3D numerical simulations of fault gouge evolution during shear: Grain size reduction and strain localization

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Abstract

Strain localization has important implications for the mechanical strength and stability of evolving fault zones. Structural fabrics interpreted as strain localization textures are common in natural and laboratory faults, however, the dynamic microscale processes controlling localization (and delocalization) are difficult to observe directly. Discrete numerical models of faulting allow a degree of dynamic visualization at the grain scale not easily afforded in nature. When combined with laboratory validation experiments and field observations, they become a powerful tool for investigating the dynamics of fault zone evolution. We present a method that implements realistic gouge evolution in 3D simulations of granular shear. The particle based model includes breakable bonds between individual particles allowing fracture of aggregate grains that are composed of many bonded particles. During faulting simulations, particle motions and interactions as well as the mechanical behavior of the entire system are continuously monitored. We show that a model fault gouge initially characterized by mono-disperse spherical aggregate grains gradually evolves, with accumulated strain, to a wide size distribution. The comminution process yields a highly heterogeneous textural signature that is qualitatively comparable to natural and laboratory produced fault gouges. Mechanical behavior is comparable to a first order with relevant laboratory data. Simulations also reveal a strong correlation between regions of enhanced grain size reduction and localized strain. Thus in addition to producing realistic fault gouge textures, the model offers the possibility to explore direct links between strain partitioning and structural development in fault zones. This could permit investigation of subtle interactions between high and low strain regions that may trigger localization–delocalization events and therefore control macroscopic frictional stability and hence the seismic potential of evolving fault zones.

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1. Introduction

Brittle faults observed in the field or generated in the laboratory often display accumulations of granular breccia or fault gouge. Structural fabrics occurring within such fault zones are commonly characterized by distinct grain size and shape distributions that are generally interpreted as strain localization indicators. The development of such structures may have important implications for mechanical strength and stability and therefore a full understanding is crucial for fault and earthquake mechanics.

Observations of natural fault zones have revealed the occurrence of characteristic shear fabrics (Rutter et al., 1986; Chester and Logan, 1987) and wide grain size distributions within these fabrics that are typically described by a power law or ‘fractal’ size distribution with exponent D(3d) reported to range between 1.8 and 5.5 (e.g. Sammis et al., 1987; Blenkinsop, 1991; Storti et al., 2003; Billi et al., 2003).

Exponents of D=2.6 are relatively common, whereas D values closer to 3.0 have been described in shear bands (Billi and Storti, 2004) or fault core (Chester et al., 1993, 2005) within the faults. The development of such grain size distributions with shear has largely been attributed to grain fracture and intense localization.

Laboratory experiments have reproduced similar shear fabrics e.g. (Byerlee et al., 1978; Logan et al., 1979) and provide opportunities to track the development of structures by e.g. serial thin section analysis at increasing increments of accumulated shear strain whilst continuously monitoring bulk mechanical response. A direct link between the appearance of ‘shear localization fabric’ and the transition from velocity strengthening (inherently stable) to velocity weakening (potentially unstable) mechanical behavior has been demonstrated e.g. (Beeler et al., 1996; Mair and Marone, 2000). The grain size distributions of gouge material within these fabrics are also reported to be fit by power law (fractal) distributions. Detailed analyses (Marone and Scholz, 1989) indicates an overall evolution towards steady state bulk values of D=2.6 but that higher D values occur in intensely deformed shear bands within these fabrics, similar to field observations.

Several theoretical models for fragmentation have been developed e.g. (Allegre et al., 1982; Turcotte, 1986; Sammis et al., 1987) and offer

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insights into the comminution processes operating in natural fault zones. One such model, the constrained comminution model (Sammis et al., 1987) where the probability of grain breakage depends on the size of the nearest neighbors, predicts power law grain size distributions with theoretical exponent $D = 2.58$. This agrees with many field and laboratory observations but does not fit the high $D$ values observed in e.g. shear bands. These high $D$ values could be attained by i) preferential breakage of large grains (Sammis et al., 1987; Blenkinsop, 1991) or ii) preferential increase of small particles by rotation enhanced abrasion of large particles during shear (Hattori and Yamamoto, 1999; Storti et al., 2003). A recent extended version of the constrained comminution model (Sammis and King, 2007) invokes collisions between large grains during granular flow to reach values of $D = 3.0$ in high-strain fault gouges.

The broad consistency of laboratory and field observations as well as the success of theoretical models in producing the oft reported gouge grain size distributions is encouraging. However, the dynamics of the micro-scale processes controlling localization are difficult to observe directly in the laboratory or field and rather only snapshot insights can readily be obtained. Numerical modelling of granular shear zones offers an excellent opportunity to visualize dynamic grain scale processes and interactions that are not readily accessible in nature or laboratory experiments. When validated with precise laboratory experiments, such models can become very useful tools in understanding the micro-scale dynamics of evolving fault zones.

Discrete particle models (e.g. Cundall and Strack, 1979; Mora and Place, 1998; Aharonov and Sparks, 1999; Morgan, 1999) of sheared granular systems have proved extremely useful in visualizing particle dynamics and interactions that may be operating in natural faults. One drawback, however, is that these models have generally been conducted in 2D and with minimal grain or particle evolution thus connecting their results directly to natural (or even laboratory) faults is somewhat challenging. Recent laboratory shearing experiments on a range of both simulated gouges and highly idealized granular materials have demonstrated the influence of grain characteristics such as grain size, shape, evolution (Mair et al., 2002; Anthony and Marone, 2005) and particle dimensionality (1D, 2D, 3D) (Frye and Marone, 2002) on bulk mechanical behavior highlighting the need to investigate these aspects numerically.

Recent numerical modelling in 3D has highlighted the importance of out of plane grain motions in setting friction level (Hazzard and Mair, 2003) and the role of heterogeneous force distributions dependent on grain size distributions (Mair and Hazzard, 2007). It has now become computationally tractable to run much higher resolution simulations and investigate gouge evolution processes in 3D (Abe and Mair, 2005).

In this article we present new high resolution 3D models of gouge evolution during shear that build on our recent granular gouge model involving fracture of aggregate grains (Abe and Mair, 2005). We focus on tracking mechanical behavior, textural evolution, fracture distributions and local strain with accumulated global shear strain for a range of normal stress conditions (reaching significantly higher shear strains than previously (Abe and Mair, 2005)). We demonstrate the development of a highly heterogeneous damage texture that resembles natural and laboratory faults and show a strong correlation between regions of preferential grain size reduction and concentration of local strain.

2. Method

2.1. Simulation approach

The Lattice Solid Model (LSM) (Mora and Place, 1994; Place and Mora, 1999) is a particle based model similar to the Discrete Element Model (DEM) developed by Cundall (Cundall and Strack, 1979). The model consists of spherical particles which are characterized by their radius, mass, moment of inertia, position and linear and angular velocity. The particles interact with their nearest neighbors, by imparting elastic and frictional forces. Particles can be linked together by elastic bonds in which case the interaction forces consist of linear elastic, bending and twisting components (Wang et al., 2006). Links between particles are irreversibly broken if the deformation of the link

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**Fig. 1.** The 3D granular gouge model. Aggregate grains (large spheres) have breakable bonds between the particles (small spheres). We show: a) an undeformed model; b) a model after significant shear strain (220%) for run b015 conducted at 20 MPa normal stress. Arrows indicate the sense of shear. In this deformed gouge, regions of intense crushing lie next to survivor grains that maintain much of their original volume.

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Table 1
Numerical simulations

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Particles</th>
<th>Initial aggregate grains</th>
<th>Normal stress (MPa)</th>
<th>Shear displacement (%)</th>
<th>Strain</th>
<th>Total bonds broken</th>
<th>Bonds broken during normal load up</th>
<th>Bonds broken during shear</th>
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<td>281</td>
<td>686,252</td>
<td>533,948</td>
<td>152,304</td>
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</tbody>
</table>

exceeds a given threshold. If two particles which are not linked together come into contact, they will interact by repulsive elastic and frictional forces. In the work presented here, the local frictional forces are calculated according to a linear Coulomb friction law. The microscopic stiffness parameters and the fracture criterion for the bonds connecting the particles are chosen such that the macroscopic elastic and frictional behavior of a test block of material (formed by particles bonded together) closely resembles that of a linear elastic solid (Wang et al., 2006).

The micro-properties of the particle interactions, i.e. bond stiffness and frictional parameters, are calibrated so that bulk elasticity and friction strength of the resulting material resemble those of the glass beads used in experiments i.e. Young's modulus $E = 25$ GPa and unconfined compressive strength UCS = 300 kPa. For details on how to calibrate the mechanical properties of a material in a DEM simulation, see for example, (Schöpfer et al., in press).

2.2. Model setup

Our model setup consists initially of a number of large, roughly spherical aggregate grains confined between two blocks of solid material (Fig. 1a). The particles within the boundary blocks and within each of the aggregate grains are fully bonded together. There are no bonds between different aggregate grains or between aggregate grains and the boundary material. The initial spherical shape of the aggregate grains has been chosen to resemble the initial conditions of laboratory shear experiments performed on spherical glass beads (Mair et al., 2002; Anthony and Marone, 2005). The aggregate grains each consist of a dense packing of random sized spherical particles bonded together. The dense packing is generated using a modified version of an insertion based algorithm (Place and Mora, 2001). In the original algorithm a new particle is generated by fitting it to either 4 existing particles or to 3 particles and a plane (in case of particles close to a planar boundary). In order to generate the spherical aggregate grains for our current models, the algorithm has been modified to also allow the fitting of a new particle to 3 existing particles and the inside of the bounding sphere of the aggregate grain. Particle have radii between 0.2 and 1 model unit and the initial aggregate grains have an approximate radius of 8 model units.

There is no deliberate variation in bond strength within the aggregate grains, however at the mesoscopic scale (i.e. larger than an individual particle and smaller than an aggregate grain) the strength of the material will vary due to the random geometric arrangement of the particles. The upper and lower boundary blocks are formed by a regular arrangement of equal sized bonded spherical particles of radius = 1.0 model unit (Fig. 1). The bond strength in this material is identical to the strength in the aggregate grains.

We apply and maintain a force to the solid boundary blocks in y-direction to maintain a constant normal stress. The outer edges of upper and lower boundary blocks are then driven at constant velocity in the +x and -x direction to generate shear in the model during the main phase of the simulations. In the initial loading phase, only the normal forces are applied until the model has reached an equilibrium state under the given normal stress. Then the shear velocity is linearly ramped up until it reaches its chosen value. Circular boundary conditions are applied to the model in the direction of the shear (x) i.e. particles that leave the model on one side return at the other side of the model (Fig. 1). In the third direction (z), fixed frictionless boundary walls are used. The applied shear velocity of $2.5 \times 10^3$ model length unit per model time unit, equivalent to several m/s in a real fault, is significantly faster than the velocities used in corresponding laboratory experiments, typically micron/s to mm/s (Mair et al., 2002; Anthony and Marone, 2005), but allow us to achieve significant

Fig. 2. Macroscopic friction (i.e. shear stress/normal stress) measured at the boundaries of the model is plotted as a function of shear strain for the range of applied normal stresses indicated.

Fig. 3. Fluctuations in friction and dilatancy rate are plotted against shear strain for a simulation conducted at 30 MPa. Y-axis scales are comparable for both datasets. Subplot summarises the mean level of friction and amplitude of fluctuations in friction (indicated as error bars showing +/- 1 standard deviation from this mean) as a function of normal stress. Data are calculated for different simulations from strains of 100%, where steady state level of friction has been reached, until the end of the simulations (i.e. strains of 220–280%).

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shear displacement using the available computational resources. The shear displacements achieved, of up to 180 model units, result in global shear strains up to 280%. Local strains are much higher in some parts of the model. Normal and shear loading induce grain fracture and gouge evolution (Fig. 1b) leading to regions of complete pulverization (intense crushing) that lie adjacent to aggregate grains that survive with relatively little damage. Simulation conditions are summarized in Table 1 for the main runs used in this paper (note however that 15 additional simulations were carried out for preliminary studies and model refinement).

For the remainder of the paper we will refer to ‘particles’ as the fundamental unit of the discrete model and ‘grains’ as ‘aggregates’ of connected particles. When comminution results in single particle grains, the two terms are synonymous.

2.3. Model evolution

During simulations, we continuously monitor macroscopic stress and displacements at the boundaries. Key quantities we derive include: friction (shear stress/normal stress); layer thickness (l); dilatation rate (dl/dt, where l is layer thickness and x is shear displacement); compaction rate (dC/dt). In addition, we also trace individual particle positions, motions and interactions (e.g. contact forces, existing versus broken bonds, sliding or non sliding contacts). To determine the size and shape of aggregate grains at different stages during the simulations, and hence monitor size and shape evolution, we use a grain tracking technique. Using snapshots of the particle bond data (collected at a given time step) we extract information on the connected components (i.e. aggregate grains) by determining which individual particles can be reached from other particles by traveling along existing bonds. We then analyze this information to determine grain size and shape. By comparing the aggregate grains and distributions of remaining or broken bonds between snapshots, we can gain information on grain fracture and grain size evolution. In general, we will present grain size data as equivalent grain diameter i.e. the cube root of the grain mass determined using this grain tracking technique.

3. Results

3.1. Mechanical behaviour

Friction measured at the boundaries of the model is plotted as a function of shear strain in Fig. 2 for the range of normal stresses indicated. Friction lies within the range 0.2 and 0.4 with all records showing an overall evolution with strain in addition to high frequency fluctuations about a mean level. Notably the low normal stress simulation shows a decrease in friction with strain whereas the high normal stress simulation starts at a lower value and increases with increased strain. Intermediate normal stress runs show intermediate behavior systematic with their normal stress.

Friction fluctuations, plotted as a closeup in Fig. 3, track closely with change in dilatancy rate. This suggests an intrinsic relationship between compaction state and sliding friction. In all simulations, the period of the dominant fluctuation of both friction and dilatancy rate are comparable to the initial aggregate grain size. The mean level of friction increases systematically with increasing normal stress (Fig. 3 subplot). Conversely, the amplitude of fluctuations in friction are inversely related to normal stress as highlighted in Fig. 3 subplot.

3.2. Microstructural observations

3.2.1. Textural evolution of the model gouge

The textural evolution of the granular gouge model is highlighted in Fig. 1. The initial configuration of the model just prior to shearing
(Fig. 1a) shows individual aggregate grains coloured as slightly different grey scales. After 220% strain, the deformation and structural evolution of the gouge model are significant (Fig. 1b). Some grains survive relatively intact (e.g. dark grain, lower middle) whereas other regions show total pulverisation and a mixture of greyscales indicating that the daughter grains or particles now mixed together originally belonged to different parent aggregate grains (e.g. light coloured particles, upper middle). Grain shape evolves from initially spherical grains to a mixture of both spherical and angular fragments.

As a result of individual (and groups of) bonds breaking, the aggregate grains change in size and shape with accumulated strain. Unsurprisingly, grain size generally decreases with accumulated strain, the effect being most significant at higher normal stress. An important observation (Abe and Mair, 2005) found in similar models, was the persistence of a number of survivor grains (defined as grains that retain a 75% of their original grain diameter) up to shear strains of 50%. In Fig. 4 we plot the number of survivor grains as a function of strain for our new simulations conducted at a range of different normal stresses and shear strains up to 280%. At low normal stresses (e.g. 10 MPa and 15 MPa) most grains in the model are survivors i.e. very few aggregate grains are completely destroyed. At higher normal stresses, there is a systematic decrease in the number of grains surviving for a given accumulated strain, however, at relatively high normal stresses, some grains do survive even after 200% shear strain. This demonstrates that the fragmentation process (and hence stress field) is highly heterogeneous and does not just result in massive pulverisation where grains are completed destroyed. Importantly, all simulations exhibit decay in the attrition rate of survivor grains with accumulated strain. From this we infer that the destruction of survivor grains is sensitive to contact geometry and hence the evolving particle size distribution of the system. Data from previous similar simulations (Abe and Mair, 2005) exhibit comparable overall trends within each suite of simulations although absolute values are slightly different due to refined boundary conditions in the current study.

The evolution of grain size distributions with accumulated strain is summarised in Fig. 5 for different normal stresses. Grain size (equivalent grain diameter determined using our grain tracking technique, is reasonably well fit by a power law distribution for grains larger than radius = 1 model unit. (This cutoff is imposed because the grains smaller than 1 model unit are predominantly single particle grains and therefore their size distribution is mainly determined by the initial model setup and not the fracturing process). Due to the limited size ratio between the initial grains and the single particles the data used for the power law fit spans only about one order of magnitude.

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magnitude. However, within this range there is a good fit (see also the graph provided as supplementary material). The resulting estimated power law exponents (Fig. 5) generally show an initial increase, reaching a peak and levelling off to a somewhat stable (or slightly decreasing) value after 100% strain. The fact that we observe a non-zero power-law exponent already at the beginning of the shear movement, i.e. at zero shear strain, is due to grain fracturing during the initial normal loading. The value of exponent reached is strongly and directly dependent on normal stress. This indicates a wider grain size distribution is achieved rapidly which we attribute to more efficient grain crushing at higher normal stress.

3.2.2. Temporal and spatial distribution of grain fracture

The rupture of bonds between adjacent particles leads to grain breakage. The number of bonds broken in different runs is summarized in Table 1 and indicates that bond breakage is greater
at higher normal stress and that much of the bond breakage actually occurs during the initial application of normal load and prior to shear deformation. The intensity of comminution (i.e. grain crushing and breakage) throughout a simulation can be evaluated by considering the number of bonds breaking (per unit time) at increasing increments of strain. Bond breakage rate is now plotted alongside bulk compaction rate (measured at the edges of the model) as a function of time in Fig. 6. Importantly, the data-sets exhibit a close correspondence suggesting that the compaction process is strongly coupled to grain breakage events rather than for example grain rearrangement. These temporal records are punctuated by episodic spikes marking enhanced bond breakage occurring over a short time window thus demonstrating strong temporal clustering of events at particular stages in the simulation. We see an overall gradual decrease in breakage rate (and compaction rate) with accumulated strain. The major spikes in bond breakage rate decay significantly after 100% strain coinciding with the approximate strain where macroscopic friction reaches a steady state value (see Fig. 2).

The spatial distribution of individual bonds breaking and the relationship to grain fracture processes is presented in Fig. 7. We show bond breakage as 3D snapshot plots early in a 20 MPa simulation (9% strain Fig. 7a, b) and after 75% strain (Fig. 7c, d). These time windows are recognised (in Fig. 6) as having relatively high and relatively low temporal clustering respectively. A side view and top view are shown for the two accumulated strains (animations A1.avi and A2.avi showing rotations of these plots to highlight 3D structure are available as an online supplement). Positions of individual bonds breaking are shown in black, and particles associated with a single grain (blue) and a second grain (red) are superimposed. A strong spatial clustering of breaking bonds (at 9% strain, Fig. 7a, b) directly coincides with the position of the single (blue) grain. The (blue) grain appears to undergo major intra-granular fracture along several sub vertical (xy- planes) and split into several distinct pieces. Some additional minor bond breakage occurs during this time window but is not spatially correlated. At 75% strain, the snapshot of bond breakage exhibits a different spatial pattern (Fig. 7c, d). Breaking bonds are distributed much more homogeneously throughout the model. Although often not completely isolated, bonds are spatially correlated on much shorter length scale than for the 9% strain snapshot. This could be attributed to small daughter fragments breaking up (in an intra-granular fashion as above) or small pieces breaking off a large survivor grain by e.g. an abrasion type mechanism.

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Fig. 9. Profiles of matrix fraction (black dotted) and local strain (grey) are plotted as a function of position in the model. Data plotted at a give y-position are average values for all x- and z-positions (i.e. essentially averages of thin horizontal slices through the model). Local strain is calculated for only the x-direction. Data are shown for 0, 10, 50, 200% shear strain (see columns) and normal stresses of 10, 15, 20 30 MPa (see rows).

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3.2.3. Fragmentation products and strain localization

To determine the extent of grain size reduction and local strain occurring in different regions of our model, we track the properties of subvolumes of the model (of size 2 × 2 × 2 model units) during the simulations. We define 'Matrix material' as material which consists of grains with a radius smaller than 1 model unit and therefore is largely made up of single particles. 'Matrix fraction' is then defined as the percentage of total mass within a subvolume contributed by grains that are smaller (in radius) than 1 model unit. A matrix fraction = 1 means that all the grains within this volume are smaller than 1 model unit, whereas a matrix fraction = 0 means that all particles within the subvolume belong to large grains i.e. those having radii greater than 1 model unit. Local strain is calculated as difference in average displacement (in x-direction) of particles contained within two adjacent subvolumes.

We summarize the spatial distribution of grain size reduction and local strain with accumulated shear strain in Figs. 8 and 9. Fig. 8 highlights the spatial distribution of matrix fraction visualized on a 2D slice cut through our 3D model. A 3D isosurface i.e. region where matrix fraction = 0.85 is superimposed to emphasise the 3D nature of the structures formed. Initially, Fig. 8a, matrix fraction is zero since only large aggregate grains exist. With increasing strain (Fig. 8a to e) the matrix fraction increases – particularly close to the upper and then the lower edges of the gouge layer. Note the boundaries i.e. where the upper and lower blocks meet the gouge layer, move inwards (in the y-direction) as the gouge layer compacts. Grain size reduction is clearly enhanced near the edges of the gouge layer, however some matrix sized material also appears close to the middle of the layer. Often this central matrix material lies as narrow oblique zone between two regions of 0 matrix fraction (e.g. Fig. 8d). Extended regions having no matrix material (i.e. dark blue colour) are interpreted as survivor grains. In Fig. 8e, the isosurface for matrix fraction = 0.85 is shown. (An animation A3.avi showing additional intermediate snapshots of data presented in Fig. 8 is available as an online supplement). In Fig. 8f we show the isosurface for matrix fraction = 0.85 with an additional isosurface of high local strain superimposed (the 2D slice is removed for clarity). A close correlation between regions of high matrix content and regions of enhanced local strain is clear.

Matrix fraction and local strain data are plotted for a range of simulations at different normal stresses and accumulated shear strain in Fig. 9. Here the data, presented as y-position profiles, are averages of thin horizontal (xz-) slices cut through the 3D model. This representation is clearly an approximation since we know there is variability in the x- and z-directions (see Fig. 8), however it provides an effective way to compare the main features of different simulations. At 0% shear strain, we see peaks in matrix fraction, indicating a concentration of matrix sized grains close to the upper or lower edges of the granular layer. This effect is systematically enhanced at higher normal stresses. It illustrates crushing at the edges of the granular layer and demonstrates the influence of initial load up on the early structure of the granular layer. With increasing applied shear strain these peaks in matrix fraction grow and generally become symmetrical on the upper and lower boundaries. The peaks gradually move towards the center of the model as the layer compacts. At low (10, 15 MPa) normal stress there is little evidence for crushing away from the boundaries. In contrast, at higher (20, 30 MPa) normal stress, the peaks near the edges are considerably wider and there is also evidence for significant grain size reduction close to the center of the layer. In general, areas of enhanced local strain correlate strongly with regions of high matrix fraction, illustrated by the peaks in local strain. The extent of strain localization is enhanced in all cases with accumulated shear strain, the strongest localization (i.e. most spatially concentrated peaks of local strain) being observed at low normal stress. Interestingly, in most cases, the peaks in local strain appear to hug the inner edges of the high matrix fraction zones.

4. Discussion

In terms of mechanical behaviour, the friction level achieved in our simulations (0.4) is clearly lower than that (0.6–0.8) generally found in laboratory experiments for sliding on bare surfaces or layers of rough angular gouge. However, to a first order, the value we obtain is comparable to laboratory friction values for shear in a granular material consisting of spherical beads e.g. (Mair et al., 2002; Anthony and Marone, 2005). This is not surprising since the smallest fragments in our models are indeed spherical. Friction in the numerical simulations is sensitive to applied normal stress and at higher normal stresses, shows an increase with accumulated strain. A similar (though significantly larger) increase in friction observed in laboratory experiments on sheared spherical beads (Mair et al., 2002; Anthony and Marone, 2005) has been attributed to an increase in grain angularity as spherical grains break up to become angular. It is likely that the increase in friction in our simulations is dominated by contact geometry due to a reduction in porosity leading to a larger number of grain contacts both within and out of the plane, in addition to having more angular intermediate sized grains. At low normal stress, there are few intermediate sized grains since few aggregate grains actually break, this results in higher porosity and therefore less grain contacts.

The fluctuations in friction we observe have a period comparable to the diameter of an original aggregate grain. They are largest in amplitude for the lowest normal stress simulation. These observations are consistent with laboratory observations (e.g. Frye and Marone, 2002) and are interpreted as aggregate grains bouncing over each other. The fluctuations become noticeably smaller at higher normal stress where the grains are smaller (sometimes individual particles) and have enhanced mobility leading to more potential for out of plane motions. Close links between friction and dilatancy rate agree with those previously observed in laboratory (e.g. Frye and Marone, 2002) and numerical simulations (Hazzard and Mair, 2003). We believe that the dominant mechanical behaviour exhibited in our models is largely consistent with the comparable laboratory experiments that exist (Frye and Marone, 2002; Mair et al., 2002; Anthony and Marone, 2005) and recent 3D numerical simulations (Hazzard and Mair, 2003).

The textural evolution of our gouge models yields structures that bear at least some of the hallmarks commonly found in natural and laboratory fault zones. Particularly important observations are the heterogeneity of deformation highlighted by survivor grains and highly localized zones of pulverisation occurring in the same model. Our observations of evolving grain size distributions are largely consistent with prior modelling (Abe and Mair, 2005) though here our data are considerably more comprehensive due to the larger strains reached and the wider range of stresses investigated. At higher normal stresses, our models show two distinct phases: initially an increase in power law exponent; then a relatively stable distribution. We suggest this illustrates a transition in the dominant grain size reduction mechanism from initial (and highly efficient) intra-grain splitting to subsequent grain abrasion (which is expected to be relatively inefficient). This transition is less pronounced (or even absent) at lower normal stress indicating that grain splitting is relatively minor and rather that abrasion is dominating at these conditions. The co-existence of these two comminution mechanisms and their varying contribution to the total grain size reduction is consistent with observations by Hattori and Yamamoto (Hattori and Yamamoto, 1999) and Storti et al (Storti et al., 2003).

In terms of dynamic behaviour we see a clear coupling between temporal and spatial distribution of fracturing. We see an evolution from localized and major intra-granular splitting events, early in a simulation, to smaller and more distributed fracturing events later in a run. These observations entirely support our interpretation above of a switch in dominant deformation mechanism and dramatic reduction in comminution rate and intensity with accumulated global shear strain.

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Previous work has indicated that force chains (or grain bridges) transmit load across sheared granular material (Sammis et al., 1987; Sammis and Steacy, 1994; Cates et al., 1998) and that (Mair and Hazzard, 2007) the style of force network distributions in 3D are highly sensitive to grain size distributions. Although an extensive investigation of force distributions is beyond the scope of the current manuscript (and will be a topic of future work), our structural observations are certainly consistent with recent ideas on force networks and fragmentation. In our models at high normal stresses where the granular model is (initially) essentially monodisperse, we expect force chains to be highly organized (Mair and Hazzard, 2007) leading to high potential for grain splitting. After a wide size distribution has been attained, the force networks would become more diffuse (Mair and Hazzard, 2007) reducing the possibility for strong stress concentrations. The granular system has arrived at a ‘cushioned state’ where neighbouring grains are buffering each other from stress and grain splitting potential is dramatically reduced. Our 30 MPa normal stress run is consistent with constrained comminution models (Sammis et al., 1987; Sammis and King, 2007) and some observations of natural and laboratory faults, however one should note that the power law exponents quoted from field observations have a wide range e.g. (Sammis et al., 1987; Marone and Scholz, 1989; Blenkinsop, 1991; Chester et al., 1993; Billi et al., 2003; Storti et al., 2003; Billi and Storti, 2004; Chester et al., 2005). In natural fault zones it has often been observed that the values of D are significantly higher within the zones of localized shear strain (Storti et al., 2003; Billi and Storti, 2004). However, in our model the zones of localized shear largely consist of material which has been ground down to single particles. Therefore the power law exponent in those zones is determined by the initial size distribution of the single particles, generated by the packing algorithm, and not by the comminution process. The cause of the observed symmetry in the position of the shear band will be investigated in future models. In particular, models with different (e.g. rougher) boundary conditions will be used to test if it is a function of the initial setup.

Some obvious limitations of our current model include the relatively small number of aggregate grains in simulations. This leads to initial porosity and significant volume collapse during initial compaction and subsequent shear. The voids may preferentially focus the pulverized fault gouge. In addition, since the individual particles in our model are spherical in shape, the mobility of fault gouge in the simulations is effectively enhanced when aggregate grains are reduced in size to become individual particles due to their preference to roll. This may generate a positive feedback that enhances strain localization. We argue that this effect would be greatest at late stages of simulations (i.e. large strains) and that the earlier stages are certainly not dominated by this effect. Future simulations conducted on larger computational resources could test these ideas. Despite these limitations, we are encouraged by the relatively realistic textures and evolution processes that our model can produce.

5. Conclusions

In summary, we have designed a new 3D granular gouge evolution model that to a first order, produces realistic fault gouge textures. Importantly, we do not just see a bulk pulverization of the simulated fault gouge in our granular model but rather highly heterogeneous deformation. Grain size evolves, with accumulated strain, to a power law size distribution where the exponent depends on normal stress and some near original sized ‘survivor’ grains persist to high strains even at high normal stresses. Both features are common traits in natural and experimental fault zones. An evolution from episodic grain fracturing (clustered in both time and space) at the start of a simulation to spatially and temporally distributed events suggests a gradual switch in dominant deformation mechanism from intra-granular fracture to abrasion with accumulated strain. Interactions of nearest neighbours support ideas from models of constrained comminution i.e. where one grain is substantially broken up it acts as a stress buffer effectively protecting its neighbour who then has a low chance of intra-granular fracture and hence a much higher survival potential. We see enhanced grain size reduction in certain regions of our model, notably the edges (but also in the middle for runs at high normal stress). These regions are strongly correlated (both temporally and spatially) with areas of enhanced local strain. It therefore appears, in our models, that grain size reduction and development of a structural fabric may be driving strain localization.

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Appendix A. Supplementary data


References


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