v)} \right) \delta_n^{1/3} F_n^{2/3} \]  
(10)

where \( G \) is the shear modulus, and \( v \) is Poisson's ratio (Table 1).
Table 1. Parameters for numerical experiments.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental variables</td>
<td></td>
</tr>
<tr>
<td>Initial gouge zone thickness (^{(1)})</td>
<td>~ 11.25 mm</td>
</tr>
<tr>
<td>Shear strain rate (^{(1)})</td>
<td>~ 8.89 \times 10^{-5}</td>
</tr>
<tr>
<td>Total shear strain</td>
<td>200%</td>
</tr>
<tr>
<td>Applied normal stress on walls</td>
<td>5-100 MPa</td>
</tr>
<tr>
<td>Grain properties</td>
<td></td>
</tr>
<tr>
<td>Grain radius</td>
<td>300, 352.9, 415.2, and 488.5 \ \mu m</td>
</tr>
<tr>
<td>Exponent for grain size distribution ((D)) (see Equation 11)</td>
<td>0.5</td>
</tr>
<tr>
<td>Grain shape distribution ((S)) (^{(2)})</td>
<td>100% (T000)</td>
</tr>
<tr>
<td></td>
<td>75% (T025)</td>
</tr>
<tr>
<td></td>
<td>50% (T050)</td>
</tr>
<tr>
<td></td>
<td>25% (T075)</td>
</tr>
<tr>
<td></td>
<td>0% (T100)</td>
</tr>
<tr>
<td>Interparticle friction</td>
<td>0.5</td>
</tr>
<tr>
<td>Shear modulus</td>
<td>29 GPa</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.20</td>
</tr>
<tr>
<td>Interparticle bond properties</td>
<td></td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.20</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>69.6 GPa</td>
</tr>
<tr>
<td>Maximum tensile strength</td>
<td>\infty (^{(3)})</td>
</tr>
<tr>
<td>Maximum shear strength</td>
<td>\infty (^{(3)})</td>
</tr>
</tbody>
</table>

(1) Depend on normal stress and grain shape.
(2) \(S\) represents the degree of grain angularity quantified by the percentage of the triangular grains. For convenience, we use T100, T075, T050, T025, and T000 to represent five granular assemblages, respectively. \(T\) represents triangular grains and the number behind it is the percentage of the triangular grains.
(3) Prevents grain fracture.

2.3.2. Experimental Design

The major purpose of this paper is to examine the influence of \(\sigma_n\) and grain shape on the sliding friction of sheared granular assemblages. In order to study the effect of grain shape on sliding friction, we generated five different grain assemblages by proportionally distributing two different types of grains: rounded grains composed of 7 close-packed circular particles of equal size, and triangular grains composed of 6 close-packed circular particles of equal size (Figure 2b). The grain assemblages contained
Figure 2. Experimental design. (a) Initial reference assemblage of circular particles with $D$ value of 0.51, created by randomly arranging a predetermined number of circular particles of four sizes within the domain with periodic boundaries. Boundaries were moved inward until equilibrium isotropic mean stress was attained; (b) Initial grain assemblage was created by replacing circular particles of the same size with rounded and/or triangular grains in certain proportions. Rounded grains define two rough-surfaced walls for all grain assemblages. Normal stress was maintained at a constant value throughout each experiment. Deformation was induced by moving the top wall to the right at a constant velocity, $v$, and keeping the bottom wall fixed. Shaded vertical and horizontal columns are strain markers.
different percentages of triangular grains, i.e., 0%, 25%, 50%, 75%, or 100%, defined by grain abundance. Four different grain sizes were created by bonding particles of four different radii, given as 100, 117.6, 138.4, and 162.8 μm. As grain size distribution during shear zone deformation evolves through cataclasis toward a power law distribution [Sammis et al., 1986, 1987], the relative abundances of four different sized grains satisfy a power law relationship. This law is defined with a fractal dimension $D$ and given by the following relationship [Turcotte, 1986; Sammis et al., 1986, 1987; Morgan and Boettcher, 1999]:

$$D = \log(N_i/N_0)/\log(R_i/R_0)$$  \hspace{1cm} (11)

where $N_i$ and $N_0$ are numbers of grains with a radius equal to $R_i$ and $R_0$, respectively (Table 1). The value of $D$ in our assemblages is held constant at 0.51.

A reference circular particle assemblage also with $D$ value of 0.51 was created (Figure 2a) by randomly arranging a predetermined number of circular particles of four sizes within the domain with periodic boundaries that were moved inward until the isotropic mean stress was attained. There are about 16 particles in a vertical column of the circular particle assemblage. The initial grain assemblages (Figure 2b) were created by proportionally replacing circular particles of a given size with rounded and/or triangular grains between two rough-surfaced walls. Only rounded grains are used within the walls so that wall surface roughness is the same for all grain assemblages. By maintaining constant wall surface roughness, initial grain configuration (i.e., positions), and grain size distribution for all the experiments, we can isolate the specific effects of grain angularity and normal stress. Before the start of the experiment, the granular assemblage was compacted by shifting the top wall back and forth under the applied
experimental normal stress until the equilibrium stress and porosity (Table 2) were reached. The granular assemblage was then deformed by moving the upper wall at constant velocity to the right, while keeping the lower wall fixed. The constant wall velocity condition equates to infinite wall stiffness, precluding velocity variations associated with the stick-slip deformation. Data on grain displacements and interactions were recorded after each 2% shear strain increment.

**Table 2.** Equilibrium porosity for granular assemblages of different grain composition sheared under various normal stresses.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Normal stress (MPa)</th>
<th>5</th>
<th>25</th>
<th>50</th>
<th>75</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>T100</td>
<td>0.602</td>
<td>0.593</td>
<td>0.582</td>
<td>0.573</td>
<td>0.57</td>
<td></td>
</tr>
<tr>
<td>T075</td>
<td>0.593</td>
<td>0.578</td>
<td>0.566</td>
<td>0.56</td>
<td>0.553</td>
<td></td>
</tr>
<tr>
<td>T050</td>
<td>0.57</td>
<td>0.566</td>
<td>0.553</td>
<td>0.546</td>
<td>0.542</td>
<td></td>
</tr>
<tr>
<td>T025</td>
<td>0.566</td>
<td>0.547</td>
<td>0.54</td>
<td>0.534</td>
<td>0.528</td>
<td></td>
</tr>
<tr>
<td>T000</td>
<td>0.533</td>
<td>0.528</td>
<td>0.523</td>
<td>0.519</td>
<td>0.516</td>
<td></td>
</tr>
<tr>
<td>C100</td>
<td>0.455</td>
<td>0.443</td>
<td>0.435</td>
<td>0.43</td>
<td>0.426</td>
<td></td>
</tr>
</tbody>
</table>

For the purpose of investigating the variation of sliding friction due to $\sigma_n$ and grain shape, the DEM experiments for each of the five grain assemblages with different grain shape characteristics were carried out under identical boundary conditions (i.e., wall surface roughness and strain rate are the same for all experiments) over a range of normal stresses, i.e., 5, 25, 50, 75, and 100 MPa. For comparison, we also carried out a similar suite of numerical experiments using the unbonded, circular particles with the same size and size distribution as the rounded grains (Figure 2a). Parameters for the numerical experiments are listed in Table 1.
2.4. Results

In this study, friction of the granular assemblage is defined as the ratio of shear stress to normal stress, i.e., \( \mu = \tau / \sigma_n \). As \( \sigma_n \) is held constant during a given experiment, \( \mu \) serves as a normalized measure of shear stress. The typical friction vs. shear strain curve of our numerical experiments is characterized by a peak friction, defined as \( \mu_{\text{peak}} \), reached within the first 40% shear strain and followed by a gradual decrease over about 10% shear strain. Friction then fluctuates about a residual value, defined as \( \mu_{\text{mean}} \) (Figure 3). The fluctuations in friction arise from stress averaging over the small number of particles in the assemblage, as well as heterogeneous interactions along the irregular shear zone walls. The amplitude of friction fluctuations generally decreases with increasing particle abundance [e.g., Morgan, 1999], approaching the smooth friction trends observed in laboratory experiments in the absence of stick-slip behavior [e.g., Mair et al., 2002]. Since all of the sheared assemblages begin to slide steadily by 60% shear strain, we refer to the friction after 60% strain increments as sliding friction in order to distinguish between \( \mu_{\text{peak}} \) and \( \mu_{\text{mean}} \). Maximum sliding friction \( \mu_{\text{max}} \), representative of shear strength of the assemblage, is calculated as the sum of \( \mu_{\text{mean}} \) and its standard deviation. Data on frictional and micromechanical properties of granular assemblage were recorded at every 2% shear strain. Again, only the data after 60% shear strain were used for the analysis of variation \( \mu_{\text{max}} \) and micromechanical properties of granular assemblage.
2.4.1. Effects of $\sigma_n$ and Grain Shape on $\mu_{\text{max}}$

Both grain shape and normal stress affect variations of $\mu_{\text{max}}$. Representative examples are shown in Figure 3. Figure 3a plots friction calculated for three assemblages composed of different shaped grains: triangular, rounded, and circular, as a function of shear strain at low $\sigma_n$ (5 MPa). The rounded grain and circular particle assemblages show similar frictional strength and behavior. However, $\mu_{\text{peak}}$ and magnitude of fluctuations of the rounded grain assemblage are slightly higher than these of the circular particle assemblage. Variations of friction for both assemblages are similar in form and magnitude to the laboratory experiments on 2-D pasta and quartz rods [Frye and Marone, 2002]. The triangular grain assemblage is markedly stronger than the other two assemblages, reaching $\mu_{\text{peak}}$ at 2.8 and $\mu_{\text{max}}$ at 1.49. Variations of friction with shear strain are characterized by longer period and greater magnitude saw-tooth fluctuations than the rounded grain assemblage, a result of the greater irregularity of particles. For high $\sigma_n$ (100 MPa) experiments (Figure 3b), friction curves of the rounded grain and circular particle assemblages match each other very well in terms of peak friction and variations in friction with shear strain. The triangular grain assemblage again exhibits higher friction values and large fluctuations in friction compared with the others, but significantly lower than observed at 5 MPa. The results show that both grain shape and $\sigma_n$ have significant effects on the magnitude of $\mu_{\text{max}}$. At low $\sigma_n$, $\mu_{\text{max}}$ of the rounded grain assemblage is about 0.49, close to results of laboratory experiments conducted on 3-D glass beads under similar conditions [Mair et al., 2002], and decreases to 0.26 when $\sigma_n$ increases to 100 MPa. The value of $\mu_{\text{max}}$ for the triangular grain assemblage also
Figure 3. Friction data for granular assemblages composed of different shaped grains under low (a) and high (b) normal stresses. Frictional behaviors of the rounded grain assemblages are similar to the circular particle assemblages. The triangular grain assemblages are much stronger than the other two.
decreases with increasing $\sigma_n$, from 1.49 at 5 MPa to 0.41 at 100 MPa (Table 3). Therefore, the effect of grain shape on friction becomes more significant as $\sigma_n$ decreases.

Table 3. Maximum sliding friction for granular assemblages of different grain composition sheared under various normal stresses.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Normal stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>5</td>
</tr>
<tr>
<td>T100</td>
<td>1.49</td>
</tr>
<tr>
<td>T075</td>
<td>1.246</td>
</tr>
<tr>
<td>T050</td>
<td>0.864</td>
</tr>
<tr>
<td>T025</td>
<td>0.753</td>
</tr>
<tr>
<td>T000</td>
<td>0.488</td>
</tr>
<tr>
<td>C100</td>
<td>0.37</td>
</tr>
</tbody>
</table>

The variation of sliding friction with both $\sigma_n$ and grain shape was rigorously quantified by carrying out a series of numerical experiments under a wide range of normal stresses. Specifically, five numerical experiments were conducted at each normal stress by systematically changing the proportion of triangular and rounded grains to constrain the effects of grain shape. Values of $\mu_{\text{max}}$ are listed in Table 3. For each grain assemblage, $\mu_{\text{max}}$ decreases nonlinearly with increasing $\sigma_n$. At each normal stress, $\mu_{\text{max}}$ decreases with decreasing proportion of triangular grains. These relationships hold true for all five grain assemblages of different grain shape compositions under all applied experimental stresses. A decreasing trend of $\mu_{\text{max}}$ with increasing $\sigma_n$ is also observed for the circular particle assemblages, but with a lower decreasing rate compared to the grain assemblages. The final results are well fit by inverse power law relationships between $\mu_{\text{max}}$ and $\sigma_n$ (Figure 4), and can be expressed by the following equation:

$$ \mu_{\text{max}} = a\sigma_n^{-b} $$

(12)
Best fit values of coefficient $a$ and exponent $b$ are listed in Table 4. Both of them tend to increase with increasing gouge angularity.

![Graph](image)

Figure 4. Maximum sliding friction as a function of normal stress for circular particle assemblage and five grain assemblages with different grain shape compositions. The decreasing trends of maximum sliding friction are fitted by inverse power laws.

**Table 4.** Best fit values of coefficient $a$ and exponent $b$ for granular assemblages of different grain composition sheared under various normal stresses.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>$a$</th>
<th>$b$</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>T100</td>
<td>2.8026</td>
<td>0.4037</td>
<td>0.9814</td>
</tr>
<tr>
<td>T075</td>
<td>2.6526</td>
<td>0.4448</td>
<td>0.9761</td>
</tr>
<tr>
<td>T050</td>
<td>1.6372</td>
<td>0.3644</td>
<td>0.9677</td>
</tr>
<tr>
<td>T025</td>
<td>1.2614</td>
<td>0.3159</td>
<td>0.9978</td>
</tr>
<tr>
<td>T000</td>
<td>0.6932</td>
<td>0.2098</td>
<td>0.9942</td>
</tr>
</tbody>
</table>

2.4.2. Effects of $\sigma_n$ and Grain Shape on Micromechanical Behavior of Granular Assemblages

Grain assemblages deformed under low $\sigma_n$ of 5 MPa develop narrow, and high porosity zones of shear bands parallel and close to the top wall. Both the gradient of grain shear displacement (i.e., calculated as the directional derivative of the horizontal grain displacement [e.g., Morgan and Boettcher, 1999]), and the distortion of the initially
vertical strain marker, denoted by the shaded column of grains (Figures 5b and c), show that grain displacement is restricted to this band. At this low $\sigma_n$, short-range grain bridges develop readily, supporting the load of the wall (Figures 5a, b, and c). This leads to high dilation and formation of high pore space near the top wall in all assemblages. Despite the localized shearing, rotating grains are uniformly distributed across the upper half of the rounded grain assemblage (Figure 5b), whereas rotating grains in the triangular grain assemblage are clustered along poorly developed high angle shear bands (Figure 5c).

In contrast, at the high normal stress of 100 MPa, deformation is more distributed throughout the whole domain, and characterized by relative homogeneous pore space and short-lived grain bridges that extend across the domain (Figures 5e and f). The high dilation of the assemblage near the top wall at the normal stress of 5 MPa is not observed. The greatest displacements still occur close to the top wall; grains also show the highest rotations in this region. In the rounded grain assemblage, there are a few nonrotating grains close to the bottom wall, while rotating grains are uniformly distributed in the triangular grain assemblage (Figures 5d and e). The most distinct difference in deformation state between circular particle assemblage and triangular and rounded grain assemblages is that the circular particle assemblage shows less dilation, lower porosity, lower abundance of rotating particles, and higher degree of localization (Figures 5a and d).

A full understanding of how $\sigma_n$ and grain shape affect $\mu_{\text{max}}$ requires a more complete knowledge of how these factors affect the micromechanical properties of granular assemblage. Statistics on grain rotations, contact sliding, coordination number,
Figure 5. Deformation state of circular particle (C000), rounded grain (T000), and triangular grain (T100) assemblages at low and high normal stresses. (a) Circular particle, 5 MPa; (b) Rounded grain, 5 MPa; (c) Triangular grain, 5 MPa; (d) Circular particle, 100 MPa; (e) Rounded grain, 100 MPa; (f) Triangular grain, 100 MPa. Left panel: grain configuration; Center panel: grain rotation. Higher degrees of rotation are indicated by darker colors; Right panel: gradient of horizontal displacement. Darker colors represent more intense shear strain. See text for discussion. Arrow points to inclined shear band.
and contact force after 60% shear strain demonstrate that $\sigma_n$ and grain shape have significant influences on these micromechanical properties.

2.4.2.1. Grain Rotation

The average percentage of rotating grains of each grain assemblage is plotted against $\sigma_n$ in Figure 6a. The percentage of rotating grains increases with increasing proportion of triangular grains, and also with $\sigma_n$, except for the rounded grain assemblage. The percentage of rotating grains in the rounded grain assemblage decreases from 74% to 70% with an increase of $\sigma_n$ from 5 to 25MPa. Further increase of $\sigma_n$ does not significantly change the number of rotating grains in the rounded grain assemblage; this value remains around 70%. The rotational tendency of triangular grains is more sensitive to $\sigma_n$, but in the opposite sense. The percentage of rotating grains in triangular grain assemblages increases nonlinearly with increasing $\sigma_n$, from 40% at 5 MPa to 91% at 100 MPa. As the percentage of rotating rounded grains changes little with $\sigma_n$, this quantity must be mainly controlled by the proportion of triangular grains in assemblages of multiple shaped grains. The percentage of rotating particle in the circular particle assemblage is much lower than the rounded grain assemblage, especially at normal stress of 5MPa, and decreases with increasing $\sigma_n$ at normal stresses higher than 25 MPa.

The variations in the average angle of grain rotation with $\sigma_n$ and grain shape (Figure 6b) show a similar pattern as noted for the percentage of rotating grains. The mean angle of grain rotation does not change significantly with $\sigma_n$ for the rounded grain assemblage. By comparison, the mean angle of grain rotation in the triangular grain assemblage is lower than that for the rounded grain assemblage at normal stress of 5MPa,
Figure 6. (a) Average percentage of rotating particles or grains for circular particle assemblage and five grain assemblages of different grain shape composition plotted against normal stress; (b) Average angle of rotation for same assemblages plotted against normal stress. All but the circular particle and rounded grain assemblages show increasing percentage of rotating grains and average angle of rotation with increasing normal stress. Rotation also increases with increasing abundance of triangular grains at normal stresses higher than 5 MPa.
but increases nonlinerly with increasing $\sigma_n$. Just as observed with the percentage of rotating grains, a transition occurs at normal stress of 25MPa. The variations in the mean angle of grain rotation of the other assemblages reflects the combined trends in rotational behavior of the rounded grain and triangular grain assemblages, dependent on the relative abundance of triangular grains (Figure 6b). The mean angle of particle rotation in the circular particle assemblage is smaller than in the rounded grains assemblage, and decreases with increasing $\sigma_n$.

2.4.2.2. Contact Sliding

Grain shape has a more significant influence on the percentage of sliding contacts than does $\sigma_n$ (Figure 7). Yet, the percentage of sliding contacts within all of the grain assemblages does not change as dramatically with $\sigma_n$ and grain shape as does the percentage of rotating grains. Contacts between triangular grains have a much greater tendency to slide than those between rounded grains. On average, about 15% of the grain contacts slide over each time step in the triangular grain assemblage, whereas only 9% slide in the rounded grain assemblage. The average percentage of sliding contacts in the triangular grain assemblage increases about 1% with increase of $\sigma_n$ from 5 to 25 MPa, but then shows little change with further increase in $\sigma_n$ (leveling off at about 15.5%). The percentage of sliding contacts in the rounded grain assemblage decreases steadily from 10.3% to 7.5% as $\sigma_n$ increases from 5 to 100 MPa. The percentages of sliding contacts of the other grain assemblages decrease with increasing abundance of rounded grains and $\sigma_n$. This trend is consistent with variations of sliding contacts in the triangular and rounded grain assemblages. The circular particle assemblage exhibits the similar
decreasing trend in the percentage of sliding contacts with increasing $\sigma_n$, but less abundance of sliding contact at each normal stress compared to the rounded grain assemblage.

![Graph showing sliding contacts percentage vs. normal stress](image)

Figure 7. Average percentage of sliding contacts for five granular assemblages of different grain shape composition and one circular particle assemblage plotted against normal stress. The percentages of sliding contacts of all the granular assemblages decrease with decreasing gouge grain angularity, and normal stress at normal stress higher than 25 MPa.

2.4.2.3. Coordination Number

A plot of average number of contacts per grain, i.e., coordination number, reveals that grain shape strongly influences grain connectivity (Figure 8). Coordination number increases proportionally with increasing abundance of rounded grains. At the same normal stress, coordination number in the rounded grain assemblages is about 20% higher than in the triangular grain assemblages. Variations in coordination number of the other grain assemblages also follow similar trends, i.e., a 25% increment of rounded grains results in about 5% increment in coordination number. Coordination numbers of
all the grain assemblages increase with increasing $\sigma_n$, in a very similar pattern: the rate of change in coordination number decreases with increasing $\sigma_n$, and coordination number increases about by a factor of 1.6 as $\sigma_n$ increases from 5 to 100 MPa. Coordination number of the circular particle assemblage also shows an increasing trend with increasing $\sigma_n$. It is greater than that of the rounded grain assemblage at normal stresses lower than 50 MPa, but becomes slightly smaller at higher normal stresses.

![Figure 8. Average coordination number for circular particle assemblage and five grain assemblages of different grain shape composition plotted against normal stress. Coordination numbers of all assemblages increase with decreasing grain angularity and increasing normal stress.](image)

2.4.2.4. Contact Force

At a given $\sigma_n$, the average contact force increases with increasing abundance of triangular grains. The contact force of the rounded grain assemblage is about 40% lower than that of the triangular grain assemblage at 5 MPa, but only 25% at 100 MPa, even though the absolute difference between the average contact forces increases by more than five times as $\sigma_n$ increases from 5 to 100 MPa. To study the effect of both $\sigma_n$ and grain
angularity on the variation of contact force, the average contact force of each assemblage at a given $\sigma_n$ is normalized by the average contact force of that assemblage at normal stress of 100 MPa. A plot of normalized average contact force for each assemblage (Figure 9) demonstrates a nearly linear relationship between $\sigma_n$ and contact force for all of the assemblages. The normalized average contact forces increase with increasing $\sigma_n$, and their rates of increase are similar and show little dependency on the proportion of rounded and triangular grains (Figure 9).

![Figure 9. Average contact force for circular particle assemblage and five grain assemblages of different grain shape composition plotted against normal stress. The average contact force is normalized by the maximum average contact force of that assemblage at 100 MPa. Normalized average contact forces increase with increasing normal stress, and their increasing rates are similar and show little dependency on the grain angularity.](image)

2.4.2.5. Volume of Assemblage

Volume changes with increasing $\sigma_n$ are markedly different for the rounded and triangular grain assemblages. The average volume of each grain assemblage at a given $\sigma_n$ is normalized by the average volume of that assemblage at normal stress of 5 MPa. In this
way, we can document the effects of $\sigma_n$ on dilation. The normalized volume of the triangular grain assemblage decreases more rapidly than for the rounded grain assemblage with increasing $\sigma_n$ (Figure 10). The normalized volumes of the mixed rounded and triangular grain assemblages at each normal stress are similar to each other in magnitude, and intermediate to those of the rounded and triangular grain assemblages. The normalized volume of the 75% triangular grain assemblage, which is higher at the normal stress of 25 MPa, decreases more rapidly than the 25% triangular grain assemblage with increasing $\sigma_n$. The normalized volume of the assemblage of equal abundance of rounded and triangular grains lies between them. The normalized volume of the circular particle assemblage tends to decrease at a slightly higher rate than the rounded grain assemblage.

Figure 10. Average volume for circular particle assemblage and five grain assemblages of different grain shape composition plotted against normal stress. Volume of each assemblage is normalized by the average volume of that assemblage at 5 MPa. Normalized average volumes decrease with increasing normal stress, and their decreasing rates increase with increasing grain angularity.
2.5. Discussion

2.5.1. Maximum Sliding Friction

Variation in friction of faults during sliding is a fundamental factor influencing the generation of earthquakes. Byerlee’s law defines a linear relationship between shear and normal stress, which presumes a constant friction coefficient under normal stress less than 200 MPa [Byerlee, 1978]. This linear friction law can be used to estimate the mean strength of natural faults. However, it neglects important second order variations in friction that may govern fault behavior. Results of our DEM simulations demonstrate a first order dependence of friction on grain angularity, as well as a second order dependence on $\sigma_n$ captured by Equation 12, both of which may contribute to the slip behavior responsible for unstable sliding that leads to earthquakes.

Several investigators have reported nonlinear friction laws similar to Equation 12 that show $\sigma_n$ dependence, providing a theoretical basis for our interpretation of the simulated friction data [Bowden and Tabor, 1964; Jaeger and Cook, 1976; Villaggio, 1979]. If surface deformation occurs entirely by the mechanism of elastic yielding of asperities, the area of contact $A$ is proportional to $f_n^{2/3}$ according to Hertzian contact law [Mindlin and Deresiewicz, 1953; Johnson, 1985]

$$A = k f_n^{2/3}$$  \hspace{1cm} (13)

where $f_n$ is normal force, and $k$ is a constant related to elastic and geometrical properties of the materials. Shear force $f_s$ can be expressed as

$$f_s = s A$$  \hspace{1cm} (14)

where $s$ is the shear strength of materials. Therefore friction is given by

$$\mu = \frac{f_s}{f_n} = s k f_n^{2/3} / f_n = s k f_n^{-1/3}$$  \hspace{1cm} (15)
For example, friction of a diamond stylus sliding on a surface of diamond was found to follow the above friction law [Bowden and Tabor, 1964].

The value for $\mu_{max}$ observed in our numerical experiments also shows an inverse power law relationship with $\sigma_n$ (Figure 4). As contact forces in our simulations are calculated using the non-linear Hertz-Mindlin contact model, our results are consistent with the above theoretical friction law. We obtain a range of power law exponents $b$, spanning from 0.21 to 0.40 (Table 4), which bracket the theoretical exponent of 1/3 (Equation 15). The variations in numerical values are systematic, however, indicating a strong dependence of grain shape. The exponent $b$ is observed to increase with increasing proportion of triangular grains. This relationship suggests that the presence of non-spherical grains changes the relationship between contact force and contact area. We propose, therefore, that the exponent $b$ is also a function of grain shape. For the same reason, the constant $k$ also appears to change with normal force in our simulations. To summarize the effect of grain shape on $\mu_{max}$, we derive the following friction law based on the best fit values of coefficient $a$ and exponent $b$ in Table 4.

$$\mu_{max} = (2.244S + 0.687) \sigma^{-(0.207S + 0.244)}$$

(16)

where $S$ is the proportion of triangular grains in range of 0 to 100%. This friction law encapsulates the dual dependence of $\mu_{max}$ on both $\sigma_n$ and grain shape. It shows that $\mu_{max}$ decreases with increasing $\sigma_n$ in a power form, and grain shape determines the rate of change by increasing both the coefficient and exponent of the friction law.

The decreasing trend of rock friction with increasing $\sigma_n$ has been observed in many laboratory experiments conducted under a wide range of normal stresses [e.g., Maurer, 1965; Murrell, 1965; Byerlee, 1967, 1968; Handin, 1969; Jaeger, 1970; Edmond
and Murrell, 1971; Saffer et al., 2001; Saffer and Marone, 2003]. In particular, Saffer and Marone [2003] reported on the coefficient of sliding friction of a series of direct shear experiments conducted on gouge materials of different compositions, i.e., quartz, smectite powder, smectite-quartz mixtures, and natural illite shale over a range of normal stresses from 5 to 150 MPa. Their results also show a strong second order dependency of sliding friction on $\sigma_n$ for all the gouge materials, in an inverse power form (Figure 11). For the direct comparison between experimental observations and the numerical friction law (Equation 16), we plot Equation 16 in Figure 11 for a fault gouge composed of 50% triangular grains and 50% rounded grains. Therefore, a value of 0.5 is assigned to the parameter $S$, and the coefficient and exponent of the numerical friction law are 1.81 and 0.35, respectively. The decreasing trend of sliding friction predicted by the numerical friction law is comparable in form to those of smectite and smectite-quartz mixture, and yields predicted sliding friction values close to those of quartz and illite.

Compared to the best fit values of coefficients and exponents for numerical sliding friction (Table 4), the best fit coefficients for the experimental data fall into a narrower range from 0.83 to 1.14, while the best fit exponents define a wider range from 0.08 to 0.54 (Table 5). Clearly, both the exponent and coefficient vary as a function of clay mineral abundance and composition, introducing first order variation in experimental sliding friction that we have not simulated. No specific data are available to examine the role of grain shape in the variation of these parameters, or to make direct comparisons between numerical and experimental results of the first order effect of grain angularity. However, alignment of platy clay minerals is suggested to be a key factor controlling the strength of clay-rich gouges [Lupini et al., 1981; Chester and Logan,
Therefore, variations in the best fit coefficient and exponent for the experimental sliding friction, particularly at low stresses, may be a function of preferred clay grain orientation.

Figure 11. Comparison between experimental sliding friction (from Saffer and Marone, 2003) and sliding friction predicted by numerical friction law (Equation 16). The decreasing trends of experimental sliding frictions are fitted in an inverse power law form. Equation 16 is plotted by assuming that fault gouge is composed of 50% triangular grains and 50% rounded grains, i.e., S = 0.5.

<table>
<thead>
<tr>
<th>Gouge</th>
<th>a</th>
<th>b</th>
<th>R²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Smectite</td>
<td>1.138</td>
<td>0.5372</td>
<td>0.9158</td>
</tr>
<tr>
<td>50% Smectite/50% Quartz</td>
<td>1.1782</td>
<td>0.3688</td>
<td>0.9666</td>
</tr>
<tr>
<td>Illite</td>
<td>0.8185</td>
<td>0.1335</td>
<td>0.9062</td>
</tr>
<tr>
<td>Quartz</td>
<td>0.8327</td>
<td>0.0762</td>
<td>0.7959</td>
</tr>
</tbody>
</table>

The first order variations of friction due to grain angularity observed in our numerical simulations are consistent with the observations made from laboratory experiments [Mair et al., 2002]. Our data also show the second order dependency of friction on σ₀, comparable to the recent laboratory results [Saffer et al., 2001; Saffer and
Marone, 2003]. Both effects of $\sigma_n$ and grain angularity on friction can be defined by an inverse power law (Equation 16) that is identical in form to the theoretical friction law derived from Hertzian contact model (Equation 15).

2.5.2 Underlying Micromechanisms

The results of our numerical experiments demonstrate that the variation of $\mu_{\text{max}}$ is a response to changes in $\sigma_n$ and grain angularity, which in turn affect on the micromechanical behavior of granular assemblage. Previous studies on circular particle assemblages suggested that the reduction in $\mu_{\text{max}}$ with increased $\sigma_n$ for the circular particle assemblage was due to the tighter grain packing, inhibited contact sliding, and enhanced particle rolling [Morgan, 1999]. Similar effects of $\sigma_n$ on micromechanical behavior of granular assemblage are also observed in our simulations. For example, dilation is inhibited at high $\sigma_n$ for all the granular assemblages (Figure 10). The coordination number also increases with $\sigma_n$ (Figure 8), whereas percentage of sliding contacts is nearly constant (Figure 7). Therefore, the absolute number of sliding contacts increases with $\sigma_n$. The effects of $\sigma_n$ on these properties are apparently small, defining the second order dependence of friction. Grain angularity may result in more significant variations in micromechanical behavior of the granular assemblage.

Grain shape variations introduce important influences on deformation mechanisms that can affect micromechanical and frictional properties of granular assemblages. At a given $\sigma_n$, the circular particle and rounded grain assemblages achieve a tighter packing than the triangular grain assemblage, as indicated by their lower porosity (Figure 5) and higher coordination number (Figure 8); strain is more frequently localized
along several rows of grains parallel to shear direction or along low angle, oblique shear bands (Figure 5); and deformation is mainly accommodated by grain rolling and sliding, resulting in lower dilation and reduced sliding friction. This observation is consistent with previous studies [Morgan, 1999; Mair et al., 2002]. In contrast, the triangular grain assemblage is characterized by a high abundance of jostling grains, bouncing against, but barely rolling over each other due to grain interlocking; strain tends to be localized along high angle, oblique shear bands or distributed across the whole domain; and deformation is mainly accommodated by grain rotation and sliding, leading to high dilation and increased sliding friction.

Our data also reproduce the first order dependency of sliding friction on grain angularity that is observed in the laboratory experiments [Mair et al., 2002]. Although at a normal stress of 100 MPa, $\mu_{\text{max}}$ of the 2-D triangular grain assemblage (0.41) is still significantly lower than typical results of 3-D laboratory experiments (around 0.6) (Figure 4). The discrepancy may be explained by differences in the abundance of gouge grains, grain size, size distribution, and boundary conditions between numerical and laboratory experiments. We have not investigated these parameters in this study. In addition, laboratory experiments on 2-D glass rods and 3-D glass beads demonstrate that 2-D friction is smaller than 3-D friction due to the lack of out-of-plane particle contacts [Frye and Marone, 2002]. Therefore, numerical experiments in 3-D [e.g., Hazzard and Mair, 2003] would need to be carried out to verify if low $\mu_{\text{max}}$ is a result of the effect of grain dimensionality on sliding friction.

Enhanced grain rolling among rounded grains has been proposed as an explanation for low macroscopic frictional strength in numerical models [Mora and
Place, 1998, 1999; Morgan, 1999; Mair et al., 2002]. Our results, however, reveal a more complicated picture. The characteristics and importance of active deformation mechanisms are influenced by both $\sigma_n$ and grain shape. With the exception of the experiments conducted under low normal stress of 5 MPa, all of the experiments show increased rather than decreased angles of grain rotation, and the greater abundance of rotating grains in assemblages with higher proportions of triangular grains (Figure 6). Furthermore, we see increasing angles of grain rotation and percentage of rotating grains with increasing $\sigma_n$ and decreasing $\mu_{\text{max}}$. These differences between lab and numerical results may arise from differences in deformation mechanisms. In direct shear experiments on thin layers of angular quartz sand and spherical glass beads [Mair et al., 2002], normal stress of 5 MPa defines a non-destructive deformation regime (i.e., with little grain comminution), where grain rolling and sliding are dominant deformation mechanisms. Under normal stresses over 20 MPa, grain fracture becomes more important. In our simulations, however, grain fracture was not allowed, so deformation must always be accommodated by grain rolling and sliding. Therefore, grain rolling, characterized by enhanced grain rotation but reduced grain translation (i.e., horizontal displacement) may be a more significant deformation mechanism in our highly angular assemblages at high normal stresses. Consequently, the low $\mu_{\text{max}}$ of fault gouge can not be explained simply by enhanced grain rolling due to grain shape, as previously argued by others [Mora and Place, 1998, 1999; Morgan, 1999; Mair et al., 2002].

In real granular shear zones, one of the fundamental observations about fault zones is that damaged wall rocks undergo grain size reduction during cataclastic flow [Sammis et al., 1986, 1987; Scholz, 1990; Blenkinsop, 1991], and angular rock fragments
are progressively rounded by abrasion [Blenkinsop, 1991; Morgan et al., 1996]. Our results have shown the significant effects of grain shape on the frictional behavior of simulated granular shear zone. Therefore, continuous changes in grain shape and size during simulation, optimally, due to the natural processes of grain fracture and abrasion, should be included in numerical simulations in order to obtain a comprehensive understanding of dynamics and evolution of natural fault zones. This topic is the subject of a subsequent paper [Chapter 3; Guo and Morgan, resubmitted].

2.6. Conclusions

DEM simulations of granular shear using irregularly shaped grains composed of bonded particles show that both normal stress, $\sigma_n$ and grain shape have significant effects on frictional strength of our simulated granular assemblages. Observed $\mu_{\text{max}}$ decreases with increasing $\sigma_n$ in a power law form as predicted by a theoretical friction law derived from the Hertzian contact law. This relationship can be represented by the best fit power law equation (Equation 16). Grain shape controls the dependence of $\mu_{\text{max}}$ on $\sigma_n$ by influencing both the coefficient and exponent of the best-fit friction law.

In the absence of grain fracture, the triangular grain assemblage at high normal stresses is characterized by enhanced grain rotation but reduced grain translation compared with the rounded grain assemblage. Grain interlocking is significant, causing grain jostling, higher dilation, more distributed deformation, and higher $\mu_{\text{max}}$. Enhanced grain rolling does reduce the macroscopic frictional strength of our simulated granular assemblages, however, grain rolling cannot adequately explain the low $\mu_{\text{max}}$ values of the triangular grain assemblage observed at a normal stress of 100MPa.
Chapter 3

The Frictional and Micromechanical Effects of Grain Communion
in Fault Gouge from Distinct Element Simulations

3.1. Abstract

Natural fault zones undergo pervasive grain comminution during faulting and shearing, producing progressive changes in fault gouge properties. We simulate the comminution process of quartz gouge using the distinct element method (DEM) to examine the influences of grain comminution and associated dynamic changes in grain characteristics on the frictional and micromechanical behavior of granular shear zones. Rounded and triangular grains are constructed from clusters of circular particles, connected by some breakable bonds, allowing for grain fracture and comminution. DEM experiments are conducted by shearing identical granular assemblages composed of either rounded or triangular grains of different strengths over a range of normal stresses from 5 to 100 MPa. The results show that grain comminution with strain changes the partitioning of different deformation mechanisms, mainly by changing grain shape and size. Grain comminution may decrease or increase gouge strength, depending on the direction and degree of change in grain shape. Increases in grain angularity lead to significant increases in frictional strength of fault gouges, while increases in grain elongation tend to decrease in frictional strength. The final strength results from the competition between strength reduction by fracturing and strength variation by changes in grain shape and grain size distribution. Our simulations also demonstrate that the intensity and probability of grain comminution in narrow grain size gouges is affected by shape, strength (e.g., due to mineralogy), and normal stress.
3.2. Introduction

Fault gouge, the product of wear and fragmentation of fault surfaces, undergoes progressive grain comminution during faulting and shearing in natural fault zones [Sammis et al., 1986; Marone and Scholz, 1989; Marone et al., 1990]. Grain comminution is a destructive deformation mechanism that accommodates shear strain, dissipates energy, reduces grain size, changes grain shape, and results in characteristic grain configurations and distributions of particle sizes [Sammis et al., 1987; Marone and Scholz, 1989]. These changes may also affect the stability of fault zones [Engelder et al., 1975; Byerlee et al., 1978; Logan et al., 1979; Moore et al., 1988; Tullis et al., 1989; Biegel et al., 1989; Marone and Scholz, 1989; Mair et al., 2002; Monzawa and Otsuki, 2003; Guo and Morgan, 2004]. Therefore, a knowledge of the effects of grain comminution on fault zone deformation is critical to understanding the conditions for unstable faulting in the earth. Overall influences of grain comminution on frictional and micromechanical properties of fault gouge, however, remain poorly understood, because of complex coupling between frictional resistance and dynamic changes in gouge microstructure and grain characteristics during frictional sliding of fault surfaces [e.g., Beeler et al., 1996].

The microstructural effects of grain comminution have been extensively studied in both field and laboratory. The comminution mechanism proposed by Sammis et al. [1987] suggests that the probability of comminution is controlled by the relative size of nearest-neighbor particles. Comminution is most likely when neighboring particles are of similar size, leading to high tensile stresses that cause particle fracture. This is argued to result in a power-law particle size distribution (PSD) in three dimensions (3-D) with
power law exponent $D \approx 2.6$. Laboratory experiments indicate that fractal gouge with a $D$ value of 2.6 sheared between smooth or rough surface blocks, exhibits distinct frictional constitutive behavior associated with localized or distributed shear strain, respectively [Biegel et al., 1989]. Assuming this comminution mechanism, a method based on analysis of particle size reduction has been developed to estimate strain accommodated by grain comminution [Hadizadeh and Johnson, 2003]. All of these efforts are fundamental to gaining a better understanding of the micromechanical processes of the onset of shear localization and the significance of the fractal PSD on frictional behavior of fault zones.

Effects of grain characteristics on frictional properties of sheared granular materials have also been studied in recent laboratory experiments [Mair et al., 2002; Anthony and Marone, 2005]. The results demonstrate that grain shape has a strong effect on the active deformation mechanisms, and may account for the first order variations in friction, and also influence the stability of granular shear zones. In addition, PSD has been observed to control the tendency for stick-slip or stable sliding, but appears to have relatively little effect on the frictional strength of the granular shear zones [Mair et al., 2002]. How changes in grain angularity and PSD due to grain comminution influence the active deformation mechanisms, such as grain rolling, sliding, and fracturing, and how these factors control frictional properties of fault gouge, and thereby, the strength and stability of granular shear, however, still needs to be resolved. This is largely due to the difficulty of studying real time correlations between gouge deformation and variations in friction in laboratory experiments.
Numerical simulations of granular shear carried out previously using the Distinct Element Method (DEM, *Cundall and Strack*, 1979) or Lattice Solid Model (LSM, *Mora and Place*, 1993) have qualitatively reproduced experimental observations of shear zone deformation, and provided insight into the frictional behavior of fault gouge (*Mora and Place*, 1998, 1999; *Morgan and Boettcher*, 1999; *Morgan*, 1999; *Place and Mora*, 2000; *Hazzard and Mair*, 2003; *Guo and Morgan*, 2004; *Abe and Mair*, 2005). Furthermore, changes in PSD, characterized by the fractal dimension $D$, which tends to increase with grain comminution, may lead to second order variations in fault strength. *Morgan* [1999] document a reduction in frictional strength with increasing $D$ in two dimensional (2-D) DEM simulations, but only up to a characteristic 2-D value for $D$ of ~1.6, which coincides with the 3-D value of 2.6 noted by *Sammis et al.* [1986, 1987]. Numerical experiments on gouge deformation using circular particles show much lower base levels for sliding friction than do laboratory studies on angular gouges (*Morgan*, 1999; *Hazzard and Mair*, 2003). Subsequent simulations of gouge composed of triangular grains yield much higher sliding friction values than those composed of either rounded grains or circular particles (*Guo and Morgan*, 2004), comparable to laboratory results under certain normal stresses (*Byerlee*, 1978). In all of these numerical experiments, however, gouge deformation is accommodated by grain rolling and sliding alone, with no grain fracture. Consequently, the effects of dynamic changes in grain shape, size, and size distribution as a result of grain comminution on frictional properties of fault gouge and underlying deformation mechanisms cannot be constrained.

Here, we examine the influences of grain comminution on frictional and micromechanical behavior of simulated fault gouge using DEM simulations, by including
breakable bonds between adjacent particles. In this way, irregularly shaped grains can be generated to reproduce more realistic fault gouge, and grain size and shape can evolve by grain comminution during granular shear. Our results indicate that grain comminution will alter the partitioning of active deformation mechanisms mainly by changing the shapes and sizes of grains, depending on the direction of change in these properties. The intensity and probability of grain comminution is influenced by shape, strength (e.g., due to mineralogy), and normal stress. Such comminution can either weaken or strengthen the fault gouge, strongly influencing the frictional behavior of the shear zone during sliding.

3.3. Numerical Methods

The distinct element method provides a foundation for studying the mechanical behavior of granular media composed of discrete particles that interact only at contact points according to fundamental contact physics [Cundall and Strack, 1979; Antonellini and Pollard, 1995; Morgan and Boettcher, 1999; Burbidge and Braun, 2002]. DEM simulations have been employed to model a wide variety of discontinuous deformation, such as deformation band formation [Antonellini and Pollard, 1995], microstructure development in simulated gouge zone [Morgan and Boettcher, 1999], block faulting [Saltzer and Pollard, 1992; Homberg et al., 1997], accretionary wedges and thrust belt growth [Burbidge and Braun, 2002], rate-state friction [Morgan, 2004], and effects of grain shape and normal stress on granular shear [Guo and Morgan, 2004].

We have used the DEM approach, combined with interparticle bonding for this study [Cundall and Strack, 1979; Guo and Morgan, 2004]. For the case of unbonded particles in contact, particle interactions through contacts is monitored and updated using
an explicit central difference scheme that calculates particle motions through Newton's second law [Morgan, 1999]. A force-displacement law relates the relative displacement between two particles in contact to the contact normal force $F_n$ and shear force $F_s$, described using a non-linear Hertz-Mindlin contact model [Mindlin and Deresiewicz, 1953; Johnson, 1985]

$$F_n = \left(\frac{2G\sqrt{2R}}{3(1-v)}\right)\delta_n^{3/2}$$  \hspace{1cm} (1)

$$F_s = \left(\frac{2\left(3RG^2(1-v)\right)^{1/3}}{(2-v)}\right)F_n^{1/3}\delta_s$$ \hspace{1cm} (2)

where $\delta_n$ and $\delta_s$ are the relative normal and shear displacements at the particle contact, respectively, $G$ is the shear modulus, $v$ is Poisson's ratio, and $R$ is the effective radius determined by the radius of two contact particles $R_1$ and $R_2$, and given by

$$R = \frac{2 \cdot R_1 \cdot R_2}{R_1 + R_2}$$ \hspace{1cm} (3)

The shear force between two particles that are not bonded is limited by the interparticle friction $\mu_p$. When $F_s$ exceeds the critical shear force $F_{s}^{\text{max}} = \mu_p F_n$, the contact undergoes frictional sliding and $F_s$ is then scaled back to $F_{s}^{\text{max}}$. $\mu_p$ is set to 0.5 in our numerical experiments (Table 1).

Interparticle bonding (Figure 1) can be envisioned as two bonded particles connected by two elastic springs and an elastic beam that transmit forces and moment, respectively [Guo and Morgan, 2004]. The interparticle bonds are assumed to deform in a linear elastic manner within the failure criteria. Normal force, shear force, and moment $M$ within the bonds are proportional to bond normal stiffness $k_n$ or shear stiffness $k_s$, and
also proportional to bond cross-sectional area $A$ and the moment of inertia of the bond cross-section $I$, respectively

$$F_n = k_n \cdot A \cdot \delta_n$$  \hspace{1cm} (4)

$$F_s = k_s \cdot A \cdot \delta_s$$  \hspace{1cm} (5)

$$M = k_n \cdot I \cdot \theta$$  \hspace{1cm} (6)

where $\delta_n$, $\delta_s$, and $\theta$ are the relative normal, shear, and angular displacements at the particle contact, respectively, $A = \pi R^2$ and $I = (AR^2)/4$.

**Table 1.** Parameters for numerical experiments.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental variables</td>
<td></td>
</tr>
<tr>
<td>Initial gouge zone thickness $^{(1)}$</td>
<td>$\sim 11.25 \text{mm}$</td>
</tr>
<tr>
<td>Shear strain rate $^{(1)}$</td>
<td>$\sim 8.89 \times 10^{-5} \text{ s}^{-1}$</td>
</tr>
<tr>
<td>Total shear strain</td>
<td>200%</td>
</tr>
<tr>
<td>Applied normal stress on walls</td>
<td>5-100 MPa</td>
</tr>
<tr>
<td>Grain properties</td>
<td></td>
</tr>
<tr>
<td>Grain radius</td>
<td>300, 352.9, 415.2, and 488.5 $\mu$m</td>
</tr>
<tr>
<td>Grain size distribution ($D$)</td>
<td>0.51</td>
</tr>
<tr>
<td>Intergranular friction</td>
<td>0.5</td>
</tr>
<tr>
<td>Shear modulus</td>
<td>29 GPa</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.20</td>
</tr>
<tr>
<td>Interparticle bond properties</td>
<td></td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.20</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>69.6 GPa</td>
</tr>
</tbody>
</table>

(1) Depends on normal stress and grain shape.

By introducing elastic bonds between circular particles, irregularly shaped grains can be generated. However, there are still restrictions on the shape of the grains due to the fact that they are composed of non-overlapping circular particles with a limited range of sizes. In particular, the surface roughness of the aggregate grains is determined by the minimum size of the basic particles, which in turn is limited by the available computational resources. DEM simulations using this bond model have been used to
Figure 1. Schematic diagram of an interparticle bond and its mechanical analogs [Modified after Guo and Morgan, 2004]. The bond between particles behaves as (a) an elastic spring that transmit normal force, and (b) an elastic spring that transmit shear force, and (c) an elastic beam that transmits moment. The interparticle bonds are assumed to deform in a linear elastic manner within the failure criteria, when bonded particles are displaced and rotated from their equilibrium positions.

investigate the effects of grain shape on frictional behavior of simulated granular shear zones [Guo and Morgan, 2004]. In this study, we take this approach one step further by allowing breakage of elastic bonds to simulate the process of grain comminution. Bonds with finite strength break if bond tensile stress, $\sigma$, equals or exceeds bond tensile strength $\sigma_{\text{max}}$, or if shear stress, $\tau$, equals or exceeds the bond shear strength $\tau_{\text{max}}$:

$$\sigma = \frac{F_n}{A} + \frac{|M|}{I} \cdot R > \sigma_{\text{max}}$$  \hspace{1cm} (7)

$$\tau = \frac{|F_t|}{A} > \tau_{\text{max}}$$  \hspace{1cm} (8)
Here, we assume that tensile normal force is positive. The contact forces between broken bond particles are then calculated as for non-bonded contacts, using equations 1 and 2.

3.4. Experimental Design

For experiments conducted here, two-dimensional (2-D) granular shear zones are constructed and deformed in the same way as described by Guo and Morgan (2004). In this way, the two sets of experiments (i.e., with and without grain comminution) can be directly compared. The initial granular assemblages are created by randomly arranging a certain number of either rounded or triangular quartz grains of four different sizes between two pre-designed, rough-surfaced walls. Grain size and relative abundance obey a power law relationship defined by a 2-D power law exponent $D = 0.51$ and given by the following relationship [Turcotte, 1986; Sammis et al., 1986, 1987; Morgan and Boettcher, 1999; Guo and Morgan, 2004]:

$$D = \log(N_t/N_0)/\log(R/R_0)$$

(9)

where $N_t$ and $N_0$ are numbers of grains with a radius equal to $R_t$ and $R_0$, respectively. The rounded grains are composed of 7 close-packed circular particles, and triangular grains are composed of 6 close-packed circular particles (Figure 2). Adjacent particles in each grain interact through elastic bonds. The initial grain assemblage (Figure 2a) was created by replacing circular particles with the rounded or triangular grains in a reference circular particle assemblage that is under an isotropic mean stress state and with $D$ value of 0.51 [Guo and Morgan, 2004]. Before the start of the experiment, the grain assemblage with infinite bond strength was compacted by shifting the top wall back and forth under the applied experimental normal stress until the equilibrium stress was reached. The
appropriate bond strength was then assigned to the grains and the granular assemblage was deformed by moving the upper wall at constant velocity to the right, while keeping the lower wall fixed. Parameters for numerical experiments are listed in Table 1.

Figure 2. Experimental design. (a) Initial grain assemblage created by randomly arranging a predetermined number of rounded or triangular grains of four sizes within the domain with periodic lateral boundaries. Boundaries were moved inward until equilibrium isotropic mean stress is attained. Rounded grains define two rough-surfaced walls for all grain assemblages. Normal stress along the walls is maintained at a constant value throughout each experiment. Deformation is induced by moving the top wall to the right at a constant velocity, \( v \), and keeping the bottom wall fixed. Shaded vertical and horizontal columns are strain markers. (b) Rounded and (c) triangular grains are generated by bonding circular particles together using various numbers of unbreakable and four breakable elastic bonds, as shown. Bond breakage of randomly oriented grains produces smaller subgrains of specific shapes in various configurations, as shown.

Previous studies [Mair et al., 2002; Nouguier-lehon et al., 2003; Guo and Morgan, 2004] demonstrate that both grain angularity and elongation may affect the behavior of granular materials. For the purpose of studying the effects of dynamic changes in these two factors, two types of bonds are defined in each grain: unbreakable bonds with infinite strength, and four breakable bonds with defined failure strengths (Figure 2). The breakage of each rounded grain, therefore, produces one rectangular and
one trapezoidal subgrain, causing grains in the rounded grain assemblages to become more angular with progressive grain comminution. The breakage of each triangular grain produces one triangular and one elongate rectangular subgrain with aspect ratio of 3:1 (Figure 2). Grain comminution, therefore, does not change the total number of triangular grains, but serves to decrease mean grain size, and increase the number of the elongate grains, i.e., the average grain elongation of the assemblage. As initial grain orientations are random, the products of grain fracture are smaller subgrains with a range of configurations.

In our numerical model, finite strength values can be assigned to all elastic bonds in each grain so that grains can fracture in any highly stressed directions, like real granular materials. If all bonds are allowed to break, either 14 or 10 possible subgrains of various shapes and sizes could be produced for each rounded and triangular grain, respectively. Consequently, grain shape and size distribution evolution could be very complex. For example, grain angularity could increase or decrease during deformation. In addition, if comminution goes to completion, the resulting subgrains would all be circular, unlike natural materials, which consist of angular particles. In this study, we do not attempt to simulate the exact fracture process of real gouge, but rather to examine frictional and mechanical effects of grain comminution that results in an increase in grain angularity and elongation. We choose the simplified rounded and triangular grain shapes because (a) we know how grain shape will change and (b) we know how they behave in a non-fracturing regime [Guo and Morgan, 2004]. In order to simplify subgrain characteristics, we define weak planes in the grains, similar to cleavages in mineral grains, by only allowing one row of bonds to break. In this way, subgrain characteristics
can be defined explicitly, and the variations in gouge properties due to comminution can be easily identified. This simplified approach toward comminution is precursory to a more complete study of rock fragmentation to form gouge [Chapters 4 and 5].

In this study, initial grain size distribution falls within a narrow range. The biggest grain is \( \sim 2.65 \) times larger than the smallest one. Although grain strength generally varies with size [\textit{Pitch}, 1953], this is not significant in our case due to the narrow size range. Therefore, the same bond strengths are assigned to all grains in each granular assemblage regardless of size. In this study, we define \( \tau_{\text{max}} \) to be 1.27 times greater than \( \sigma_{\text{max}} \), although most rocks typically exhibit values of \( \tau_{\text{max}} \) that are one to two times \( \sigma_{\text{max}} \) [e.g., \textit{Attewell and Farmer}, 1976]. Because each grain can only break into two sub-grains, the evolving grain shape and size distribution can be easily derived. Once all of the grains have broken, comminution will cease. For these simulations, however, we ensure that grain sizes continue to evolve by choosing finite bond strengths such that bond breakage occurs throughout the duration of an experiment; total bond breakage after 200% shear strain must lie between 1% and 99% of possible breakable bonds (Table 2).

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
Experimental set & Tensile strength (MPa) & Shear strength (MPa) \\
\hline
R\(\infty\) & \(\infty\) & \(\infty\) \\
R1100 & 1100 & 1400 \\
R550 & 550 & 700 \\
R413 & 412.5 & 525 \\
R275 & 275 & 350 \\
R220 & 220 & 280 \\
T\(\infty\) & \(\infty\) & \(\infty\) \\
T1100 & 1100 & 1400 \\
\hline
\end{tabular}
\caption{Bond strength for numerical experiments.}
\end{table}

*\(T\) and \(R\), followed by bond tensile strengths, represent the triangular and rounded grain assemblages of certain strengths, respectively.
Two suites of experiments are carried out to examine the influence of initial grain shape and normal stress ($\sigma_n$) on grain comminution. In the first, all granular assemblages are composed of either 100% rounded grains or 100% triangular grains, and have the same bond strengths. Assemblages are sheared under identical boundary conditions, i.e., with the same wall surface roughness, over a normal stress range from 5 to 100 MPa. The results are also compared to experiments carried out without grain comminution, i.e., with bonds of infinite strength, as described by Guo and Morgan [2004]. In addition, a subset of rounded grain assemblages are constructed, each with different intergranular bond strengths, but all sheared at a normal stress of 25 MPa, for the purpose of studying the effects of bond strength on grain comminution, and gouge frictional and micromechanical properties. For convenience, we use the letters R and T, followed by bond tensile strength, to represent the rounded and triangular grain assemblages with a given bond strength. For example, R275 refers to the rounded grain assemblage with the bond tensile strength of 275 MPa, and T1100 refers to the triangular grain assemblage with the bond tensile strength of 1100 MPa. All of the simulations carried out for this study, and their tensile and shear strengths, are listed in Table 2.

3.5. Results

3.5.1. Comminution Induced Evolution of the Sheared Assemblages

The breakage of the rounded and triangular grains leads to distinctly different changes in grain characteristics, i.e., increased grain angularity and elongation, respectively. It is desirable to compare assemblages of each type after they have undergone the same degree of grain breakage, i.e., within the 200% shear strain of the
experiment. The rounded grain assemblage (R275) and the triangular grain assemblage (T1100) sheared under a normal stress of 25 MPa results in 63% and 41% grain breakage, respectively. The results of the two experiments show the effects of initial grain shape and characteristics of comminution products, i.e., subgrains, on the behavior of granular assemblages during shear.

The evolving configuration of the rounded assemblage, R275-25, is plotted in Figure 3. The concentration of rotating grains along the top wall indicates that deformation within the first 2% shear strain is localized along the moving wall (Figure 3c). Additionally, broken bonds occur in several of the smallest grains adjacent to the top wall (Figure 3a), and a nearly horizontal slip surface develops below the top wall (Figure 3d), as denoted by the high gradient in the horizontal displacement field [described by Morgan and Boettcher, 1999]. Grain contact stresses are distributed heterogeneously (Figure 3e) and higher stresses tend to build up along the contacts between grains with large contrasts in size (Figure 3b). Low angle stress chains are more likely developed close to the top wall, while high angle stress chains are concentrated in the middle of the assemblage. Contact stresses adjacent to the bottom wall are relatively low (Figure 3e). With continuing grain comminution and increasing number of angular subgrains, deformation migrates downward, but by 20% shear strain is still localized within the upper part of the assemblage (Figure 3d). The abundance of rotating grains increases with increasing shear strain (Figure 3c). Grain breakage (Figures 3a and b) is concentrated within zones of higher shear strain and degree of grain rotation. The failure planes within the grains are randomly oriented, and not always coincident with, or parallel to, major slip surfaces (Figures 3b and d). Several distinct stress chains are developed close to the
Figure 3. Evolution of the rounded grain assemblage (R275) with increasing shear strains of 2%, 20%, and 200% under normal stress of 25 MPa. (a) Grain configuration. Black dots are mid-points of broken bonds over the previous 2% shear strain increments. (b) Magnification of the boxed areas in (a). Dotted lines parallel to particle contacts denote the locations of bonds broken over the previous 2% shear strain increments, representing completely failed or partially failed failure surfaces within grains. Solid lines denote grain contact stress as shown in (e). Darker colors indicate higher contact stresses. (c) Grain rotation. Darker colors indicate higher degrees of rotation. (d) Gradient of horizontal displacement. Darker colors indicate greater gradient of horizontal displacement. See text for explanation and discussion. (e) Grain contact stress. Higher contact stress is denoted by lines of darker color that connect the centers of particles in contact.
bottom wall and the orientations of high stresses become more diverse (Figure 3e). The intense deformation eventually extends down to the lower part of the assemblage at 200% shear strain as indicated by the distribution of rotating grains and broken bonds. Overall, the smaller grains and grains close to the moving wall show the highest probability of breakage. Similar sized grains in contact do not show obviously higher probabilities of breakage (Figure 3b).

Figure 4 shows the progressive deformation of the triangular assemblage, T1100-25. Initially, over the first 2% shear strain increments, bond breakage is intense, and occurs nearly uniformly across the entire domain (Figure 4a). Over these increments of strain, about 14% of total 2768 bonds break in T1100-25, whereas less than 1% (i.e., 0.18%) break in R275-25. The rate of bond breakage drops significantly after 2% shear strain, and bonds tend to break within localized zones of high shear strain and stress that extend across the whole domain (Figures 4c-e). With continued reduction in grain size and increase in grain elongation, the abundance of rotating grains varies slightly (Figure 4c). The elongate grains highlighted in Figure 4b, at 200% strain, show a tendency to align parallel to the slip surface. In contrast to experiment R275-25 (Figure 3), T1100-25 is characterized by generally more distributed deformation, developing relatively uniform distributions of pore space (Figure 4a) and rotating grains (Figure 4c), and localized distribution of intensified stress along broad zones across the whole domain (Figure 4e) by 200% shear strain. Again, smaller grains are subject to higher stresses and show higher probabilities of breakage, rather than similar sized grains in contact. Although the triangular grains are oriented randomly, they do not show any apparent preferential breakage direction (Figure 4b).
Figure 4. Evolution of the triangular grain assemblage (T1100) with increasing shear strains of 2%, 20%, and 200% under normal stress of 25 MPa. Symbols are the same as in Figure 3. Dashed line in (b) at 200% shear strain denotes a slip surface inferred from the high gradient of horizontal displacement highlighted in (d). Elongate subgrains are observed to align parallel or subparallel to this slip surface.
Figure 5 shows the detailed evolution of mechanical and micromechanical properties for R275-25. For the purpose of comparison, these data are plotted with results from R∞-25, i.e., without grain comminution, but sheared under the same σ_n of 25 MPa as R275-25. Figure 5a shows the ratio of shear stress to normal stress, defined as friction μ, for R275-25. A pronounced peak of μ ~ 0.85 occurs at 6% shear strain, followed by a residual phase in which μ fluctuates about a mean value of ~0.35 with a standard deviation of 0.08. Although the friction distribution is similar, the residual value of μ for R∞-25 varies around a smaller mean value of 0.31 with the standard deviation of 0.05 (Figure 5a).

As shown in Figures 3C and 4C, all of the particles in a given grain usually exhibit similar rotations over 2% shear strain increments. Thus, the rotational properties of grains can be quantified by the rotations of particles in the granular assemblages. Initially, the percentage of rotating grains in R275-25 is lower than that in R∞-25, but it increases gradually and reaches a level comparable to R∞-25 after 120% shear strain (Figure 5b). The angle of rotation in R275-25 is similar to that in R∞-25 before 120% shear strain, but increases to a higher magnitude with increasing shear strain (Figure 5c). R275-25 also shows a higher average percentage of sliding contacts and volume strain than R∞-25 (Figures 5d and e). The abundance of sliding contacts and volume strain also increase with increasing shear strain, i.e., with increasing grain angularity and decreasing grain size.

Grain comminution and associated variations in grain characteristics tend to correlate with gouge frictional and mechanical properties. As shown by the vertical lines on Figure 5f, distinct peaks in the incremental percentage of broken grains usually
Figure 5. Evolution of frictional and micromechanical properties of the breakable rounded grain assemblage (R275) with shear strain at normal stress of 25 MPa, compared to R\(\infty\) (unbreakable). (a) Friction. (b) Percentage of rotating grains. (c) Angle of rotation. (d) Percentage of sliding contacts. (e) Volume strain. (f) Percentage of broken grains over 2% strain increments and mean grain size.
coincide with troughs or drops in friction within the first 50% strain, but subsequently, tend to coincide with peaks in friction. The distinct peaks in the incremental percentage of broken grains also coincide with peaks or rises in rotational properties and volume strain, and mostly with peaks and rises in the percentage of sliding contacts (Figure 5).

A similar plot of evolving gouge properties is made for T1100-25, and compared with T∞-25 without grain comminution, both sheared under σn of 25 MPa (Figure 6). T1100-25 undergoes the accumulation of elongate subgrains due to fracture of the triangular grains, and shows a lower residual friction value, μ ~ 0.48, compared to that of the T∞-25 of 0.56 (Figure 6a). The rotational and sliding properties are comparable in both T1100-25 and T∞-25, except for the slightly lower abundance of rotating grains and lower mean angle of grain rotation over the first 40% shear strain for T1100-25 (Figures 6b, c and d). In addition, much lower average volume strain is observed in T1100 than in T∞-25 (Figure 6e). After initial dilation, T1100-25 shows an overall decrease in volume strain. Pronounced peaks in the percentage of broken grains generally, but not exclusively, coincide with troughs or drops in friction, and with peaks and rises in rotational properties and volume strain, but do not show clear correlations with either highs or lows in the percentage of sliding contacts (Figure 6).

3.5.2. Assemblage Property Statistics

As shown in Figures 5 and 6, assemblages in which grain fracture occurs exhibit contrasts in behavior compared to those without grain comminution. As grain fracture is the only addition, the differences can be attributed to the effects of grain comminution during strain, including grain fracture itself, grain size reduction, and in particular, grain
Figure 6. Evolution of frictional and micromechanical properties of the breakable triangular grain assemblage (T1100) with shear strain at normal stress of 25 MPa, compared to T\(\infty\) (unbreakable). (a) Friction. (b) Percentage of rotating grains. (c) Angle of rotation. (d) Percentage of sliding contacts. (e) Volume strain. (f) Percentage of broken grains over 2% strain increments and mean grain size.
shape changes. This is further demonstrated by comparisons of the average properties of the assemblages in which systematic variations of bond strength and of normal stress can be applied. Due to progressive comminution, assemblage properties evolve throughout the experiment. However, the most rapid changes occur in the first 60% strain (Figures 5 and 6). Although the shearing assemblages are still subject to modest changes in properties after this point (Figures 5 and 6), we can approximate the remaining portion of the experiments as "residual" sliding, and calculate statistics for comparison.

Frictional strengths of grain assemblages during residual sliding demonstrate a wide range, but systematic variations are evident, corresponding to variations in bond strength, initial grain shape, and $\sigma_n$ (Figure 7). To distinguish between friction fluctuations throughout the experiment, and the maximum values of friction that define the residual frictional strength of the assemblage, we define $\mu_{\text{max}}$ as the mean value of $\mu$ after 60% shear strain, plus its standard deviation. The triangular grain assemblages are much stronger than the rounded grain assemblage for any given $\sigma_n$, and both systems show decreasing $\mu_{\text{max}}$ with increasing $\sigma_n$ (Figure 7). All of the triangular grain assemblages, i.e., T1100, have consistently lower strengths than T∞. The rounded grain assemblages, i.e., R1100, are slightly weaker at lower normal stresses, but stronger at higher values of $\sigma_n$, compared to R∞ (Figure 7). At normal stress of 25 MPa, decreasing bond strength leads to a progressive increase in $\mu_{\text{max}}$ (Figure 7, inset), reflecting the increasing tendency for grain breakage and its effects, i.e., increases in grain angularity.

Volume strains of our simulated fault gouges are functions of both $\sigma_n$ and grain shape, and show generally compactional responses (given as positive values) (Figure 8).
Figure 7. Maximum sliding friction ($\mu_{\text{max}}$), calculated as the ratio of wall shear stress to normal stress, plotted against normal stress for all rounded and triangular grain assemblages. Error bars plotted below $\mu_{\text{max}}$ values show average drops in sliding friction during stick slip events. Inset shows suite of the rounded grain assemblages with different bond strengths deformed under normal stress of 25 MPa. Interpolated lines are fit to data points by eye, but only for assemblages with grain comminution.

Figure 8. Average volume strain for all rounded and triangular grain assemblages plotted against normal stress. Inset shows suite of the rounded grain assemblages with different bond strengths deformed under normal stress of 25 MPa. Error bars show the standard deviation. Interpolated lines are fit to data points by eye.
An increase in $\sigma_n$ leads to a systematic decrease in volume strain for gouges composed of unbreakable grains of both shape, i.e., gouges in $R_\infty$ and $T_\infty$. The effects on $T_\infty$ are most significant. This decreasing trend is also observed for $R_{1100}$, but not so clearly for $T_{1100}$. At a normal stress of 25 MPa, a decrease in bond strength in the rounded grain assemblages leads to an increase in volume strain (Figure 8, inset). Again, $R_{1100}$ and $R_\infty$ show very similar volume strain for all values of $\sigma_n$. Evidently, changes in grain shape characteristics with comminution in assemblages $T_{1100}$ lead to non-systematic variations in volume strain, compared to $T_\infty$.

Grain comminution in the rounded and triangular assemblages has very different effects on the grain rolling tendency and magnitude (Figure 9). Rounded grain assemblages generally show slight decreases in incremental percentages of rotating grains with increasing $\sigma_n$ values. Percentages for $R_{1100}$ are very similar to $R_\infty$, except for the highest $\sigma_n$ values where more grains rotate in $R_\infty$ (Figure 9a). In contrast, triangular grain assemblages show a rapid increase in incremental percentage of rotating grains for $\sigma_n < 25$ MPa (Figure 9a), and a more gradual increase thereafter. Percentages for $T_{1100}$ diverge from and become measurably higher than those of $T_\infty$ for $\sigma_n > 25$ MPa. These trends reflect the important role of particle interlocking and rotational coupling at high normal stresses in the triangular assemblages, which is suppressed at lower normal stresses and in the rounded grain assemblages (Guo and Morgan, 2004). Furthermore, the increasing elongation of grains due to breakage in the $T_{1100}$ at high $\sigma_n$ appears to increase grain interlocking and resulting grain rotation relative to $T_\infty$ (Figure 9a).

Varying bond strengths for the rounded grain assemblages sheared at normal stress of 25 MPa leads to a nonlinear variation in the percentage of rotating grains (Figure
9a, inset). The abundance of rotating grains decreases with increasing bond strength from 220 to 413 MPa, but increases gradually thereafter. Experiment R220, with the lowest bond strength, undergoes the most intense comminution, and correspondingly, shows the highest percentage of rotating grains.

![Graph](image_1.png)

(a)

![Graph](image_2.png)

(b)

Figure 9. Average percentage of rotating grains (a) and mean angle of rotation (b) for all rounded and triangular grain assemblages, plotted against normal stress. Insets show suite of the rounded grain assemblages with different bond strengths deformed under normal stress of 25 MPa. Error bars show the standard deviation. Interpolated lines are fit to data points by eye.
The mean angles of grain rotation show different response patterns to changes in grain shape, size, and size distribution with grain comminution for the rounded and triangular grain assemblages (Figure 9b). The angle of grain rotation is not sensitive to $\sigma_n$ for the rounded grain assemblages. A substantial increase in the angle of rotation is observed only for R220, which undergoes the most intense grain comminution and associated changes in grain shape. Triangular grain assemblages, in contrast, show nearly linear increases in their angles of rotation with $\sigma_n$, and the increasing rate for T1100 is much higher than that for T$\infty$ (Figure 9b). Correspondingly, T1100 shows significantly higher magnitudes of rotation than T$\infty$ at $\sigma_n > 25$ MPa.

The instantaneous proportions of sliding contacts also show dependence on initial grain shape, bond breakage, and $\sigma_n$ (Figure 10). The grains in our numerical experiments actually interact at the contacts between particles. Thus, grain pairs can have multiple sliding contacts, but generally no more than 2 per pair. R$\infty$ experiments show decreases in the abundance of sliding contacts with increasing $\sigma_n$, while T$\infty$ experiments show only slight increases with increasing $\sigma_n$. At low normal stresses, the small amount of grain comminution does not lead to remarkable variations in the abundance of sliding contacts in either rounded or triangular grain assemblages. Only at normal stresses higher than 50 MPa does grain comminution lead to a noticeable increase in the abundance of sliding contacts in both R1100 and T1100, even though grain shapes change in different ways for these two types of assemblages. Increases in bond strength in the rounded grain assemblages at a normal stress of 25 MPa lead to steady decreases in the abundance of sliding contacts.
Figure 10. Average percentage of instantaneous sliding contacts for all rounded and triangular grain assemblages, plotted against normal stress. Inset shows suite of the rounded grain assemblages with different bond strengths deformed under normal stress of 25 MPa. Error bars show the standard deviation. Interpolated lines are fit to data points by eye.

3.5.3. Comminution and Grain Size Evolution

The cumulative abundance of broken grains (i.e., once all four breakable bonds in grains break) after 200% shear strain in our simulated fault gouge is strongly dependent on initial grain shape, bond strength, and \( \sigma_n \) (Figure 11). For the same bond strength, and the same values of \( \sigma_n \), the triangular grains in T1100 undergo much more intense grain comminution than the rounded grains in R1100, although the abundance of broken grains increases with increasing \( \sigma_n \) for both suites of experiments. Decreases in bond strength in the rounded grain assemblages at normal stress of 25 MPa also lead to increases in the abundance of broken grains in a nonlinear fashion.

The rates, and changes in rates, of grain breakage also prove to be influenced by initial grain size. For both the rounded and triangular grains, the probability of grain
breakage increases with decreasing grain size (Figure 12). To demonstrate this, we compare two simulations that result in similar total grain breakage, R275-25 and T1100-25. Rounded grains in R275-25 (Figure 12a) show nearly linear increases in cumulative abundance of broken grains. The likelihood of a small grain breaking is nearly twice that of the largest grain (i.e., 78% compared to 39%). In contrast, triangular grains in T1100-25 (Figure 12b) initially show very high rates of grain breakage that decrease with shear strain. The likelihood of a small grain breaking is more than 10 times that of the largest grain (i.e., 79% compared to 6%). We have also compared the statistics of bond breakage with grain breakage to test for the possibility of grain damage with incomplete breakage (fewer than four bonds break). The two ratios prove to be quite similar to each other, except for during the early stages of deformation, where the triangular grains appear to undergo significant damaged, but incompletely fracture. This difference disappears by 60% shear strain and so does not affect our statistics at 200% shear strain significantly.

Figure 11. The cumulative percentage of broken grains after 200% shear strain for all assemblages with finite bond strengths. Inset shows suite of the rounded grain assemblages with different bond strengths deformed under normal stress of 25 MPa. Error bars show the standard deviation. Interpolated lines are fit to data points by eye.
Figure 12. Cumulative abundance of broken grains for four different grain sizes in R275 (a) and T1100 (b) shear at normal stress of 25 MPa plotted again shear strain. In both the rounded and triangular grain assemblages, the smallest grains show the highest probability of breakage.

The influence of initial grain shape, bond strength, and $\sigma_n$ on the evolution of grain size distributions can be explored by plotting the normalized statistics of broken grains (Figure 13). We calculate the abundance of broken grains, and compare the
partitioning of grain breakage among the four different sizes. We note that grain comminution is limited to the initially rounded and triangular grains in our simulated fault gouge, whereas real fault gouge may undergo continued breakage of subgrains. This limitation affects the associated changes in grain character (i.e., grain shape, size, and size distribution) in the simulated gouge that might be influenced by additional grain breakage. Therefore, to minimize these influences, we use grain breakage data for each assemblage at the point at which 32% of the smallest grains have broken. Also, we exclude data from experiments in which fewer than 6% of the total grains have broken within 200% shear strain, i.e., assemblages R1100 at normal stresses between 5 and 25 MPa. The abundance of broken grains is further normalized by dividing each size fraction by the total number of broken grains.

In general, the normalized abundances of broken grains show a strong dependence on grain size, i.e., abundance decreases as grain size increases in both the rounded and triangular grain assemblages (Figure 13). The broken grain abundances do not always show systematic variations with changing shape, bond strength, or normal stress, but the data do tend to fall into clusters, denoted by the different geometric outlines in Figure 13. For the rounded grain assemblages, bond strength appears to have a more significant effect on the normalized abundance of broken grains for a given size than does $\sigma_n$. The low strength assemblages, i.e., R275 and R220 (solid square outline) show the least change in normalized grain size abundance with increasing size, and this change occurs in a nearly linear fashion (Figure 13). The triangular grain assemblages sheared at the lower normal stresses, T1100-5, -25, and -50 (dashed circle outline) also have similar high normalized abundances of broken smallest grains, i.e., $\sim$60%, whereas the higher
Figure 13. Percentage of broken grains of four different sizes in the rounded and triangular grain assemblages, normalized and plotted in bins denoting initial grain size. Lateral position of points within a bin is arbitrary. The smallest grains show the highest probability of breakage. High bond strengths and rounded grain shapes favor breakage of the smallest grains. Variations in normal stresses do not result in systematic changes in breakage of the smallest grains in the rounded grain assemblages, but fewer of smallest grains break at normal stresses higher than 50 MPa in the triangular grain assemblages. Data points are divided into subgroups to demonstrate patterns in their variations with bond strength, grain shape, and normal stress.
normal stress triangular experiments, T1100-75 and -100 (solid circle outline), show values close to 51-52%. Generally, the decrease in the normalized abundance of broken grains with increasing size is faster in R1100 than in T1100.

3.6. Discussion

3.6.1. Frictional Effects of Grain Communion

The results of our DEM experiments of grain breakage demonstrate that grain comminution can have several first-order effects on frictional behavior during granular shear, primarily due to changes in grain shape, size, and size distribution. As noted previously, the primary control appears to be the degree of grain angularity [Guo and Morgan, 2004]. Grain breakage in rounded grain assemblages generates angular subgrains. The angularity increases with increasing the abundance of grain breakage as bond strength decreases under normal stress of 25 MPa, which leads to systematic increases in sliding friction (e.g., Figure 7 inset). Similarly, grain breakage in triangular grain assemblages produces elongate grains, as well as smaller triangular grains. However, this trend leads to systematic decreases in sliding friction (Figure 7). Finally, we also see that the frictional strength of granular shear zones is more sensitive to changes in grain shape (i.e., initially rounded grain verse initially triangular grain) at low normal stresses than at high normal stresses (Figure 7), due to the effects of assemblage dilation at low σn [Guo and Morgan, 2004]. This leads to a narrower range of friction values at the larger normal stresses, despite the higher rates of grain comminution.

The frictional strength of our simulated shear zones is also affected by the process of grain fracture itself, this appears to be a second order effect. Grain fracture may
decrease the frictional strength of the granular shear zone, by decreasing frictional resistance and assemblage dilation. For example, during the early stages of R275-25 peaks in the incremental abundance of broken grains correlate with sudden drops in frictional strength (Figure 5), and generally, the same correlation is evident for T1100-25 (Figure 6). However, because of the competing effects of increasing grain angularity (e.g., R275-25), which increases frictional strength and dilation, this predicted correlation is not as obvious during the later stages of the experiments (e.g., Figure 5).

These numerical results generally corroborate previous laboratory and numerical experiments. Shear zones composed of rounded gouge grains tend to be significantly weaker than those composed of angular grains [e.g., Mair et al., 2002; Nouguier-lehon et al., 2003; Guo and Morgan, 2004]. The presence of elongate grains also tends to weaken natural assemblages, as has been observed in ductile shear zones [Lister and Snoke, 1984], natural clay-bearing fault gouges [Chester and Logan, 1987], and synthetic clay-rich gouges [Saffer et al., 2001; Saffer and Marone, 2003]. The low friction values in these natural systems are generally interpreted to result from the preferred orientation of inequant grains and platy clay minerals [Lupini et al., 1981; Chester and Logan, 1987; Saffer et al., 2001; Saffer and Marone, 2003]. Our observations are consistent with this interpretation. We see that elongated subgrains in TS1100, sheared at normal stress of 25 MPa, tend to align parallel to slip surfaces (Figure 4b), facilitating localized deformation along these surfaces. The enhanced localized shear together with other weakening mechanisms, such as grain fracture, result in a progressive reduction in strength. The peak friction is as high as 0.8 at early stage of the simulation, but decrease to ~0.5 by end (Figure 6).
Several previous studies have explored the role of evolving grain size, and particle size distribution, described by fractal dimension $D$, on shear zone friction. For example, laboratory experiments have suggested that a change in $D$ value due to grain comminution may cause second order variations in fault frictional strength [Mair et al., 2002]. Monzawa and Otsuki (2003) argue that comminution of fault gouge is likely to start at a fractal dimension $D$ close to 2.5 in three dimensions; in this condition, a given grain is supported by the maximum number of surrounding grains possible, and the gouge is at its strongest. However, as grains begin to fracture, the fractal dimension $D$ will increase and the shear strength will decrease. In this way, they suggest that grain comminution itself is a slip weakening mechanism. Morgan [1999] draws a similar conclusion on the basis of 2-D numerical simulations of shear zones with different particle size distributions, but demonstrates that fault strength decreases with $D$ only over low $D$ values up to a value of 2.6 (1.6 in 2D), beyond which frictional strength remains at nearly constant levels. The results of our numerical simulations demonstrate that grain comminution can both decrease and increase the gouge frictional strength, dependent mainly on direction and degree of change in grain shape, consistent with previous laboratory studies. Thus, we suggest that weakening or strengthening of granular shear zone due to grain comminution is primarily dependent on the competition between the reduction in strength by fracturing and the frictional effects resulting from changes in grain shape and size distribution. Changes in $D$ value are truly a secondary factor in gouge strength evolution.
3.6.2. Micromechanical Effects of Grain Comminution

As demonstrated by previous studies, grain characteristics including grain shape, size, and size distribution, also play an important role in the partitioning of deformation mechanisms among rotation, translation, sliding, and fracture, all of which influence the micromechanical behavior of granular materials [Morgan, 1999; Mair et al., 2002; Nouguier-lehon et al., 2003; Guo and Morgan, 2004]. Our results show that ongoing grain comminution during shear causes dynamic changes in these characteristics, and therefore leads to distinctive and evolving micromechanical behaviors (Figures 5 and 6). Grain comminution affects the micromechanical behavior of our sheared granular assemblages in two distinct ways: (1) by changing grain characteristics (e.g., shapes and sizes), and (2) by accommodating deformation in preference to other deformation mechanisms, such as grain rolling and sliding.

Both R275-25 and T1100-25 show lower degrees of grain rotation, but similar abundances of sliding contacts, over the first 20% shear strain compared to $R_\infty$ and $T_\infty$, respectively (Figures 5b-d and 6b-d). They also show a strong correlation between pronounced peaks in the incremental abundance of broken grains and rises in rotational properties, although the abundance of broken grains does not correlate well with the abundance of sliding contacts. These results may be explained by the need to reorganize grain packing following fracture to better fill the space. Grain rotation can do this very efficiently, reducing the need for intergranular sliding.

Grain angularity plays an important role in the partitioning of deformation mechanisms in our simulated fault gouges. The percentage of sliding contacts (Figure 10) and the volume strain (Figure 8) both tend to increase with increasing grain angularity in
the rounded grain assemblages, consistent with previous simulations [Guo and Morgan, 2004]. Also, previous studies have demonstrated that the abundance of rotating grains is highly sensitive to grain angularity. Spherical particles promote particle rolling, whereby particles rotate as they translate, thus decreasing shear zone strength [Morgan, 1999; Mair et al., 2002]. Angular grains, in contrast, experience enhanced grain rotation but reduced grain translation (i.e., they jostle back and forth), accounting for their higher strength [Guo and Morgan, 2004]. In most cases, it appears that the abundances of rotating grains in the rounded grain assemblages do not increase significantly with small increases in grain angularity, compared to R∞ (Figure 9a), indicating that the abundance of rotating grains is not sensitive to a small variation in grain shape. However, in at least one case, the enhanced comminution in experiment R220 leads to increased abundance of rotating grains (76%), probably because of the high number of angular subgrains generated by breakage of the weak grains (Figure 9a). Enhanced grain rotation may also result from the production of these smaller subgrains. This interpretation is consistent with studies that show that smaller particles exhibit greater angles of rotation than larger particles at a given σn [Morgan, 1999].

Grain elongation also significantly affects the micromechanical behavior of our simulated fault gouges. Mean grain rotation in the experiment T1100-5 MPa is lower than that of T∞ conducted under the same σn (Figure 9). This implies that grain fracturing in T1100-5 is suppressing the mechanism of grain rotation in T∞, which cannot fracture. With increases in σn, and correspondingly, the abundance of elongate grains, however, grain rotation in breakable T1100 is enhanced dramatically, in terms of both the
abundance of rotating grain and the rotation angle, and becomes measurably higher than T\(\omega\) (Figure 9).

Previous studies have shown that the influence of grain elongation on the behavior of granular materials is highly dependent on loading direction [Nouguier-lehon et al., 2003], i.e., elongate grains show lower values of mean rotation angle and dilatancy rate when loading direction is perpendicular to their long axis, but higher values when loading direction is perpendicular to their short axis. Thus, there is a tendency of elongate grains to rotate into their most stable orientations, regardless of their initial orientations. In our granular assemblages, elongate subgrains are initially randomly oriented, because the triangular grains and potential fracture planes are also initially randomly oriented (Figure 4b). With continuing shear strain, these subgrains rotate into preferred orientations parallel to slip surfaces to facilitate localized deformation (Figure 4b). For this reason, we can attribute the enhanced grain rotation in T1100 partly to the rotation of the initially randomly oriented elongate grains, and partly to the greater abundance of smaller subgrains. The presence of elongate subgrains in the fractured T1100 assemblages also appears to lead to increases in the abundance of sliding contacts at normal stresses higher than 25 MPa (Figure 10), but to non-systematic variations in volume strain (Figure 8). This possibly results from initially random orientations of the elongate grains, because their initial orientations will determine the direction and magnitude of rotation, and the associated volume change during shear.
3.6.3. Comminution Mechanisms

Laboratory and field investigations of gouge comminution mechanisms show that loading conditions and lithology affect the processes of gouge grain breakage [Marone and Scholz, 1989]. It was found that quartz grains under hydrostatic loading undergo spalling and fracture along their edges. During shearing deformation, quartz grains experience much more intense comminution, by grain crushing at $\sigma_n$ of 100 MPa, and mainly by spalling at $\sigma_n$ of 25 MPa. Analysis of poorly lithified sediments from the Rio Grande rift reveal that the mechanisms of grain breakage are also dependent on mineralogy and relative grain strength, i.e., the comminution of quartz occurs by flaking and spalling along grain edges, feldspar grains undergo transgranular fracturing facilitated by cleavage, and lithic fragments exhibit distributed microcracking and transgranular fracturing [Rawling and Goodwin, 2003]. In our numerical experiments, we also observed a dependence of grain breakage intensity on normal stress and grain strength (i.e., bond strength). The highest degrees of grain breakage occur at high normal stresses or low bond strengths (Figure 11).

Although both normal stress and grain strength affect the intensity of grain breakage, the significances of their effects are different. For example, although the ratios of normal stress to bond tensile strength are similar for experiments R275-25 and R1100-100, many more grains break in R275-25 than R1100-100 (Figure 9). This is due to the effect of $\sigma_n$ on the grain packing, and consequently, on the internal stresses of the grains. The simulated granular shear zones are more dilated at lower normal stresses (Figure 8). Consequently, the coordination number (i.e., number of contacts per grain) is higher in R275-25 than in R1100-100. This results in higher differential stress and therefore higher
intensity of grain breakage in the first simulation. In addition, our results show that the periodicity in the breakage rate that might be associated with the periodicity of dilation and compaction (Figures 5f and 6f). When the assemblage undergoes dilation, granular differential stresses in the assemblage are high, resulting in higher rates of grain breakage. This is indicated by the correlation between the peaks in the abundance of broken bonds and the peaks or rises in volume strain (Figures 5 and 6).

![Diagram showing configurations of rounded and triangular grains under a given normal stress $\sigma_n$. The triangular grains have a higher tendency to break because they interact through fewer contacts and are subject to higher differential forces than the rounded grains.](image)

Figure 14. Configurations of (a) rounded grains and (b) triangular grains under a given normal stress $\sigma_n$. The triangular grains have a higher tendency to break because they interact through fewer contacts and are subject to higher differential forces than the rounded grains.

Our results also indicate that initial grain shape plays an important role in the intensity of grain breakage over 200% shear strain in our simulated fault gouges. Triangular grains (i.e., T1100) show a much higher tendency to break than do rounded grains at the same bond strength (i.e., R1100) for a given $\sigma_n$ (Figure 11). For example, many more grains break in T1100-25 than do in R275-25 during the first 2% shear strain
(Figures 3a and 4a). Again, we can explain this by the fact that different grain geometries result in distinct granular packings, contact force distributions, and internal grain stresses. As the triangular grains interact through fewer contacts than the rounded grains [Guo and Morgan, 2004], they are subject to more intense contact forces (Figure 14), leading to higher tendencies for breakage. An additional factor that comes into play is intense bond breakage through grain crushing at the onset of the experiment. This occurs because assemblage consolidation conducted with infinite bond strength can lead to high intergranular forces when finite bond strength is applied. This effect is particularly significant for T1100 experiments due to the higher contact stresses.

Previous models have suggested that the probability of grain comminution is controlled by the relative size of nearest-neighbor particles and is not very sensitive to particle strength. The constrained comminution model [Sammis et al., 1987] assumes that equidimensional particles (i.e., spheres) will break through tensile failure. Consequently, fracture probability should be independent of grain size and strength in a gouge in which adequate small particles are available to surround large particles and support them isotropically, thereby reducing the high axial stresses that favor tensile failure. In our granular assemblages, initial gouges are composed of grains of only four sizes with a PSD defined by $D = 0.51$. The smallest grains are surrounded by larger grains and/or grains of the same size (Figures 3b and 4b at 2% shear strain), and therefore subject to higher loads (Figures 3b and 4b). This more open packing may account for the high degree of breakage of small grains overall (Figure 13), as well as early in experiments (Figure 12). With continued deformation, the breakable grains become surrounded by an increasing number of smaller unbreakable subgrains (Figures 3b and 4b at 200% shear.
strain), which impose a more isotropic grain stress and reduce the probability of bond breakage. However, at the same time with increasing strain, the rate at which broken bonds accumulate decreases for the smallest grains, but increases for the biggest grains (Figure 12). These observations are consistent with previous studies showing that larger grains are forced to break to accommodate deformation when the smallest grains reach their grinding limits or have higher fracture strengths than large grains [Petch, 1953; An and Sammis, 1994; Marone and Scholz, 1989; Storti et al., 2003].

In real materials, $D$ values of natural and artificial gouges from different source rocks under various experimental loading conditions fall into a broad range from 1.7 to 5.52, but show a prominent mode of ~2.6 in 3 dimensions [Sammis et al., 1987; Marone and Scholz, 1989; Biegel et al., 1989; Blenkinsop, 1991; An and Sammis, 1994; Storti et al., 2003; Billi et al., 2003; Rawling and Goodwin, 2003]. Other studies have shown that $D$ value also increases with increasing confining pressure [Morrow and Byerlee, 1989; Blenkinsop, 1991], and $D$ values of rounded sedimentary gouge grains in poorly lithified, immature sediments [Rawling and Goodwin, 2003] are lower than those of more angular gouge grains [Sammis et al., 1987; Blenkinsop, 1991], and also lower than that of stronger pure quartz gouge grains [Marone and Scholz, 1989]. By changing the loading conditions, and gouge grain geometrical and mechanical properties, the results of our simulated gouge deformation also suggest that the probability of grain comminution is sensitive not only to grain size, but also to grain strength (i.e., mineralogy), shape, and $\sigma_n$ at least for the narrow range of grain sizes we consider here (Figure 12).

We can examine the PSD evolution resulting from our simulations as well, although the interpretations are limited by the restricted grain size and fracture options
available. Representative curves defining PSD (i.e., cumulative grain abundance versus equivalent grain radius) are shown in Figure 15 for R275-25 and T1100-25. Both assemblages start with essentially the same PSD, although initial grain sizes differ slightly. Upon breakage, each rounded grain produces two subgrains of unequal sizes, whereas the breakage of each triangular grain yields two equal sized subgrains with different shapes (Figure 2) (Note: We approximate the radius for a given grain or subgrain as for an equivalent circle with the same area of all circular particles that constitute the grain or subgrain). R275-25 displays relatively more intense breakage of large and intermediate sized grains, and rapidly accumulates larger subgrains. In contrast, T1100-25 undergoes more intense breakage of intermediate and small sized grains, which generates smaller subgrains. Therefore, the slope of the PSD curve is nearly constant for the rounded grain assemblage, but migrates toward smaller grain sizes with increasing shear strain, while the triangular grain assemblage shows progressive decrease in the slope of the PSD curve. The variations in PSD evolution primarily result from the differences in subgrain sizes relative to original grain sizes in these two types of assemblages, but also from grain strength, shape, and \( \sigma_n \). Distinct evolutionary patterns of PSDs in the rounded and triangular assemblages suggest that the \( D \) value is controlled not only by the probability of grain comminution, but also by the size of comminution products (Figure 15).

In our numerical model, the prescribed fracture mechanism limits the possible shapes of resulting subgrains, which may influence the other properties of the assemblage. If the triangular grains were allowed to break in arbitrary ways, breaking off single corner particles would be a distinct possibility, leading to grain rounding. The
Figure 15. PSD curves plotted for different strains in representative experiments (a) R275-025 and (b) T1100-025. Bold line represents initial PSD. For R275-25, the slope of the PSD curve is nearly constant, but migrates toward smaller grain sizes with increasing shear strain, while T1100-25 shows progressive decrease in the slope of the PSD curve associated with more intense breakage of intermediate sized and small grains. Note: the horizontal to low slopes at small grain sizes result from the limited fracture potential of grain and subgrains, and are not representative of natural gouge PSDs.
numerical experiments presented here do not explore the importance of this plausible fracture mechanism. However, the results of our experiments do allow us to infer its effect. As this fracture mechanism will produce a circular particle and a trapezoidal subgrain, the overall angularity of the granular assemblage will decrease after fracture. Comminution itself, combined with the reduced angularity, would lead to a decrease in grain rotation, sliding, and fracturing, and a drop in frictional strength of the granular assemblage. Further, DEM studies of PSD evolution during rock fracture and shearing have also been carried out to examine such alternative fracture and comminution mechanisms [Chapters 4 and 5].

3.7. Conclusions

Natural shear zones undergo grain comminution that leads to progressive changes in gouge grain characteristics. DEM simulations of grain comminution in simplified granular assemblages demonstrate that grain comminution, by itself, is an efficient way to accommodate shear strain, thereby reducing the frictional resistance and weakening granular shear zones. However, comminution also produces smaller grains with different shapes that may significantly affect frictional strength of granular shear zone. Rounded grains may become angular through fracture, thereby strengthening the shear zone. Alternatively, angular grains may become rounded, thereby weakening the shear zone. Increases in grain elongation in a highly angular gouge may decrease the frictional strength of the gouge zone, because elongate grains may develop preferred orientations that facilitate localized deformation. In addition, changes in particle size distribution by grain comminution may also affect shear zone strength. Therefore, the ultimate variations
in frictional strength due to grain comminution are dependent on the combined effects of these factors.

The frictional response to grain comminution can be better understood by analyzing the underlying micromechanical process. As it is a destructive deformation mechanism, grain comminution not only accommodates deformation like grain rotation and sliding, but more importantly, it also causes changes in grain characteristics that affect the partitioning of deformation mechanisms during granular shear, and therefore the micromechanical behavior of fault gouge. Deformation partitioning in our simulated fault gouges reflects the combined effects of dynamic changes in both grain shape and size on the abundance and degree of active deformation mechanisms under a given $\sigma_n$. Increases in grain angularity may lead to enhanced grain rotation, sliding, and fracturing, whereas increases in grain elongation may result in reduced translation and enhanced grain rotation and sliding, dependent on normal stress. Small grains favor higher degrees of rotation.

Previous studies have demonstrated that grain comminution may be affected by loading conditions and gouge properties. The intensity of grain comminution in our simulations is also dependent on $\sigma_n$, grain (i.e., bond) strength, and grain shape. Higher $\sigma_n$, lower grain strength, and more angular grains lead to higher degrees of grain breakage. The smallest grains in our simulated fault gouges with a narrow size range show the highest tendency for breakage. The probability of grain comminution is also dependent on grain shape, strength, and $\sigma_n$. These numerical studies are precursory to more detailed investigates of wholesale rock fracture, and gouge production and comminution, which will reveal further aspects of fault zone evolution.
Chapter 4

Fault Gouge Evolution and Its Dependence on Normal Stress and Rock Strength:

Results of Discrete Element Simulations

1. Gouge Zone Properties

4.1. Abstract

In order to study the process of gouge zone evolution, and its dependence on normal stress, $\sigma_n$, and uniaxial compressive strength, $\sigma_{ucs}$, we simulate the break down of fault blocks and growth of fault gouge zones using the Distinct Element Method (DEM) in 2-dimensions. Elastic bonds were added between adjacent, closely packed particles to generate the fault blocks with a given $\sigma_{ucs}$ in a range from 100 to 260 MPa. DEM experiments were conducted by shearing the fault blocks along an initially flat surface for a range of $\sigma_n$ from 10 to 100 MPa. The simulated fault gouge zones experience two distinct stages of evolution, i.e., fast growth and slow growth, distinguished by a switch in deformation mechanism from dominantly wear of the fault blocks to dominantly shearing of existing fault gouge. The rate of the gouge zone thickening decreases exponentially during the fast growth stage (to about 20\% shear strain), and then reaches a relatively constant value, marking the beginning of the slow growth stage. The thickening rate is proportional to $\sigma_n$ and inversely proportional to $\sigma_{ucs}$ during the fast growth stage, but the dependency reverses during the slow growth stage. The mean grain size of the gouge shows a first order dependence on shear displacement, and varies slightly with $\sigma_n$ and $\sigma_{ucs}$. In our simulated shear zones that undergo both surface wear and grain comminution, gouge grains develop a power law size distribution characterized by a 2-D fractal dimension $D$ ranging from 0.6 to 2.4.
4.2. Introduction

Natural faults at shallow depth undergo continual wear of fault surfaces during slip, which leads to a progressive increase in the thickness of the fault gouge zone with net slip [Scholz, 1987; Power et al., 1988]. In the meantime, gouge microstructure and grain characteristics (i.e., grain shape, size, and size distribution) vary with fault shear displacement as a result of grain reorganization and comminution [Marone and Scholz, 1989; Beeler et al., 1996]. These changes in gouge zone features during fault deformation may affect fault strength, stability [Byerlee and Summers, 1976; Sammis et al., 1986; Marone et al., 1990; Beeler et al., 1996], and earthquake characteristics [Heermance et al., 2003]. The effects of fault gouge on fault zone behavior have been studied extensively, both experimentally and numerically under a wide range of conditions [Engelder et al., 1975; Marone and Scholz, 1989; Morrow and Byerlee, 1989; Beeler et al., 1996; Mora and Place, 1998, 1999; Morgan and Boettcher, 1999; Morgan, 1999; Mair et al., 2002; Guo and Morgan, 2004, resubmitted; Anthony and Marone, 2005]. The dependence of strength and stability of the fault on fault gouge, however, remains poorly constrained, because gouge properties change progressively during frictional sliding, and are also dependent on many factors, such as wall rock strength, confining pressure (i.e., depth), and shear displacement [Engelder, 1974; Anderson et al., 1980, 1983; Sammis and Osborne, 1982; Scholz, 1987].

Studies of natural fault zones have yielded many important observations on the nature of fault gouge. It was found that fault gouge develops characteristic shear fabrics [Berthe et al., 1979; Chester and Logan, 1987], and gouge grains obey either a non-fractal [Wilson et al., 2005] or a fractal size distribution characterized by a fractal
dimension $D$ in a range of 1.7 to 5.52 [Sammis et al., 1987; Blenkinsop, 1991; An and Sammis, 1994; Storti et al., 2003; Billi et al., 2003; Rawling and Goodwin, 2003]. These observations are important to infer the mechanical processes of gouge formation [Sammis et al., 1987; Wilson et al., 2005], the frictional and mechanical effects of gouge [Storti et al., 2003; Monzawa and Otsuki, 2003], fault zone stress state, and deformation history [Lin, 2001; Rawling and Goodwin, 2003]. However, field studies can only capture the properties of fault gouge at a single evolutionary stage, and therefore, offer limited information about the dynamic processes of gouge zone evolution.

Important insights for understanding the effects of variations in gouge properties on fault behavior during fault growth are provided by fault process studies in the laboratory. By shearing experimental faults with artificial gouge, laboratory experiments demonstrate that fault gouge affects the stability of slip [Byerlee and Summers, 1976; Scholz et al., 1972], and the transition from stable to unstable sliding appears to be related to gouge grain shape [Mair et al., 2002], grain size [Dieterich 1981], grain size distribution [Biegel et al., 1989], gouge thickness [Byerlee and Summers, 1976; Anthony and Marone, 2005], composition [Morrow et al., 1992; Saffer et al., 2001; Saffer and Marone, 2003], and the shear localization features [Byerlee et al., 1978; Logan et al., 1979; Tullis et al., 1989; Beeler et al., 1996]. Because of limitations in laboratory shear displacements, preventing the natural formation of thick gouge layers, artificial fault gouge is usually introduced between shearing wall rocks in the laboratory experiments. Consequently, the frictional and mechanical effects of sliding surface wear and continual growth of gouge zone on fault slip are excluded in these types of experimental studies.
Numerical simulations of fault zone deformation can also provide views into the role of fault gouge in evolving faults. By shearing circular or irregularly shaped grains (i.e., fault gouge) in a configuration similar to direct shear laboratory experiments, numerical experiments show that the strength of simulated fault zones is correlated with gouge grain configuration [Mora and Place, 1998, 1999], grain size distribution [Morgan, 1999], and grain shape [Morgan, 1999; Guo and Morgan, 2004]. In addition, recent simulations of granular shear using the Distinct Element Method (DEM) also demonstrate that gouge grain comminution can either strengthen or weaken the granular shear zone, dependent on the competing effects of reduced frictional resistance by fracturing and changes in grain characteristics by comminution [Guo and Morgan, resubmitted]. Again, in these numerical simulations, fault gouge is created artificially rather than by the progressive break down of wall rocks in these numerical simulations.

Recognizing the importance of evolving structural and physical properties of fault gouge for understanding its frictional and mechanical effects on fault zone sliding, and therefore earthquake processes, we carry out DEM experiments in two dimensions to simulate the break down of fault blocks and the evolution of fault gouge zones, starting from bare rock surfaces. The purpose of this study is to (1) map out the spatial and temporal distribution of deformation, gouge grain characteristics, and structures that develop within the gouge as it deforms; (2) examine the variation of gouge properties (i.e., gouge zone thickness, porosity, gouge grain size, and size distribution) with shear displacement; (3) investigate the dependency of gouge zone evolution on normal stress $\sigma_n$ and rock uniaxial compressive strength $\sigma_{uc}$r. The data presented here, together with the frictional and micromechanical properties of our simulated shear zones described in an
accompanying paper [Chapter 5], may help to understand the processes of gouge zone
development and their mechanism of stabilizing effects on fault zones.

4.3. Numerical Methods

Our numerical experiments are carried out using the DEM technique [Cundall
and Strack, 1979]. DEM was designed originally to determine the mechanical behavior of
assemblies of discrete particles. Particle interactions occur only at contacts and particle
motion is determined using Newton’s second law of motion. In this study, we generate
fault blocks from assemblages of circular particles of different sizes, connected by elastic
bonds [Guo and Morgan, 2004; Guo and Morgan, resubmitted]. Each bond acts as two
elastic springs and an elastic beam that transmit contact normal force $F_n$, shear force $F_s$,
and moment $M$, respectively (Figure 1). The forces and moment acting on the bond are
proportional to bond normal stiffness $k_n$ or shear stiffness $k_s$, and also proportional to
bond cross-sectional area $A$ or the moment of inertia of the bond cross-section $I$,
respectively, i.e.,

$$F_n = k_n \cdot A \cdot \delta_n$$  \hspace{1cm} (1)

$$F_s = k_s \cdot A \cdot \delta_s$$  \hspace{1cm} (2)

$$M = k_n \cdot I \cdot \theta$$  \hspace{1cm} (3)

$$A = \pi \cdot R^2$$  \hspace{1cm} (4)

$$I = \frac{1}{4} \cdot A \cdot R^2$$  \hspace{1cm} (5)
where $\delta_n$, $\delta_s$, and $\theta$ are the relative normal, shear, and angular displacements of the particles at the contact, respectively. $R$ is the effective radius determined from the radius of the two contacting particles, $R_1$ and $R_2$, given by

$$R = \frac{2 \cdot R_1 \cdot R_2}{R_1 + R_2}$$

(6)

A bond breaks if the bond tensile stress, $\sigma$, equals or exceeds the bond tensile strength $\sigma_{\text{max}}$, or if the shear stress, $\tau$, equals or exceeds the bond shear strength $\tau_{\text{max}}$, i.e.,

$$\sigma = \frac{F_n}{A} + \frac{|M|}{I} \cdot R > \sigma_{\text{max}}$$

(7)

Figure 1. Schematic diagram of an interparticle bond and its mechanical analogs [Modified after Guo and Morgan, 2004]. The bond between particles behaves as (a) an elastic spring that transmit normal force, and (b) an elastic spring that transmit shear force, and (c) an elastic beam that transmits moment. The interparticle bonds are assumed to deform in a linear elastic manner within the failure criteria, when bonded particles are displaced and rotated from their equilibrium positions.
\[ \tau = \frac{|F|}{A} > \tau_{\text{max}} \] (8)

Here, we assume that the tensile normal force is positive. When one of the above failure criteria is satisfied, bonded particles lose their cohesion and become unbonded.

For unbonded particles in contact, the contact force is calculated using a non-linear Hertz-Mindlin contact model

\[ F_n = \left( \frac{2G\sqrt{2R}}{3(1-v)} \right) \delta_n^{3/2} \] (9)

\[ F_s = \left( \frac{2 \left( 3R G^2 (1-v) \right)^{3/2}}{(2-v)} \right) F_n^{1/3} \] (10)

where \( G \) is the shear modulus and \( v \) is Poisson’s ratio [Mindlin and Deresiewicz, 1953; Johnson, 1985; Morgan and Boettcher, 1999; Guo and Morgan, 2004]. The contact undergoes frictional sliding when \( F_s \) exceeds the critical shear force for slip.

4.4. Experimental Design

Fault blocks are constructed by randomly generating a specified number of circular particles of four different sizes within a 2-D domain (Figure 2 and Table 1). In order to create a closely packed particle assemblage, the domain is compressed under a high isotropic confining pressure until an equilibrium stress state is reached. The confining pressure is then decreased gradually to a point where the average absolute distance \( S \) between adjacent particles is minimal. \( S \) is defined by the following equation:

\[ S = \left( \frac{\sum_{i \neq j} |l - R_i - R_j|}{n} \right) / n \] (11)
where \( n \) is the number of adjacent particle pairs, and \( l \) is the center distance between two adjacent particles with radius equal to \( R_i \) and \( R_j \), respectively. Elastic bonds with uniform properties are added between adjacent particles (Table 1), if \( S \) is smaller than a given threshold (0.001% of the radius of the smallest particle). A few particles (4%) do not satisfy this criterion, so they do not have bonds and behave as noncemented particles in pore spaces. The resulting block of bonded particles, with a height of 36mm, equates to cemented rock (Figure 2). A flat fault surface is defined in the middle of the block by deleting bonds between particles if lines connecting their centers cross the central line of the block. Top and bottom layers of particles (shown in gray) represent fault zone boundaries (Figure 2). They transmit stress during fault zone deformation, but move at constant velocities without damage.

<table>
<thead>
<tr>
<th>Table 1. Parameters for numerical experiments.</th>
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<tbody>
<tr>
<td>Parameter</td>
</tr>
<tr>
<td>Experimental variables</td>
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<tr>
<td>Shear strain rate (s(^{-1}))</td>
</tr>
<tr>
<td>Total shear strain (%)</td>
</tr>
<tr>
<td>Applied normal stress (MPa)</td>
</tr>
<tr>
<td>Particle properties</td>
</tr>
<tr>
<td>Porosity (%)</td>
</tr>
<tr>
<td>Size in radius (mm)</td>
</tr>
<tr>
<td>Mean size in area (mm(^2))</td>
</tr>
<tr>
<td>Size distribution ((D))</td>
</tr>
<tr>
<td>Interparticle friction</td>
</tr>
<tr>
<td>Shear modulus (GPa)</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
</tr>
<tr>
<td>Interparticle bond properties</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
</tr>
<tr>
<td>Young’s modulus (GPa)</td>
</tr>
</tbody>
</table>
Figure 2. Experimental design. (a) Particle assemblage is compressed under a high confining pressure $\sigma_m$. $\sigma_m$ is then decreased gradually to a near zero value. (b) Rock is generated by adding elastic bond between adjacent particles (see text for details). Top and bottom layers of grey particles are defined as fault zone boundaries. A flat fault surface is predefined in the middle of the rock by deleting bonds across the surface as indicated by color contrast. Deformation is induced under constant normal stress $\sigma_n$ and variable shear stress $\tau$ by moving top boundary to the right and bottom boundary to the left at constant velocity $v$. The maximum principal stress $\sigma_f$ and the least principal stress $\sigma_s$ are $45^\circ$ and $135^\circ$ to the fault surface, respectively. Shaded vertical column is strain marker.

Initial particle size in our generated fault blocks follows a fractal distribution described by a power law defined with a fractal dimension $D$. The $D$ value is given by the following relationship [Turcotte, 1986; Sammis et al., 1986, 1987; Morgan and Boettcher, 1999; Guo and Morgan, 2004]:

$$D = \log \left( \frac{N_{i+1}}{N_i} \right) / \log \left( \frac{R_i}{R_{i+1}} \right)$$  \hspace{1cm} (12)

where $N_{i+1}$ and $N_i$ are numbers of particles with a radius equal to $R_{i+1}$ and $R_i$, respectively. The $D$ value of the initial particle distribution is set to 1 in our fault blocks.
Shear strength for most rocks is typically one to two times the tensile strength [e.g., Attewell and Farmer, 1976]. In our bond strength definition, $\tau_{\text{max}}$ is 1.27 times greater than $\sigma_{\text{max}}$ (Table 2), consistent with our previous study [Guo and Morgan, resubmitted]. Five sets of bond strengths are employed to yield $\sigma_{\text{ucs}}$ values of fault blocks in a range from 100 to 260 MPa (Table 2), comparable to strengths of fine-grained sandstone or granite [Attewell and Farmer, 1976]. In order to study the separate effects of $\sigma_{\text{ucs}}$ and $\sigma_n$ on gouge zone evolution, one suite of experiments involved shearing these five pairs of fault blocks under a $\sigma_n$ of 25 MPa, and a second suite involved shearing the fault blocks with $\sigma_{\text{ucs}}$ of 183 MPa under $\sigma_n$ of 10, 40, 55, 70, and 100 MPa. The experiments carried out to examine the effects of $\sigma_{\text{ucs}}$ are labeled using the letter C (i.e., compressive strength), followed by the $\sigma_{\text{ucs}}$ value for the fault blocks, and the experiments conducted to explore the effects of $\sigma_n$ are labeled using the letter N (i.e., normal stress), followed by the applied experimental value for $\sigma_n$. Therefore, N25 and C183 refer to the same experiment that is carried out at normal stress of 25 MPa by shearing the fault block with $\sigma_{\text{ucs}}$ value of 183 MPa.

Table 2. Mechanical properties of fault blocks in numerical experiments.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Bond strength (MPa)</th>
<th>Uniaxial compressive strength (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Tensile</td>
<td>Shear</td>
</tr>
<tr>
<td>C100*</td>
<td>143</td>
<td>182</td>
</tr>
<tr>
<td>C140</td>
<td>206.25</td>
<td>262.5</td>
</tr>
<tr>
<td>C183 (N25*), N10, N40, N55, N70, N100</td>
<td>275</td>
<td>350</td>
</tr>
<tr>
<td>C220</td>
<td>332.75</td>
<td>423.5</td>
</tr>
<tr>
<td>C260</td>
<td>393.25</td>
<td>500.5</td>
</tr>
</tbody>
</table>

* C refers to fault block compressive strength, and N refers to experimental normal stress. The number behind the C or N is either the fault block compressive strength or applied normal stress of represented experiment.
DEM experiments are conducted by moving the upper fault zone boundary to the right and the bottom to the left, at constant and equal velocities, while maintaining $\sigma_n$ on the boundaries. A periodic boundary condition is applied in the horizontal direction, i.e., when a particle leaves the domain from the right boundary, it re-enters through the left boundary, or vice versa. In this deformation configuration, the maximum principal stress $\sigma_1$ and the least principal stress $\sigma_3$ lie at approximately 45° and 135° to the fault surface, respectively (Figure 2). The total shear strain for each experiment is 200%. The deformation state of the fault zone was recorded at each 2% shear strain increment, including stress, fault strength and dilation, bond breakage, gouge deformation mechanisms (i.e., translation, rotation, sliding, and fracture), gouge zone thickness, gouge grain size, and size distribution.

4.5. Deformation Visualization and Gouge Zone Analysis

In order to visualize shear zone deformation, we plot grain size, particle rotation, and particle shear displacement gradient for each 2% shear strain increment. Particle rotations and displacements in our numerical experiments are either in the same sense of the fault block displacement or in the opposite direction. We define these two senses of motion as synthetic and antithetic particle displacements and rotations, respectively. The gradient of particle shear displacement is calculated as the directional derivative of the horizontal particle displacement [e.g., Morgan and Boettcher, 1999]. Grains are defined as single particles or clusters of bonded particles that are connected to the fault blocks or the fault zone boundaries by bonds, due either to their initial configuration or to bond breakage during deformation. In our simulated shear zones, the grains are found either
within damaged zones in the fault blocks or between the fault surfaces (Figures 3b-5b). In the first case, the grains are not part of the gouge zone and undergo minimal rotation or slip after formation. Here, we define gouge grains as those that experience repeated high magnitude rotation or translation within a high displacement gradient zone. The gouge zone boundaries are interpreted based on this definition of fault gouge (Figures 3b-5b).

Changes in volume (i.e., area in 2-D) of our simulated shear zones during deformation, \( \Delta V \), results primarily from variations in the volume of the gouge zone as a result of dilation, compaction, gouge grain comminution, and rearrangement, and secondarily from variations in the volume of the damaged fault blocks as a result of opening and closing of fractures and elastic compression and decompression of the fault blocks (Figures 3a-5a). As the latter contribution is small, we assume that volume change only occurs in the gouge zone; gouge porosity \( \eta_g \) and gouge zone thickness \( T \) can be calculated approximately by the following equations, respectively:

\[
\eta_g = \{ 1 - A_g / [ \Delta V + (A_g / A_p) \cdot V_o] \} \cdot 100\% \\
T = [A_g / (1 - \eta_g / 100)] / L
\]

where \( A_g \) is the area of the gouge grains and \( A_p \) is the area of all particles that constitute the fault blocks. These are the actual areas occupied only by circular particles and do not include the void space between them. \( V_o \) is the original area of the fault blocks including void space, and \( L \) is the length of the fault blocks, which remains constant.

Grain size analysis of the gouge includes (1) the calculation of mean grain size, give by the ratio of \( A_g \) to the number of gouge grains, and (2) the calculation of grain radius, i.e., the radius of an equivalent circular area for a given grain shape. Compared to natural fault gouge zones, our simulated gouge zones are composed of a limited number
Figure 3. Snapshot of gouge zone evolution at 2% shear strain for experiments N100, N25, C260, and C100. (a) Fault zone configuration. Red and green domains denote the two fault blocks or fault gouge derived from them. Yellow particles define initially vertical strain markers. Black lines denote distinct fractures defined by the linear arrangements of void and broken bonds. (b) Gouge grain size contour. Dotted lines are the interpreted gouge zone boundaries (see text for details). (c) Incremental particle rotation over 2% shear strain. White indicates no rotation. (d) Directional derivative of the horizontal component of the residual displacement [Morgan and Boettcher, 1999].
Figure 4. Snapshot of gouge zone evolution at 20% shear strain for experiments N100, N25, C260, and C100. Same as in Figure 3.
Figure 5. Snapshot of gouge zone evolution at 200% shear strain for experiments N100, N25, C260, and C100. Same as in Figure 3. Y-shear and R-shear surfaces are indicated by horizontal and low angle synthetic slip surfaces in red color in (d), respectively.
of gouge grains and grain sizes. To best represent this narrow size distribution, we compare the cumulative grain abundance to grain radius to quantify the fractal dimension $D$, i.e., Equation 15:

$$D = \log \left[ \left( \frac{N_{i+1}}{N_i} \right) + 1 \right] / \log \left( \frac{R_i}{R_{i+1}} \right)$$  \hspace{1cm} (15)

where $R_i$ is greater than $R_{i+1}$.

4.6. Results

Our simulated shear zones show two distinct stages of gouge zone development: a fast growth stage (i.e., gouge zone thickness increases at a high rate) and slow growth stage (i.e., gouge zone thickness increases at a low rate once a well developed gouge zone has formed). The transition from the fast growth stage to the slow growth stage occurs at about 20% shear strain for most experiments, varying slightly with $\sigma_n$ and $\sigma_{u3s}$. Each evolutionary stage exhibits characteristic fabrics, micromechanical behavior, and distinct $\sigma_n$ and $\sigma_{u3s}$ dependence of gouge zone evolution. In order to show the principal features of simulated gouge zone evolution, we present the snapshots of the deforming gouge zones for four representative experiments (i.e., C100, C260, N25, and N100) at 2%, 20%, and 200% shear strain. The effects of $\sigma_n$ and $\sigma_{u3s}$ on gouge zone development are then demonstrated by comparing the intrinsic properties of the gouge zone for each suite of experiments, i.e., gouge porosity, gouge zone thickness, mean grain size, and grain size distribution.
4.6.1. Characteristics of Gouge Zone Evolution

In general, all of the numerical experiments show similar characteristics of gouge zone evolution with variations in details. During the fast growth stage, the fault surfaces are separated by a poorly developed thin gouge zone. Shear strain is accommodated primarily by wear of the fault surfaces (i.e., plucking of grains from the sliding surfaces), gouge grain comminution, and secondarily, by the development of fractures within the fault blocks. Other deformation mechanisms, such as grain rolling and sliding, become more significant as the fault gouge accumulates. The typical deformation fabrics developed during this stage are failure surfaces in fault blocks orientated sub-parallel to \( \sigma_1 \). These general observations can be seen in the snapshots of shear zone deformation at 2\% shear strain for all experiments (e.g., Figures 3-5).

The high \( \sigma_n \) experiment N100 shows a slightly different behavior at 2\% shear strain, characterized by highly interlocked asperities and small horizontal displacement along the fault surfaces (i.e., little distortion of the yellow strain marker) (Figure 3a). Initial shear strain is accommodated by multiple fractures that develop, mostly within the upper fault block. These fractures are recognized by linear arrangements of voids in Figure 3a and are generally parallel or sub-parallel to \( \sigma_1 \). Modest grain rotation (Figure 3c) and slip, indicated by locally high shear displacement gradients (i.e. red bands in Figure 3d), is evident along the fractures, as well as within the gouge zone. For the low \( \sigma_n \) experiment N25, in contrast, the degree of asperity interlocking along fault surfaces is low, whereas dilation is high, leading to higher porosity within the gouge zone, higher magnitudes of gouge grain rotation, and larger shear displacement along fault surfaces (Figures 3a, c, and d). The interiors of the fault blocks experience very little damage and
most loose grains outside the gouge zone were not initially bonded to the fault blocks (Figure 3b). Distinct fractures, oriented parallel or sub-parallel to $\sigma_1$, typically initiate at interlocked asperities along the fault surfaces and propagate into the fault blocks (Figure 3a). Correlated high displacement gradients in the fractured areas indicate that some shear strain is accommodated by slip along these fractures (Figure 3d).

The two experiments conducted on different $\sigma_{uuc}$ fault blocks at normal stress of 25 MPa also exhibit distinct variations in deformation. Compared with N25 (i.e., C183), the high $\sigma_{uuc}$ experiment C260 shows broader damage zones in both fault blocks (Figure 3a). Fractures within these zones are defined by wider void spaces, i.e., greater dilation (Figure 3a), and undergo smaller amounts of slip (Figure 3d). Gouge grains exhibit pronounced synthetic rotations (Figure 3c). The low $\sigma_{uuc}$ experiment C100, on the other hand, shows the formation of a thicker gouge zone and a large damage zone within the upper fault block (Figures 3a and b). Porosity in the shear zone is relatively low. Significant grain rotation and slip occur, not only along the fault surfaces, but also along fractures within the damaged fault blocks (Figures 3c and d).

The transition from the fast growth to the slow growth stage coincides with a decrease in the significance of deformation within the fault blocks, as shown by rare fractures and fracture-related grain rotations and sliding (Figure 4). More strain is accommodated within the gouge zone by grain comminution, rolling and sliding.

In the high $\sigma_\tau$ experiment N100, the gouge zone undergoes compaction and gouge grains experience little vertical translation, i.e., the boundary between red and green particles remains relatively flat (Figure 4a). Smaller grains concentrate in the middle of the gouge zone, and exhibit the most significant rotation and sliding (Figures 4b-d).
Larger grains arise from plucking along the fault surfaces. In contrast, the gouge zone in the low $\sigma_n$ experiment N25 undergoes dilation. The boundary between red and green particles becomes irregular, as grains translate vertically and mix (Figure 4a). In the gouge zone, smaller grains scatter among the big grains (Figure 4b). Deformation, i.e., grain rolling and contact sliding, is more distributed (Figures 4c and d).

The characteristics of deformation also vary with $\sigma_{uc}$ at a normal stress of 25 MPa. For the high $\sigma_{uc}$ experiment C260, the gouge zone undergoes greater dilation and has more large grains, compared to experiment C183 (Figures 4a and b). The large grains generally exhibit noticeable rotation (Figure 4c), but slip surfaces between them are usually less well developed (Figure 4d). For the low $\sigma_{uc}$ experiment C100, the gouge zone undergoes less dilation and has more small grains (Figures 4a and b). Grain distribution is not uniform and the smaller grains tend to concentrate in the lower part of the gouge zone (Figure 4b). Grains in the upper part of the gouge zone show relatively little rotation and sliding, at least for this increment of strain (Figures 4c and d).

During the slow growth stage represented at 200% shear strain, the predefined fault surfaces become irregular and separated by a well developed gouge zone (Figure 5). The rate of fracturing within the fault blocks, the wear rate of the fault surfaces, and the intensity of gouge grain comminution all decrease significantly with increasing shear displacement. Shear strain is mainly accommodated within the gouge zone by grain rolling and sliding. Gouge zone properties are more heterogeneous, for example, grain size is greater and porosity is higher along the gouge zone boundaries. Common shear fabrics seen in natural or experimental fault gouge [e.g., Logan et al, 1979, 1992; Marone and Scholz, 1989; Marone et al., 1990; Gu and Wong, 1994; Beeler et al., 1996; Morgan
and Boettcher, 1999] are well developed in the gouge zone, including discrete boundary shears, low angle synthetic R-shears, and horizontal Y-shears.

For the high $\sigma_n$ experiment N100, the gouge zone at 200% shear strain is highly compacted (Figure 5a). Gouge porosity is about 12%, lower than that of the original fault blocks (15%). Small gouge grains of relatively uniform size (i.e., relative well sorted) are distributed within the gouge zone, while large grains are scattered along the gouge zone boundaries (Figure 5b). Incremental deformation within the fault block is minor. Regions with high magnitudes of grain rotation and high displacement gradients are sparse, although some detached grains are present in the damaged zones within the fault blocks (Figures 5b-d). Deformation within the gouge zone is intense and heterogeneous. Grains distributed along well developed slip surfaces within the gouge show the highest magnitude of rotation, mostly in a synthetic sense (Figure 5c). A long horizontal slip surface (i.e., Y-shear) is developed in the middle of the gouge zone. Slip surfaces are less well developed along the gouge zone boundaries (Figure 5d).

The gouge zone in the low $\sigma_n$ experiment N25 is highly dilated and thicker (Figure 5a). Gouge porosity is about 21%. The heterogeneity of porosity is visible: larger void spaces are dispersed along the gouge zone boundaries. Grain size in the interior of the gouge zone falls within a wider range (i.e., relatively poorly sorted), and, on average, is greater than that in N100. Fewer large grains occur along the gouge zone boundaries (Figure 5b). More grains show high magnitude synthetic or antithetic rotations than in N100 (Figure 5c). The wide range of grain sizes tends to favor the development of short oblique and sub-horizontal slip surfaces. Both synthetic (red) and antithetic slip surfaces
(blue) are well developed close to the more irregular upper gouge zone boundary (Figure 5d).

Differences in $\sigma_{acs}$ at normal stress of 25 MPa do not seem to affect the fault block damage, which is minor, but do influence the heterogeneity of deformation within the gouge zones (Figure 5). For the high $\sigma_{acs}$ experiment C260, gouge porosity is about 20%, similar to that in experiment C183 (i.e., N25). Gouge grains in the interior of the gouge zone are better sorted than for C183 (Figure 5b). Long, continuous, and straight slip surfaces are rare in the gouge zone (Figure 5d). For the low $\sigma_{acs}$ experiment C100, gouge porosity decreases further, and is down to about 19%. Gouge grains in the interior of the gouge zone are less well sorted than for N100, but more well sorted than for C183 (Figure 5b). Again, grain rotations are heterogeneous and correlated with the slip surfaces. Grains clustered along pronounced slip surfaces show higher magnitude rotations (Figure 5c). A low angle slip surface (i.e., synthetic R-shear) is well developed in the gouge zone (Figure 5d).

4.6.2. Gouge Zone Porosity and Thickness

Within the first 4% shear strain, gouge porosities, calculated using Equation 13, increase or decrease in response to the initial dilation or compaction, and the opening or closing of failure surfaces (Figure 6). With continued shear strain, the effects of fault block fracture on porosity become much less significant; the gouge porosities for all experiments decrease non-linearly, and eventually settle out to fluctuate around constant values. Except for high $\sigma_n$ experiments N100 and N75, the gouge porosities in our simulated shear zones are higher than that of the initial fault blocks (15%). Gouge
porosity depends on both $\sigma_n$ and $\sigma_{ucs}$; Porosity decreases with increasing $\sigma_n$ (Figure 6a), and with decreasing $\sigma_{ucs}$ (Figure 6b).

As noted in Figures 3-5, the thickness of the simulated gouge zone varies significantly with shear strain (Figure 7). All of the experiments show a rapid increase in

![Graph](image)

Figure 6. Effects of (a) normal stress and (b) uniaxial compressive strength on gouge porosity plotted against shear strain.
gouge zone thickness within the first 20% shear strain, i.e., the fast growth stage. Gouge zone thickness then increases at a much lower rate with continued shear strain. The evolution of gouge zone thickness is also strongly dependent on both $\sigma_n$ and $\sigma_{nCS}$. Within the first 20% shear strain, experiment N100 shows the most rapid increase in gouge zone thickness. The rate of gouge thickening decreases with decreasing $\sigma_n$, with the exception
of experiment N40, which shows an anomalously low rate of thickening. Over the last 180% shear strain, i.e., the slow growth stage, and the rate of gouge thickening tends to decrease with increasing $\sigma_n$ (Figure 7a). Experiments N10 shows the fastest increasing rate in the gouge zone thickness. The dependence of gouge zone thickness on $\sigma_{ucs}$ is similar to the change in $\sigma_n$ but in the opposite direction (Figure 7b). For example, experiment C100 show the fastest gouge growth rate within the first 20% shear strain, while experiment C260 show the highest rate of increase over the last 180% shear strain. The rate of the gouge zone thickening appears to be proportional to $\sigma_{ucs}$ within the first 20% shear strain, but inversely proportional to $\sigma_{ucs}$ over the remaining shear strain.

4.6.3. Gouge Grain Size and Size Distribution

Mean gouge grain size evolves systematically with shear strain for all experiments (Figure 8). In general, mean grain sizes reach peak values within the first 4% shear strain, and then fall exponentially with increasing shear strain. Both $\sigma_n$ and $\sigma_{ucs}$ have secondary effects on the mean gouge grain size (Figure 8). Mean gouge grain size tends to decrease with increasing $\sigma_n$ and decreasing $\sigma_{ucs}$, but varies within a very narrow range. Although grain size is noticeably higher in experiment C260 than in the other experiments, and about two times larger than the mean particle size of the initial particle assemblage at 200% shear strain (Figure 8b).

The evolution of grain size distribution with shear strain is a sensitive indicator of mechanical processes of gouge deformation. A representative log-log plot of cumulative grain abundance versus equivalent grain radius for experiment N25 shows generally linear increases in log cumulative grain abundance with decreasing log grain size in
Figure 8. Effects of (a) normal stress and (b) uniaxial compressive strength on mean grain size, plotted against shear strain. Dotted lines denote the mean particle size of the initial particle assemblage (Figure 2a).

radius (Figure 9). This observation suggests that grain size follows a fractal size distribution that can be quantified by the fractal dimension $D$ (Equation 15). The grain size distribution curves can be divided into a linear portion to the right and a nonlinear portion to the left. The linear portion describes the distribution of large grain sizes (i.e.,
radius > 2.8mm) where grains are still breakable. The nonlinear portion includes both breakable and unbreakable grains. Thus, the nonlinearity results from the accumulation of unbreakable grains (i.e., single particles).

![Graph showing grain size distribution curves for different strains in experiments N25.](image)

**Figure 9.** Grain size distribution curves for different strains in experiments N25. Breakable grains to the right of dotted line give an unbiased measure of grain size distribution, and $D$ values are estimated from the slopes of these linear portions of the curves. Grain size distributions to the left of dotted line are skewed by the presence of unbreakable particles. In this particular example, crushing of gouge grains is a dominant mechanism for grain size reduction, resulting in progressive steeping of PSD curve.

In order to eliminate the effect of unbreakable grains on the size distribution, $D$ values defined by Equation 15 were calculated from the best-fit to the linear portion of the gouge grain size distribution. Our numerical experiments generally yield increasing $D$ values during the fast growth stage (Figure 10). $D$ values then vary in a wide range from 0.9 to 2.4, but occasionally reach plateaus that last as long as 20% shear strain. Both $\sigma_n$ and $\sigma_{acs}$ affect the $D$ values. The $D$ values tend to be higher in low $\sigma_n$ experiments within
the first 110% shear strain, but increases in the $D$ values for experiment N100 and decreases for experiment N10 weaken this tendency within the remaining shear strain (Figure 10a). No systematic variation in the $D$ values is observed with $\sigma_{act}$ in our numerical experiments (Figure 10b).

![Graph](image)

Figure 10. Effects of (a) normal stress and (b) uniaxial compressive strength on fractal dimension $D$ value, plotted against shear strain.
4.7. Discussion

4.7.1. Structural Evolution of Shear Zone

Our numerical experiments demonstrate that shear zones show different characteristics of structural evolution during the fast growth and the slow growth stages. These two stages are distinguished by a change in the dominant deformation structures from tensile fractures within the fault blocks, to shear fracture arrays within a well-developed fault gouge zone. In our numerical experiments, the earliest phase of the fast growth stage is characterized by the development of $\sigma_1$ parallel or sub-parallel fractures in the fault blocks, especially for the high $\sigma_n$ and low $\sigma_{uc}$ conditions (Figure 3a). As low strength brittle materials easily yield by fracturing at high stress, the longest and most abundant fractures are observed in high $\sigma_n$ and low $\sigma_{uc}$ experiments. The tensile fractures observed during initial shearing are common features in a simple shear configuration [Knipe and White, 1979; Scholz, 1990; Wibberley et al., 2000]. Once the gouge zones in our numerical experiments reach a sufficient thickness to completely separate the opposing fault surfaces, the slow growth stage initiates, generally at about 20% shear strain. The dominant deformation mechanism changes from damage (i.e., wear and fracturing) of fault blocks, to shearing within the well-developed fault gouge zone. The shearing of gouge grains produces heterogeneously distributed shear surfaces, such as R-shears and Y-shears, in the gouge zones (Figure 5d). In well-developed, naturally-occurring or simulated gouge zones, deformation is characterized by the development of characteristic shear fabrics within the fault gouge [e.g., Logan et al, 1979,1992; Marone and Scholz, 1989; Marone et al., 1990; Gu and Wong, 1994, Beeler et al., 1996; Morgan and Boettcher, 1999]. Our results are consistent with this observation.
Our experiments also reveal that the types and geometries of the shear surfaces that develop during shearing are strongly dependent on gouge grain sorting, i.e., the range of gouge grain sizes around the mean. Visual inspection of grain size distribution in the interiors of the gouge zones at 200% shear strain shows that sorting increases with increasing \( \sigma_n \) and decreasing \( \sigma_{ucS} \) (Figure 5b). This is because large grains are readily crushed under high \( \sigma_n \) and low \( \sigma_{ucS} \) conditions. Associated with this increase in grain sorting, the initial shear fractures change from short curved surfaces, to short oblique linear surfaces, long oblique linear surfaces, and finally to long horizontal linear surfaces (Figures 5d). This correlation suggests that well sorted gouge, favored by high \( \sigma_n \) and low \( \sigma_{ucS} \), facilitates the formation of long linear shear surfaces oriented parallel to or at low angles to the fault zone boundaries, i.e., Y-shears or low angle Reidel shears [Scholz, 1990]. In poorly sorted gouges, favored by low \( \sigma_n \) and high \( \sigma_{ucS} \), shear surfaces wrap around large grains, probably in less favored orientations for the simple shear configuration, and thus are short-lived before being replaced by new, more favorably oriented slip surfaces. Therefore, short curved slip surfaces are common in less well sorted gouges.

Nearly all of our numerical experiments exhibited more intense wear and fracturing in the upper fault block than in the lower fault block (Figures 3a-5a). As the fault blocks are created in the same way and have the same physical properties, symmetric block deformation would be expected. In fact, the formation process results in a rather heterogeneous particle packing which determined the bond distribution, causing strength variations in the fault blocks. This can be seen in Figure 11a, where the right side of the upper fault block is weaker because of its relatively low bond density. In addition,
the stress distribution in the fault blocks is very heterogeneous (Figure 11b), dependent on the orientation, geometry, and location of asperities along the fault surfaces, as well as particle and bond arrangements within the fault blocks. Therefore, fractures develop preferentially in the weaker zones under higher tensile stress, especially within the upper fault block.

![Image](image.png)

Figure 11. (a) Spatial distribution of bonds in undeformed fault blocks. Bonds are denoted by lines that connect the centers of particle pairs. The upper fault block, especially to the right, shows a lower bond density than the lower fault block. (b) Contact normal stress distribution in the fault blocks at 0.1% shear strain for experiment N25. Stresses are denoted by lines that connect the centers of particles in contact. Darker colors denote higher normal stresses. The stress distribution is very heterogeneous.

### 4.7.2. Gouge Zone Thickness

The thickness of natural and experimental fault gouge zones is primarily a function of the wear rate of the fault surfaces. Theoretical and experimental studies of gouge zone thickness have demonstrated that wear during continued shearing is characterized by an exponential decay in wear rate during the early stage of sliding, i.e.,
the "conditioning" stage, and finally, a nearly steady-state wear rate during the duration of fault slip [Queener et al., 1965; Scholz, 1987; Power et al., 1988; Scholz, 1990]. We observe a similar pattern of wear with shear displacement, i.e., a rapid increase in gouge zone thickness that decays with increasing shear strain, followed by a more gradual linear increase in the gouge zone thickness (Figure 7). We also found that $\sigma_n$ and $\sigma_{ucc}$ have little effect on this fundamental characteristic of gouge zone growth (Figure 7), although the fast growth stage tends to last longer in the low $\sigma_n$ and high $\sigma_{ucc}$ experiments, apparently because of relatively low wear rates in these experiments. The high wear rates during the early stages of sliding are thought to be a result of greater roughness of the initial fault surfaces, than during late stages of steady-state wear [Queener et al., 1965; Scholz, 1990]. This cannot be true for our experiments, however, because the fault surfaces are essentially flat at the onset of our experiments (at least at the scale of the largest particles in our simulated fault blocks), whereas they become more irregular and rougher as grains are plucked during sliding (Figures 3a-5a). Instead, the transition in wear rate in our experiments is apparently associated with a transition in shear zone configuration, thickness, and dominant deformation mechanisms. During the early phase of sliding, the fault gouge zone is poorly developed and asperities along the fault surfaces are highly interlocked. This leads to intensive fault block fracture and surface wear (Figure 3). The progressive accumulation of fault gouge gradually changes the dominant deformation mechanisms from wear of the fault surfaces to shearing of the fault gouge. Eventually, shear strain is accommodated mainly by gouge grain rolling and sliding when a gouge zone is well developed (Figures 5).
Previous studies of the wear process during shear deformation demonstrated that wear rate is dependent on $\sigma_n$ and rock bulk strength [Kessler, 1933; Yoshioka, 1986; Scholz, 1987; Wibberley et al., 2000]. Scholz [1987] proposed a wear model that neglects porosity change within the gouge zone. The model predicts that gouge thickness $T$ is linearly proportional to shear displacement $S$ and $\sigma_n$, and inversely proportional to rock hardness $H$, i.e.,

$$T = c\sigma_n S / 3H$$

(16)

where $c$ is a dimensionless parameter that is expected to be in the range of 0.1-1 for abrasion dominated wear and much lower for adhesion involved wear [Rabinowicz, 1965; Scholz, 1987]. In the direct shear experiments by Yoshioka [1986], the wear rates for sandstone and granite are in rough agreement with the prediction of the model [Scholz, 1987].

The dependence of wear rate on $\sigma_n$ and $\sigma_{ucs}$ that we observe appears to be much more complex than that described by Scholz's model, and in fact is shear displacement dependent. During the fast growth stage, the wear rate tends to increase nonlinearly with increasing $\sigma_n$ and decreasing $\sigma_{ucs}$ (Figure 7). This observation is qualitatively consistent with Scholz's model that describes a linear dependence of the wear rate on $\sigma_n$ and $\sigma_{ucs}$. During the slow growth stage, however, the wear rate dependence on $\sigma_n$ and $\sigma_{ucs}$ reverses in our simulations. The higher wear rates are achieved in the low $\sigma_n$ and high $\sigma_{ucs}$ experiments. Consequently, fault gouge thickness in the low $\sigma_n$ and/or high $\sigma_{ucs}$ experiments can exceed those in the high $\sigma_n$ and/or low $\sigma_{ucs}$ experiments, if shear displacement is high enough (as shown in Figure 7). The dependence of $T$ on $\sigma_n$ and $\sigma_{ucs}$ in our experiments can be described by the following best fit equation:
\[ T = 9.54S_f^{0.48} \sigma_n^{-0.035} / \sigma_{ucs}^{0.25} + 0.054S_f \sigma_{ucs}^{0.23} / \sigma_n^{0.18} \]  
(17)

\[ S_f = 0.39\sigma_{ucs}^{0.68} / \sigma_n^{0.088} \]  
(18)

where \( S_f \) and \( S_s \) are the shear displacement over the fast growth and slow growth stages, respectively. This derived numerical model is conceptually similar to a theoretical wear model suggested by Power et al. (1988), i.e., both models predict a similar evolutionary path of gouge zone thickness, i.e., nonlinear increase followed by a linear, lower rate growth. But the numerical model presented here more explicitly describes the dependence of gouge zone thickness on \( \sigma_n \) and \( \sigma_{ucs} \).

For natural faults, the gouge zone thickness to displacement ratios fall between 0.1 to 0.001 [Robertson, 1983]. Gouge zone thickening rates for our simulated shear

![Figure 12. Gouge zone thickness as a function of shear displacement predicted by Equation 17. Equation 17 defines the highest and lowest slopes (i.e., ratios of thickness to displacement) during the slow growth stage under the experimental conditions (i.e., normal stress and rock uniaxial compressive strength) for experiments N10 and N100, respectively. The slope predicted by Equations 17 is close to the upper bound (i.e., 0.1) observed from natural faults [Robertson, 1983]. The gouge zone thicknesses for experiment N10 and N100 are also plotted as reference for Equation 17.](image-url)
zones, predicted by Equation 17, lie in a range from 0.08 to 0.12 during the slow growth stage, dependent on the contrast between $\sigma_n$ and $\sigma_{u_{cs}}$ (Figure 12). Compared to natural fault zones, the shear displacements in our numerical experiments are relatively short (about 74 mm). Although the thickening rates of our simulated gouge zones are relatively constant during the slow growth stage (Figure 7), further accumulation of fault gouge beyond 200% shear strain may allow more strain to be accommodated within the gouge zone and consequently lead to relatively lower wear rates. This is supported by observed exponential decreasing abundances of bond breakage with increasing shear strain in these experiments, summarized in the accompanying paper [Chapter 5].

4.7.3. Gouge Grain Size and Size Distribution

The mean gouge grain size in our numerical experiments is primarily controlled by shear strain, decreasing with increasing shear displacement after reaching a peak value within the first 4% shear strain (Figure 8). This observation is consistent with the results of laboratory experiments, for example, triaxial tests on Sidobre granite that show increasing abundance of smaller grains with increasing shear displacement [Amitrano and Schmittbuhl, 2002]. Our results also show secondary variations in gouge mean grain size with $\sigma_n$, and also with $\sigma_{u_{cs}}$, i.e., mean gouge grain size tends to decrease with increasing $\sigma_n$ and with decreasing $\sigma_{u_{cs}}$. This is again consistent with lab studies, e.g., Wibberley et al. [2000] observed that the mean grain size of gouge decreases with increased $\sigma_n$ in shear box tests on low porosity sandstone samples. In our numerical experiments, mean gouge grain size depends on the relative activity of two failure mechanisms: fault surface wear and grain comminution (Figures 3b-5b). Initially, high $\sigma_n$ and low $\sigma_{u_{cs}}$ facilitate the
production of bigger gouge grains by inducing widely spaced and long fractures in the fault blocks with continuing shear strain, however, high $\sigma_n$ and low $\sigma_{ucs}$ also induce substantial grain comminution by crushing (Figures 3a-5a, 3b-5b). In contrast, low $\sigma_n$ and high $\sigma_{ucs}$ experiments exhibit less grain plucking, and subsequently low rates of grain comminution. Thus, the dependence of mean gouge grain size on $\sigma_n$ and $\sigma_{ucs}$ must vary with shear displacement as a result of variation in wear and comminution rate.

Grain sizes in many natural and artificial fault gouges follow power law grain size distribution, characterized by the fractal dimension $D$ defined in Equation 12 [Sammis et al., 1987; Marone and Scholz, 1989; Biegel et al., 1989; Blenkinsop, 1991; An and Sammis, 1994; Storti et al., 2003; Billi et al., 2003; Rawling and Goodwin, 2003, Abe and Mair, 2005]. Sammis et al. (1987) proposed a constrained comminution model that predicts that gouge grains tend to evolve toward a characteristic size distribution with a $D$ value of about 2.6 in three dimensions, or 1.6 in two dimensions [Turcotte, 1986]. The grain sizes in our numerical experiments also follow fractal distributions (Figure 9). The grain size distributions, given in terms of $D$, vary in step-like fashion with shear strain, and never evolve to a single steady state value. Primarily, this reflects the unsteady wear of the sliding surfaces, and secondarily the unsteady rate of grain comminution. However, the grain size distribution measured by $D$ also varies with both $\sigma_n$ and $\sigma_{ucs}$ because wear and comminution rates are functions of both $\sigma_n$ and $\sigma_{ucs}$.

The 2-D $D$ values in our numerical experiments fall into a wide range from 0.9 to 2.4 during the slow growth stage (Figure 10). There are several possible explanations for the difference in grain size distribution observed in our numerical experiments and these predicted by the constrained comminution model. The constrained comminution model
assumes that the grain size distribution varies only because of grain size reduction by comminution. In our numerical experiments, however, the grain size distribution evolves as a result of both grain comminution and wear of the sliding surfaces. While grain comminution serves to reduce grain sizes, wear tends to introduce grains of various sizes, but preferentially larger than the mean size, and preferentially along the gouge zone boundaries. The abundance and size of the wear products varies significantly with shear displacement, $\sigma_n$ and $\sigma_{ucs}$ (Figures 3b-5b). In the constrained comminution model, the probability of grain breakage is controlled by the relative size of nearest-neighbor grains and is assumed not to be sensitive to $\sigma_n$ and $\sigma_{ucs}$ [Sammis et al., 1987]. In our numerical experiments, we find more abundant large gouge grains surviving in low $\sigma_n$ and high $\sigma_{ucs}$ experiments (Figure 5b). Therefore, the probability of grain comminution is affected by both $\sigma_n$ and $\sigma_{ucs}$. In the constrained comminution model, grains never reach a grinding limit. In our numerical experiments, gouge grain size is limited by the sizes of single particles. Although we only used the abundance of breakable grains to calculate $D$ value, the presence of unbreakable grains (i.e., particles at their grinding limits) force the breakage of the breakable grains [Petch, 1953; An and Sammis, 1994; Marone and Scholz, 1989; Storti et al., 2003; Guo and Morgan, resubmitted], and therefore affect the size distribution of the breakable grains (i.e., the calculated $D$ values). Finally, for the constrained comminution model, $D$ value is calculated using incremental abundances of grains (Equation 12), whereas, we calculate $D$ using cumulative grain abundance, i.e., Equation 15 that defines a slightly higher $D$ value than equation 12. Nonetheless, the range of $D$ values observed here is comparable with these documented for natural and artificial fault gouges [Sammis et al., 1987; Marone and Scholz, 1989; Biegel et al., 1989;
Blenkinsop, 1991; An and Sammis, 1994; Storti et al., 2003; Billi et al., 2003; Rawling and Goodwin, 2003, Abe and Mair, 2005] as well as executed numerically by others [e.g., Morgan and Boettcher, 1999].

In addition, our experiments demonstrate that the spatial and temporal distribution of grain size is not homogeneous in the simulated fault gouge zones (Figures 3b-5b). Large grains tend to be concentrated along the gouge zone boundaries, i.e., the source of new grains, during the slow growth stage. The observed heterogeneity suggests that \( D \) values may also vary from the boundary to gouge zone center in natural fault zones. An increase in \( D \) value from fault damage zones, to breccia zones, and into the middle of gouge zones has been observed in Death Valley fault rocks [Morgan et al., 1996] and in carbonate cataclastic rocks [Storti et al., 2003]. The variability of \( D \) value is attributed to a progressive change of the dominant fragmentation mechanism, an increased contribution of surface abrasion, and the variation of particle strength with size and shape, and also increasing shear strain in the center of gouge zone.

4.8. Conclusions

DEM simulations of growth of fault gouge zones demonstrate that the gouge zone evolution involves two distinct stages, i.e., the fast growth and the slow growth, associated with transitions in the dominant deformation mechanisms and in shear zone configuration. During the first stage, the gouge zones are poorly developed, and deformation is characterized by the development of tensile fractures parallel or subparallel to \( \sigma_7 \) in the fault blocks. Fracture of the wall rock, which is more significant in high \( \sigma_n \) and low \( \sigma_{lus} \) experiments, is the dominant deformation mechanism. Shear
strain is mainly accommodated by wear of the fault surfaces. With increasing gouge zone thickness, grain sliding and rotation are enhanced while fracturing is reduced. The beginning of the second evolutionary stage is marked by the significant reduction in wear rate at about 20% shear strain and well-developed gouge zones. Deformation during this later stage is characterized by the development of transient shear fractures within fault gouge. Shear strain is mainly accommodated by shearing within the gouge through grain sliding, rolling, and crushing. Gouge grain sorting affects the types and geometries of the shear structures that develop. Well sorted gouge favors the development of long linear horizontal and sub-horizontal shear surfaces.

The rate of the gouge zone thickening in our numerical experiments decreases exponentially during the fast growth stage and becomes approximately constant during the slow growth stage. The dependence of the gouge zone thickness on $\sigma_n$ and $\sigma_{ucs}$ varies with shear displacement. During the fast growth stage, the rate of gouge zone thickening is proportional to $\sigma_n$ and inversely proportional to $\sigma_{ucs}$. The dependency reverses during the slow growth stage. The entire wear process can be described by a wear model (i.e., Equation 17) that predicts thicker fault gouge in high $\sigma_{ucs}$ shear zones deformed under low $\sigma_n$ if shear displacements are high enough.

Mean gouge grain size in our numerical experiments is primarily dependent on shear strain, and decreases exponentially with increasing shear displacement after reaching a peak value within the first 4% shear strain. The mean gouge grain size also shows a secondary dependence on $\sigma_n$ and $\sigma_{ucs}$ and tends to decrease with increasing $\sigma_n$ and decreasing $\sigma_{ucs}$. Grains in our simulated fault gouges follow a fractal size distribution. The 2-D $D$ values fall into a wide range from 0.6 to 2.4, and vary
unsystematically with shear displacement, $\sigma_n$, and $\sigma_{ucs}$. Our results demonstrate that surface wear preferentially generates large grains along the gouge zone boundaries, causing fluctuations in grain size distribution during a simulation. The properties (i.e., abundance and size) of the wear products are strongly dependent on shear displacement, $\sigma_n$, and $\sigma_{ucs}$. Therefore, wear together with grain comminution plays an important role in producing the characteristics of the grain size distribution observed in our numerical experiments.
Chapter 5

Fault Gouge Evolution and Its Dependence on Normal Stress and Rock Strength:

Results of Discrete Element Simulations

2. Gouge Zone Micromechanics

5.1. Abstract

We simulate the break down of fault blocks using the Distinct Element Method (DEM) in two-dimensions in order to study the frictional strength, mechanical behavior, and stress and strain state of evolving fault gouge, and their dependence on normal stress \( \sigma_n \) and uniaxial compressive strength \( \sigma_{uc3} \). The fault blocks were generated by adding elastic bonds between adjacent circular particles to obtain a given \( \sigma_{uc3} \) in a range from 100 to 260 MPa, and deformed in a direct shear configuration over a range of \( \sigma_n \) from 10 to 100 MPa. The simulated shear zones experience two growth stages: fast and slow. During the fast growth stage, they exhibit a peak friction value reached within the first 2% shear strain. The peak friction value and the magnitude of fluctuation in residual friction associated with volume strain are enhanced in low \( \sigma_n \) and high \( \sigma_{uc3} \) experiments. The residual sliding friction decreases nonlinearly with increasing \( \sigma_n \) and does not show a strong dependence on \( \sigma_{uc3} \). The peaks in friction during the slow growth stage coincide with lows in related micromechanical properties and are associated with localized deformation dependent on gouge thickness, shear strain, as well as \( \sigma_n \) and \( \sigma_{uc3} \). The intensity of bond breakage decreases exponentially with shear displacement. It also increases with increasing \( \sigma_n \) and decreasing \( \sigma_{uc3} \) during the fast growth stage, but this dependence reverses during the slow growth stage. Stress and strain distributions in our
simulated shear zones are heterogeneous and vary with progressive accumulation of fault
gouge

5.2. Introduction

Frictional sliding of brittle shear zones produces non-cohesive wear detritus called fault
gouge. Much of the shear strain may be accommodated within the fault gouge zone
by gouge grain rolling, sliding, and comminution. Consequently, gouge physical and
structural properties evolve during shear zone deformation. Variations in these properties
may change the stress state, the strain response, and the mechanical behavior of the shear
zone, potentially leading to unstable frictional sliding [Engelder et al., 1975; Byerlee et
al., 1978; Logan et al., 1979; Moore et al., 1988; Tullis et al., 1989; Mair et al., 2002;
Anthony and Marone, 2005]. In order to gain a better understanding of the complex
effects of evolving fault gouge on fault stability, this paper details the frictional behavior
and associated micromechanical processes of simulated fault gouge zones that develop
from bare fault surfaces and grow in a natural way. The evolution of structural and
physical properties of the gouges is reviewed in the accompanying paper [Chapter 4].

Numerical simulations of shear zone deformation based on discontinuum
mechanics [Mora and Place, 1998, 1999; Morgan and Boettcher, 1999; Morgan, 1999;
Place and Mora, 2000; Hazzard and Mair, 2003; Morgan, 2004; Abe and Mair, 2005;
Guo and Morgan, resubmitted], provide a unique way for real time study of fault zone
evolution and offer a rare opportunity to visualize the micromechanical processes of
gouge zone deformation and associated fault zone dynamic behavior. Recent numerical
simulations have yielded many informative observations on fault zone process and fault
mechanics. Studies of earthquake faults using the Lattice Solid Model (LSM) [Mora and Place, 1993] indicate that self-organization of fault gouge results in shear localization in a narrow zone that enhances particle rolling, and therefore causes fault weakening [Mora and Place, 1998, 1999; Place and Mora, 2000]. Simulations of fault gouge deformation using the Distinct Element Method [DEM, Cundall and Strack, 1979] demonstrate that mechanical behavior and strength of granular shear zones are influenced by particle size distribution and interparticle friction [Morgan and Boettcher, 1999; Morgan, 1999].

An unrealistically high degree of particle rolling in two dimensional numerical systems is thought to be the major reason for the much lower strengths of simulated faults than those observed in the laboratory experiments [Mora and Place, 1998; Morgan and Boettcher, 1999; Mair et al., 2002; Frye and Marone, 2002]. Subsequent efforts have been made to find proxies to reduce particle rolling or employ irregularly shaped grains in the numerical systems and to make numerical simulations more realistic [Morgan, 2004; Guo and Morgan, 2004]. Compared to experimental or natural shear zones that undergo fracturing and dynamic variation in grain characteristics [Sammis et al., 1986; Marone and Scholz, 1989; Marone et al., 1990], numerical shear zones in which contact deformation is only accommodated by elastic yielding of particles with invariable shape and size are too simple to reproduce important rate and state dependent frictional phenomena [e.g., Scholz, 1998]. The latest simulations have introduced more complex contact laws to simulate grain comminution [Abe and Mair, 2005; Guo and Morgan, resubmitted]. Numerical experiments have been carried out to simulate the break down of particle aggregates that are generated by adding elastic bonds between adjacent particles [Abe and Mair, 2005; Guo and Morgan, resubmitted]. The simulations demonstrate that
grain comminution affects the partitioning of different deformation mechanisms and
gouge zone frictional strength mainly by changing grain characteristics [Guo and
Morgan, resubmitted].

Here, we take this approach one step further to simulate the break down of fault
blocks that are approximated by assemblages of bonded particles [e.g., Chapter 4]. In this
way, we can study the stress-strain history and variations in dynamic behavior of the
simulated shear zones during fault gouge zone evolution, and their dependence on normal
stress and rock strength. In particular, the simulations allow us to examine the mechanical
and frictional effects of sliding surface wear and associated variations in gouge
properties, which could not be done in previous shear zone simulations with
undeformable sliding boundaries.

5.3. Numerical Methods and Experimental Set-up

Natural rocks, in a general sense, are composed of interlocking or cemented
mineral grains. If stress acting on a rock exceeds its strength, the rock will lose its
cohesion, undergo fracture, and produce rock detritus. Therefore, mechanically, the rock
can be approximated by an assemblage of circular particles of different sizes with finite
cohesive forces between particles in contact (Figure 1). Its deformation can be simulated
using the DEM technique, which determines particle interaction using appropriate contact
laws and monitors particle motion using Newton's second law [Cundall and Strack,
1979]. In this study, adjacent particles are connected by elastic bonds that simulate
cohesion [Guo and Morgan, 2004; Guo and Morgan, resubmitted]. Bonded particle lose
their cohesion and become unbonded if the bond tensile stress equals or exceeds the bond
tensile strength, or if the shear stress equals or exceeds the bond shear strength. The contact normal force and shear force for noncohesive contact (i.e. contact between unbonded particles) are calculated using a non-linear Hertz-Mindlin contact model that provides a more realistic description of spherical elastic contact deformation than does a linear Hookian model [Mindlin and Deresiewicz, 1953; Johnson, 1985]. Frictional sliding occurs when contact shear force exceeds the critical shear force for slip. Model details are described in Chapter 4.

![Diagram of fault zone](image)

**Figure 1.** Configuration of numerical experiments. Rock is an assemblage of circular particles linked by breakable elastic bonds. A planer fault surface is predefined in the middle of the rock, as indicated by color contrast. Fault blocks are deformed under constant normal stress $\sigma_n$ and variable shear stress $\tau$ by moving the top and bottom undeformable fault zone boundaries (layers of grey particles) at constant velocities $v$, but in opposite directions. The maximum principal stress $\sigma_I$ and the least principal stress $\sigma_3$ are approximately $45^\circ$ and $135^\circ$ to the fault zone boundaries, respectively. The light-colored vertical column is a strain marker.
Numerical direct shear experiments designed for this study are identical to those described in Chapter 4. As shown in Figure 1, rock in the numerical experiments is an assemblage of randomly distributed and closely packed circular particles connected by elastic bonds. The particles have four different sizes (0.3, 0.25, 0.2083, and 0.1736 mm in radius) that follow a fractal distribution defined with a fractal dimension $D$ [Turcotte, 1986; Sammis et al., 1986, 1987; Morgan and Boettcher, 1999; Chapter 4]. $D$ value equals to 1 in our fractal size rock block.

A flat noncohesive sliding surface (i.e., fault surface) is defined in the middle of the rock by deleting bonds between pairs of particles with centers on opposite sides of the dividing line. The resulting two fault blocks are then deformed under defined constant values of $\sigma_n$ by moving the top and bottom undeformable fault zone boundaries (particles shown in gray in Figure 1) at constant velocities, but in opposite directions to induce right-lateral shear. In this simple shear configuration, the maximum principal stress $\sigma_1$ and the least principal stress $\sigma_3$ are approximately $45^\circ$ and $135^\circ$ to the fault zone boundary, respectively (Figure 1). The left and right boundaries of the domain are periodic, i.e., when particles exit one boundary, they reenter the domain through the other.

Five sets of rocks with uniaxial compressive strength ($\sigma_{ucs}$) of 100, 140, 183, 220, and 260 MPa were created by assigning appropriate bond strengths (Table 1). These assemblages were sheared under normal stress of 25 MPa. These experiments are labeled using the letter C (abbreviation for compressive strength), followed by rock $\sigma_{ucs}$ value. The rock with $\sigma_{ucs}$ of 183 MPa was also deformed under normal stresses of 10, 40, 55, 70, and 100 MPa. This suite of experiments is labeled using the letter N (abbreviation for
normal stress), followed by experimental value for $\sigma_n$. The bulk shear strain for each experiment is 200%, i.e., the displacement of the upper fault zone boundary relative to the lower boundary is twice as long as the initial spacing between these two boundaries.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Bond strength (MPa)</th>
<th>Uniaxial compressive strength (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Tensile</td>
<td>Shear</td>
</tr>
<tr>
<td>C100*</td>
<td>143</td>
<td>182</td>
</tr>
<tr>
<td>C140</td>
<td>206.25</td>
<td>262.5</td>
</tr>
<tr>
<td>C183 (N25*), N10, N40, N55, N70, N100</td>
<td>275</td>
<td>350</td>
</tr>
<tr>
<td>C220</td>
<td>332.75</td>
<td>423.5</td>
</tr>
<tr>
<td>C260</td>
<td>393.25</td>
<td>500.5</td>
</tr>
</tbody>
</table>

*C refers to fault block compressive strength, and N refers to experimental normal stress. The number behind the C or N is either the fault block compressive strength or applied normal stress of represented experiment.

### 5.4. Results

Fault surface wear during frictional sliding of our simulated fault shear zones produces fault gouge [Chapter 4]. The progressive accumulation of the gouge changes shear zone stress and strain state. Wear rate is initially very high, and then reduced significantly at about 20% shear strain. The change in the wear rate divides the process of gouge zone evolution into two stages, i.e., fast growth stage and slow growth stage [Chapter 4]. The frictional and micromechanical properties of the shear zones, their dependence on $\sigma_n$ and $\sigma_{acc}$, and stress strain history are distinct during each evolutionary stage, as shown below.
5.4.1. Frictional Strength and Behavior

Friction, $\mu$, for our simulated shear zones is defined as the ratio of shear stress $\tau$ to normal stress $\sigma_n$ acting on the fault zone boundaries (Figure 1). All of the shear zones display a peak $\mu$ value at 2% shear strain (Figure 2). The peak is enhanced in the lower $\sigma_n$.

![Figure 1](image)

(a)

![Figure 2](image)

(b)

Figure 2. Effects of (a) normal stress and (b) uniaxial compressive strength on friction plotted against shear strain. Inset shows residual friction calculated as the sum of mean friction over the last 180% shear strain and its standard deviation. Error bars show the standard deviation. Interpolated line is fit to data points by eye.
or higher $\sigma_{ucs}$ experiments. In general, friction decreases throughout the fast growth stage, and then tends to vary around a relatively constant value or increases for high $\sigma_{ucs}$ experiments throughout the slow growth stage.

The effect of $\sigma_n$ and $\sigma_{ucs}$ on $\mu$ is systematic (Figure 2a). The residual friction, $\mu_{\text{max}}$, calculated as the sum of mean friction and its standard deviation over the last 180% shear strain, decreases with increasing $\sigma_n$ in a nonlinear fashion. The magnitude of $\mu$ fluctuations, measured as the standard deviation, also decreases with increasing $\sigma_n$. In contrast, increase in $\sigma_{ucs}$ leads to a wider range of variation in $\mu$ (Figure 2b). Both peak friction and the magnitude of $\mu$ fluctuations increase with increasing $\sigma_{ucs}$.

**5.4.2. Deformation Mechanisms**

The frictional strengths and their evolution in natural and experimental fault zones are related to the degree of shear localization within the fault gouge [Marone and Scholz, 1989; Morrow and Byerlee, 1989; Marone et al., 1990; Logan et al., 1992; Gu and Wong, 1994; Beeler et al., 1996]. The numerical experiments presented here allow us to examine the effects of deformational characteristics on gouge frictional behavior. Deformation in our simulated shear zones is accommodated by several mechanisms, in particular, volume change (i.e., dilation and compaction), particle rotation, contact sliding, and bond breakage. The significance of each deformation mechanism is shear strain dependent, and also associated with variations in $\sigma_n$ and $\sigma_{ucs}$. 
5.4.2.1. Volume Strain

Figure 3 shows volume strain for all experiments defined as the fractional change in initial area between predefined fault zone boundaries (Figure 1). Volume changes in our simulated shear zones are strongly dependent on $\sigma_n$. Generally, the simulated fault

![Graph showing volume strain vs shear strain for normal stress and compressive strength](image)

Figure 3. Effects of (a) normal stress and (b) uniaxial compressive strength on volume strain plotted against shear strain. Inset shows mean volume strain for different parameter values over 200% shear strain. Error bars show the standard deviation. Interpolated lines are fit to data points by eye.
zones in our numerical experiments dilate at the onset of shear, with the exception of experiment N100. The initial dilation is more significant at lower $\sigma_n$ (Figure 3a). The gouge zone continues to dilate for all experiments with $\sigma_n$ less than 40 MPa, but contracts for higher $\sigma_n$. Mean volume strain over 200% shear strain decreases with increasing $\sigma_n$ (Figure 3a, inset); $\sigma_{ucs}$ also influences volume strain variations, but in a different way (Figure 3b). The initial dilation, greatest for higher $\sigma_{ucs}$, is maintained throughout each experiment. Mean volume strain is proportional to $\sigma_{ucs}$ (Figure 3b, inset).

5.4.2.2. Grain Rotation

Nearly all of the grains that detach from fault blocks exhibit rotation during shear zone deformation. Grains consist of either single circular particles or particle aggregates connected by elastic bonds. In most cases, all of the particles in a given grain exhibit similar rotations over 2% shear strain. Rotational properties for the aggregate are therefore approximated by the average rotational properties for all the particles. Figure 4 shows the statistics for the percentage of rotating grains and the mean angle of rotation over 2% shear strain increments for all experiments. We also plot the mean rotational properties over 200% shear strain in insets.

Rotational properties are dependent on $\sigma_n$ and $\sigma_{ucs}$. Generally, the percentage of rotating grains varies around a nearly constant value throughout each experiment, and its mean value decreases with increasing $\sigma_n$ (Figure 4a). The mean angle of rotation and its standard deviation also decreases with increasing $\sigma_n$ (Figure 4b). The rotational properties vary with $\sigma_{ucs}$ in the opposite way (Figures 4c and d). The mean percentage of rotating grains, the mean angle of rotation, and their standard deviations increase with
increasing $\sigma_{ucs}$. In addition, the low $\sigma_{ucs}$ experiments, e.g., C100, show an increase in the percentage of rotating grains with shear strain, while the high $\sigma_{ucs}$ experiments, e.g., C260, exhibit a decrease (Figure 4c). The mean angle of rotation decreases with shear strain for all experiments (Figures 4b and d).
Figure 4. Rotational properties of grains as a function of normal stress and uniaxial compressive strength plotted against shear strain. (a) Percentage of rolling grains for different normal stresses. (b) Mean angle of grain rotation for different normal stresses. (c) Percentage of rolling grains for different uniaxial compressive strengths. (d) Mean angle of grain rotation for different uniaxial compressive strengths. Insets show mean rotational properties over 200% shear strain. Error bars show the standard deviation. Interpolated lines are fit to data points by eye.
5.4.2.3. Contact sliding

During the shearing of our simulated gouge zones, slip occurs at noncohesive contacts between unbonded particles, if the contact shear force exceeds a threshold value. We plot the sliding contact data for the four end member experiments (Figure 5). The percentage of sliding contacts increases throughout the 200% shear strain for all experiments, with the highest rate of increase during the fast growth stage. The percentage of sliding contacts appears to vary slightly with $\sigma_n$ and $\sigma_{act}$, but asymmetrically.

Figure 5. Percentage of sliding contacts plotted against shear strain for experiments N10, N100, C100, and C260. The percentage of sliding contacts increases more rapidly during the fast growth stage than during the slow growth stage.
5.4.2.4. Bond Breakage

The abundance of broken bonds that accumulate over 2% shear strain increments varies systematically with shear strain for all of the experiments, with little apparent dependence on $\sigma_n$ or $\sigma_{ucs}$. Only the end members are plotted in Figure 6, showing that the incremental number of broken bonds fluctuates over a big range, but generally decreases with increasing shear strain. The rate of decrease is greatest during the fast growth stage.

Interestingly, $\sigma_n$ and $\sigma_{ucs}$ do seem to determine the abundance of bond breakage at different evolutionary stages, but in opposite directions (Figure 7). During the fast growth stage (<20% shear strain), the total number of broken bonds increases with increasing $\sigma_n$, but during the slow growth stage, the abundance decreases (Figure 7a). In contrast, the total number of broken bonds decreases with increasing $\sigma_{ucs}$ during the fast growth stage, but increases during the slow growth stage (Figure 7b). The total number of broken bonds after 200% shear strain, however, shows a little variation with either $\sigma_n$ or $\sigma_{ucs}$ (Figure 7).

![Graph showing log of incremental broken bonds vs. shear strain](image)

**Figure 6.** Number of bonds broken over 2% shear strain increments plotted against shear strain for experiments N10, N100, C100, and C260. The rate of bond breakage decreases more rapidly during the fast growth stage than during the slow growth stage.
Figure 7. Bond breakage statistics for the fast growth stage, the slow growth stages, and entire experiment. (a) Dependence on normal stress. (b) Dependence on uniaxial compressive strength. Interpolated lines are fit to data points by eye.
5.4.3. Correlation between Friction and Deformation Mechanisms

Frictional strength variations in our simulated fault gouges are a response to changing micromechanical processes during deformation (Figure 8). Surprisingly, friction shows a poor correlation with dilatancy rate (the ratio of volume change to shear displacement). Most of the pronounced peaks in friction coincide with lows in volume strain (e.g., denoted by dashed lines). Interestingly, micromechanical properties (i.e.,

Figure 8. Evolution of fault gouge properties with shear strain in experiment N25. (a) Friction and fault zone dilatancy rate derived from volume strain. (b) Volume strain. (c) Percentage of rotating grains over 2% strain increments. (d) Mean angle of rotation over 2% strain increments. (e) Percentage of sliding contacts. (f) Abundance of broken bonds over 2% strain increments.
rotational properties, sliding contacts, and bond breakage) correlate with friction throughout the experiments, but show opposite dependencies during the two evolutionary stages (Figure 8). During the fast growth stage, the pronounced peaks in friction tend to coincide with peaks in the micromechanical properties, but correlate with troughs during the slow growth stage. The peaks and troughs in the micromechanical properties are generally well correlated with each other during the fast growth stage, but are less well correlated during the slow growth stage (Figure 8).

5.4.4. Stress State

The spatial distribution of contact stresses and broken bonds in our simulated shear zones varies as shear zone configuration transforms during shear by the progressive accumulation of grains (i.e., fault gouge) detached from the fault surfaces. We show plots of contact stresses for representative experiment N25 at different stages of the simulation to demonstrate the characteristics of stress evolution during fault gouge zone development (Figures 9a and b). The contact stresses are defined as the average stresses acting on the cross-sectional areas of the bonds [Chapter 4]. Only stresses on bonded contacts are shown. We also plot the positions of broken bonds over the previous 2% shear strain increments to show the spatial distribution and orientation of fractures that are associated with stress concentration and relief (Figures 9c and d).

The stress distribution is heterogeneous during the earliest stage of fault zone deformation (at 2% shear strain) where only a few gouge grains have been produced (Figures 9a and b). Locally high compressive stresses (in red) span the fault gouge zone and extend into the fault blocks (Figure 9a). High tensile stresses (blue) tend to be
Figure 9. Stress state and distribution of incremental bond breakage at 2%, 20%, and 200% shear strains for experiment N25. Dotted lines are the interpreted gouge zone boundaries [Guo and Morgan, this issue]. Magnitudes of (a) normal stress and (b) shear stress are denoted by the colors of the lines that connect the centers of bonded particles or particles in contact. (c) Spatial distribution and orientation of broken bonds over 2% shear strain. Lines plotted tangent to the contacts denote broken bonds. (d) Rose diagrams show preferred orientations of broken bonds.
clustered in domains adjacent to the sliding surfaces and fault zone boundaries, where the compressive stresses are relatively low (Figure 9a). As expected, compressive and tensile stresses are orientated parallel or sub-parallel to \( \sigma_1 \) (\( \sim 45^\circ \)) and \( \sigma_2 \) (\( \sim 135^\circ \)), respectively. High shear stresses correlate with high compressive stresses, and do not show strong preferred orientations (Figure 9b). Broken bonds denote the positions of tensile and shear fractures, and are preferentially developed along the fault surfaces and concentrated in fault gouge (Figure 9c). Rose diagrams show that the preferred orientation of the tensile fractures corresponds to \( \sigma_1 \) (\( \sim 45^\circ \)), and the preferred orientation of the shear fractures is about 40° to \( \sigma_1 \) (Figure 9d).

The stress distribution changes with the progressive accumulation of fault gouge, and is strongly affected by irregularity of the gouge zone boundary at high shear strains (Figures 9a and b). The compressive and tensile stresses vary significantly with the roughness of the gouge zone boundaries, and orientations, shapes, and sizes of asperities. For example, high compressive stresses can lie at angles much greater than 45° to the fault zone boundaries (Figure 9a). Fractures are also developed either along the gouge zone boundaries or within the gouge zone (Figure 9c). Neither tensile nor shear fractures show strong preferred orientations over 2% shear strain increments during the late stages of the experiments (Figure 9d).

5.4.5. Cumulative Shear Strain Distributions

Deformation in our simulated fault gouges is heterogeneous. The heterogeneity (i.e., localized versus distributed deformation) and its dependence on shear displacement, \( \sigma_n \) and \( \sigma_{uct} \) can be analyzed by quantifying shear strain variation across the gouge zone.
Shear strain in our simulated brittle shear zones is accommodated by many different mechanisms. In increasing order of importance, the dominant mechanisms are gouge grain rotation and translation, volume change (dilation and compaction), fracturing (surface wear and gouge grain comminution), and fault surface sliding. As the majority of shear strain occurs in the fault gouge zone by the displacement of gouge grains, the cumulative shear strain state at any point within the shear zone can be quantified roughly by the relative motion of corresponding particles, without considering the last three mechanisms. Cumulative shear strain was, therefore, calculated as the average ratio of the horizontal displacement of each particle to the distance between the particle and corresponding fault zone boundary.

Figure 10a shows strain profiles at various bulk shear strains for experiment N25. The sawtooth character of the strain profiles at high bulk shear strains, particular in the upper block, may reflect strain localization, i.e., a discontinuity in gouge displacement. The strain profiles are not symmetric about the initial predefined fault surface. Shear strain above the fault surface is significantly larger and extends further away from the fault plane. The discrepancy between the two fault blocks increases with increasing bulk shear strain. The shear zone thickens most rapidly within the upper block; the base of the shear zone remains almost fixed just below the initial predefined fault surface. The highest shear strains occur just above and below the initial fault surface.

The characteristics of the strain profiles and their evolution are strongly dependent on the relative wear rates of the sliding fault surfaces in our simulated shear zones. Generally, the strain profiles do not show systematic variations with $\sigma_r$ and $\sigma_{acs}$. Nearly all of the experiments display comparable strain profiles at 200% bulk shear
Figure 10. Profiles of cumulative shear strain magnitude across the simulated shear zone. Dashed line denotes the initial location of the predefined fault surface. (a) Strain profiles at different bulk shear strains for experiment N25. (b) Strain profiles at 200% bulk shear strain for experiments N10, N100, C140, and C260.
strain, with greater growth within the upper fault block (Figure 10b). The exception is Experiment C140 which shows a higher wear rate in the lower block, a thinner gouge zone, and also the highest local shear strain (227%). Maximum shear strains for the other experiments are all lower than 200%. In addition, strain profile for experiment C260 shows the highest frequency of fluctuation.

5.5. Discussion

5.5.1. Fault Zone Strength

Frictional strengths of our simulated fault gouge zones are highly variable, showing significant variations with $\sigma_r$ and $\sigma_{isc}$, and fluctuations with shear strain. The peak friction value is reached within the first 2% shear strain and is followed by a drop in friction (Figure 2). This result is similar to observations made in laboratory experiments during the sliding of dry granite under triaxial compression [Byerlee, 1967] and laboratory direct shear tests [Ohnaka, 1975]. In these lab studies, friction reaches a maximum value after a short displacement and then decreases to a nearly constant value for the rest of the experiment. The decrease in friction with increased strain was thought to result from rolling of wear particles between the sliding surfaces [Byerlee, 1967]. Our simulations show that the drop in the initial peak friction is correlated with an increase in the incremental abundance of rotating grains, the angle of rotation, the abundance of sliding contacts, and also with a decrease in the rate of bond breakage (Figure 8). This indicates that rolling of gouge grains may not be entirely responsible for the drop in the initial peak friction, at least for our experiments. The friction decrease is more likely a result of the transition from a configuration of highly interlocked asperities to a state in
which deformation can be efficiently accommodated by gouge grain rotation, contact sliding, and compaction, instead of fracturing and dilation.

In addition, the initial peak friction is enhanced for our low \( \sigma_n \) or high \( \sigma_{u cs} \) experiments (Figure 2). A decrease in the maximum value of friction with increasing \( \sigma_n \) also has been observed in the laboratory experiments, and the load dependence of friction was attributed to a finite shear strength of interlocking asperities on the sliding surfaces [Byerlee, 1967]. Our results are consistent with this explanation. As suggested by the greater abundance of broken bonds within the first 2% shear strain in high \( \sigma_n \) or low \( \sigma_{u cs} \) experiments (Figure 6), interlocking of the sliding surfaces is more easily destroyed by fracture. The initial peak friction values, therefore, are lower for high \( \sigma_n \) or low \( \sigma_{u cs} \) experiments.

We observed that the residual friction, \( \mu_{max} \) of our simulated shear zones decreases nonlinearly with increasing \( \sigma_n \) (Figure 2a). A similar \( \sigma_n \) dependence of sliding friction was observed in previous DEM simulations, in which fault gouges are composed of pre-designed, irregularly shaped grains, and the wear of wall rocks is prohibited [Guo and Morgan, 2004; Guo and Morgan, resubmitted]. This result is confirmed by a theoretical friction law [Bowden and Tabor, 1964; Jaeger and Cook, 1976; Villaggio, 1979; Guo and Morgan, 2004], and consistent with the results of many rock friction experiments in the laboratory [Maurer, 1965; Murrell, 1965; Byerlee, 1967, 1968; Handin, 1969; Jaeger, 1970; Edmond and Murrell, 1971; Saffer et al., 2001; Saffer and Marone, 2003].

Interestingly, \( \mu_{max} \) does not show a strong dependence on \( \sigma_{u cs} \) in our numerical experiments (Figure 2b). A dependence of rock friction on rock hardness has been
observed in direct shear laboratory experiments [Ohnaka, 1975], but no explicit relationship has been established between these two parameters. Observations from laboratory experiments also demonstrate that the real area of contact during rock frictional sliding is strongly dependent on rock hardness [Logan and Teufel, 1986; Stesky and Hannan, 1987]. The mean stress acting on a contact is independent of load, and approximately equal to $\sigma_{\text{ucs}}$ or the penetration hardness of the dominant mineral in the wall rocks [Logan and Teufel, 1986]. This suggests that rock hardness has a more important effect on the mechanism of friction than on the magnitude of friction [Scholz, 1990], because contact area adjusts to maintain contact stress. Results of our numerical experiments show that an increase in $\sigma_{\text{ucs}}$ does not result in any pronounced changes in $\mu_{\text{max}}$ during the slow growth stage, but does lead to a marked increase in friction fluctuations that is well correlated with the volume changes of our simulated shear zones, i.e., experiments that exhibit higher magnitude of fluctuation in friction also show greater volume strain (Figures 2 and 3).

5.5.2. Friction and Dilation

The correlation between friction and dilation (change in volume) has been observed in many rock friction laboratory experiments [Morrow and Byerlee, 1989; Marone et al., 1990; Beeler et al., 1996]. It was found that change in dilatancy rate can be used to explain friction velocity dependence because of the positive correlation between dilatancy rate and friction [Marone et al., 1990]. Dilatancy rate, however, does not always quantitatively account for the variation in friction with slip rate observed in laboratory experiments [Beeler et al., 1996]. Our results show poor correlations between
friction and dilation rate, both in magnitude and in variation with shear strain [Figure 8a]. Studies of the strength of granular materials reveal that the peak friction is a combined contribution of several different factors: sliding resistance at particle contacts, particle crushing, particle rearrangement, and dilation [Rowe, 1962; Mitchell, 1993]. To date, it has not been clear how the first three factors affect the correlation between friction and dilation in the laboratory experiments.

The results of our simulations demonstrate that the effect of gouge deformation on the correlation between friction and dilation is dependent on gouge zone thickness. During the fast growth stage, where few gouge grains are produced, the most pronounced peak in friction at 2% shear strain for experiment N25 shows a strong positive correlation with dilatancy rate (Figure 8a). The most intense bond breakage also occurs within the first 2% shear strain, and the strong correlation suggests that fracture, as a dominant deformation mechanism, may strengthen or weaken the positive correlation between dilation and friction, but does not change it. During the slow growth stage, where fracture becomes a less significant deformation mechanism, the most pronounced peak in friction at 178% shear strain for experiment N25 shows a negative correlation with dilatancy rate, but does not correlate with the most pronounced variations in gouge grain rotational and sliding properties (Figure 8). This suggests that gouge grain rearrangement can lead to a significant variation in friction.
5.5.3. Friction and Shear Localization

Friction variation due to changes in gouge fabric (i.e., gouge grain rearrangement related to localized and distributed deformation) is a common observation in laboratory experiments [Marone and Scholz, 1989; Morrow and Byerlee, 1989; Marone et al., 1990; Logan et al., 1992; Gu and Wong, 1994; Beeler et al., 1996]. It was found that the onset of shear localization, characterized by the development of shear fabrics' occurs at about the peak stress [Marone et al., 1990; Logan et al., 1992]. Our experiments also show that the peaks in friction coincide with the lows in the micromechanical properties at the slow growth stage and are associated with shear localization. For example, the peak in friction at 178% shear strain for experiment N25 corresponds to a relatively localized deformation state that is characterized by relatively lower abundances of rotating grains, sliding contacts, and broken bonds (Figure 8), and the development of localized shear surfaces, such as R-shears (Figure 11a). In contrast, the trough in friction at 180% shear strain corresponds to a more distributed deformation state where more grains undergo rotation, sliding, and fracture (Figure 8), and few localized shear surfaces are present (Figure 11b).

Gouge laboratory experiments demonstrate that the degree of shear localization is shear displacement dependent as the gouge develops and deforms [Beeler et al., 1996]. Our results show that shear localization is not only dependent on shear displacement, but also on \( \sigma_n \) and \( \sigma_{wss} \). Since the abundance of sliding contacts and broken bonds varies in a relatively narrow range during the slow growth stage (Figures 5 and 6), changes in rotational properties can be used as measures of the degree of shear localization in our numerical experiments (Figure 4).
Figure 11. Gradient of particle shear displacement at (a) 178% shear strain and (b) 180% shear strain for experiment N25. (a) Localized slip surfaces, indicated by continuous dark lines, such as low angle R-shears, are well developed at 178% shear strain. (b) Long and continuous slip surfaces are less well developed at 180% shear strain, suggesting more distributed deformation.

Analysis of grain rotation data show that the abundance of rotating grains and the angles of rotation are noticeably higher during the first 60% shear strain and tend to decrease with continued shear (Figure 4), i.e., deformation is distributed. This observation suggests that strain localization initiates once the gouge reaches a certain thickness. The degree of shear localization increases with shear displacement (i.e., gouge thickness) when the gouge is thick enough to accommodate strain by localized deformation. The abundance of rotating grains and the mean angles of rotation in our numerical experiments also decrease with increasing $\sigma_n$ and decreasing $\sigma_{isc}$, suggesting that these conditions favor more localized deformation. The higher degree of shear
localization probably results from the higher volume strain in these experiments because the grains are betterable to reorganize (Figure 3).

5.5.4. Fracture

Unlike nondestructive deformation mechanisms, such as grain rotation and contact sliding, fracture of the fault blocks and gouge grains not only accommodates shear strain, but more importantly, causes changes in gouge properties. Previous studies of granular shear without surface wear showed that dynamic changes in gouge grain characteristics due to grain comminution affect the partitioning of deformation mechanisms, and therefore, the frictional behavior of fault gouge [Mair et al., 2002; Guo and Morgan, resubmitted]. Our new simulations presented here demonstrate the added role of surface wear, which further affects the micromechanical behavior of shear zones by increasing gouge zone thicknesses and grain distributions. The progressive accumulation of fault gouge allows more strain to be accommodated within the gouge by contact sliding and grain rotation, and leads to a rapid decrease in the intensity of fracture within the fault blocks (Figures 4-6). A considerable decrease in wear rate when gouge layers were sufficiently thick to separate the sliding surfaces was also observed during experimental fault deformation in lab [Power et al., 1988; Beeler et al., 1996]. It was also found that when wear rate decreases, the majority of deformation is accommodated within the gouge layer, as long as its shear failure strength is lower than that of wall rocks [Beeler et al., 1996]. Our results are consistent with this observation.
The intensity of fracture in our numerical experiments also varies systematically with both $\sigma_n$ and $\sigma_{ucs}$ (Figure 7). The correlations are shear displacement dependent. During the fast growth stage, where the sliding surfaces are highly interlocked by asperities or gouge grains [Chapter 4], the lower stresses acting on stronger asperities and gouge grains are more likely to be relieved by nondestructive deformation mechanisms, such as dilation (Figure 3), instead of by brittle failure. Consequently, the intensity of fracture increases with increasing $\sigma_n$ or decreasing $\sigma_{ucs}$ (Figure 7a). During the slow growth stage, when the sliding surfaces are separated by a weaker gouge layer, deformation is more localized within the gouge zones in low $\sigma_n$ and high $\sigma_{ucs}$ experiments, as indicated by the less abundant rotating grains in them (Figure 4). Localized deformation promotes local stress levels and therefore enhances brittle failure. Thus, the intensity of fracture decreases with increasing $\sigma_n$ and with decreasing $\sigma_{ucs}$ (Figure 7b).

5.5.5. Stress and Strain Distributions

The stress fields in our simulated shear zones evolve with shear displacement and lead to distinct patterns of fracture distributions at each evolutionary stage (Figures 9 and 12). During the fast growth stage, stress distributions within the fault blocks are mainly controlled by the external force configuration. High compressive and tensile stresses chains are oriented parallel or sub-parallel to $\sigma_1$ and $\sigma_3$, respectively (Figure 9a). Tensile fractures, therefore, show a strong preferred orientation nearly coincident with the orientation of $\sigma_1$, i.e., about 45° to the fault zone boundaries (Figure 12a). Shear fractures show relatively weak preferred orientations. The mean orientation is about 40° to $\sigma_1$
(Figure 12b). During the slow growth stage, stress distributions within gouge zone, or adjacent to the gouge zone boundaries, are much more heterogeneous, being affected by gouge zone boundary geometry and contact orientation. High compressive stresses are more likely to deviate to higher angles greater than 45° to the fault zone boundaries (Figure 9a), leading to a concentration of tensile fractures at about 60° to the fault zone boundaries, although a wide range of orientations occur (Figure 12c). Interestingly, shear fractures show a strong preferred orientation that is nearly parallel to \(\sigma_l\) (Figure 12d).

![Rose diagrams showing the orientation distribution of fractures](image)

**Figure 12.** Rose diagrams showing the orientation distribution of fractures (i.e., broken bonds) and their abundance during the fast (a and b) and slow (c and d) growth stages. Fracture orientations are given as tangents to formerly bonded contacts, e.g., Figure 9c. Arrows show the mean preferred orientations relative to the fault zone boundaries.

Cumulative shear strain distributions in our simulated brittle shear zones are heterogeneous and asymmetric about the initial fault surface (Figure 10). Other than minor changes with shear zone thickness, the strain field does not vary systematically with either \(\sigma_n\) or \(\sigma_{u,cs}\). The heterogeneity of cumulative shear strain is genetically related to the nature of discontinuities during brittle deformation, and the rates and timing of shear zone thickening. Locally high shear strains, indicated by the zigzags in the strain
profiles (Figure 10), represent slip planes preserved during shearing. Shear strains are highest near the center of the gouge zone, and gradually decrease toward the gouge zone boundaries. The outward decrease in shear strain is similar to shear intensity variations observed at the brittle Punchbowl fault zones, where it is attributed to higher strain rates at the core [Chester and Logan, 1986]. In contrast, the asymmetry of shear strain in our simulations is caused mainly by uneven wear of the fault blocks. The uneven wear leads to a continuous shift of the center of the gouge zone, and therefore the highest cumulative shear strain, toward the fault block that undergoes more intense wear.

Unlike ductile shear zones that show predictable relationships between displacement and strain within the shear zones [Ramsay and Graham, 1970; Simpson, 1983], we see little correlation between local shear strain and shear displacement in our simulated brittle shear zones (Figure 10). The highest local shear strain can be either less or greater than the applied shear strain. The difference between them varies with shear displacement, $\sigma_n$, and $\sigma_{tcs}$, but in an unsystematic way. In our simulated brittle shear zones, shear strain is accommodated in a highly nonuniform way by grain sliding, rotation, and fracture. Each deformation mechanism leads to a different shear strain rate of the deforming body. In addition, slip surfaces frequently develop in different domains of fault gouge zone, which also alters the local shear strain rate. Therefore, local shear strain varies with shear displacement in an unpredictable way.
5.6. Conclusions

Natural shear zones are subject to a wide variety of deformation conditions. The study presented here demonstrates that variations in these conditions, including shear displacement, $\sigma_n$, and $\sigma_{ucs}$, can significantly affect the frictional and micromechanical properties of shear zones in complicated ways. Our simulated fault gouge zones exhibit peak frictional strengths within the first 2% shear strain, followed by drops in frictional strength, which correspond to a transition in gouge zone structure from highly interlocked configurations to states where strain is more efficiently accommodated by grain rotation and contact sliding. The initial peak friction values are enhanced in high $\sigma_n$ and low $\sigma_{ucs}$ experiments. The residual friction shows a decreasing trend with increasing $\sigma_n$ in a nonlinear fashion, but does not strongly depend on $\sigma_{ucs}$.

The correlation between friction and micromechanical properties is dependent on shear displacement. The peaks in friction coincide with the lows in micromechanical properties during the fast growth stage. The correlation reverses during the slow growth stage, denoting the onset of more localized deformation. The degree of shear localization increases with increasing shear displacement (i.e., gouge thickness) after gouge reaches a certain thickness. Shear localization is more significant in low $\sigma_n$ and high $\sigma_{ucs}$ experiments that exhibit higher volume strain. This indicates that higher volume strain promotes more localized deformation by allowing a higher degree of grain rearrangement, and therefore results in higher magnitude fluctuations in friction.

The activity of possible deformation mechanisms in our simulated shear zones varies with shear displacement. The abundance of sliding contacts increases exponentially with increasing shear strain, but the variation is insensitive to both $\sigma_n$ and
\( \sigma_{ucs} \). All experiments show noticeably higher abundances of rotating grains and higher angles of rotation during the first 60% shear strain. The rotational properties then decrease with continued shear. The abundance of rotating grains and the mean angles of rotation are strongly dependent on \( \sigma_n \) and \( \sigma_{ucs} \). They increase with decreasing \( \sigma_n \) and increasing \( \sigma_{ucs} \). Fracture also accommodates strain, but importantly, causes changes in gouge properties, especially gouge thickness, which strongly affects the partitioning of deformation mechanisms and therefore the frictional behavior of our simulated shear zones. The intensity of fracture decreases exponentially with increasing shear displacement. It also shows a strong correlation with \( \sigma_n \) and \( \sigma_{ucs} \), dependent on shear displacement. The intensity of fracture increases with increasing \( \sigma_n \) and decreasing \( \sigma_{ucs} \) during the fast growth stage, but the dependence reverses during the slow growth stage.

Bond stress distribution in our simulated shear zones evolves with shear displacement. During the fast growth stage, the stress distribution is similar to that of a simple shear configuration. High compressive and tensile bond stresses are oriented parallel or sub-parallel to \( \sigma_l \) and \( \sigma_3 \), respectively. During the slow growth stage, stress orientation is highly affected by the gouge zone boundary geometry and contact orientations. High compressive stresses tend to orient at high angles to the fault zone boundaries. The change in stress orientation leads to distinct distributions of fractures. Shear strain distributions in our simulated shear zones are heterogeneous and asymmetric. The highest local shear strain occurs near the center of the gouge zone and may be greater or less than the applied shear strain. Neither \( \sigma_n \) and \( \sigma_{ucs} \) affect the basic pattern of stress and strain distribution and evolution.
REFERENCES

Chapter 1


**Chapter 2**


Chapter 3


Chapter 4


**Chapter 5**


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