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2D Distinct Element Modeling of the Structure and Growth of Normal Faults in Multilayer Sequences. Part 2: Impact of Confining Pressure and Strength Contrast on Fault Zone Growth and Geometry

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Abstract

The growth of normal faults in periodically layered sequences with varying strength contrast and at varying confining pressure is modeled using the Distinct Element Method. The normal faulting models are comprised of strong layers (bonded particles) and weak layers (non-bonded particles) that are deformed using a predefined fault at the base of the sequence. The model results suggest that faults in sequences with high strength contrast at low confining pressure are highly segmented due to different types of failure (extension vs. shear failure) in the different layers. The degree of segmentation decreases as the strength contrast decreases and confining pressure increases. Faults at low confining pressure localize as extension (Mode I) fractures within the strong layers and are later linked via shallow dipping faults in the weak ones. This leads to initial staircase geometries that, with increasing displacement, cause space problems that are later resolved by splaying and segmentation. As confining pressure increases the modeled faults show a transition from extension to hybrid and to shear fracture and an associated decrease in fault refraction, with a consequent decrease in fault surface irregularities. Therefore the mode of fracture, which is active in the strong layers of a mechanical multilayer at a particular confining pressure, exerts an important control on the final fault geometry.
Introduction

Outcrop and experimental studies suggest that the geometry of faults is strongly dependent on the strength contrast of the layers, layer stacking and (effective) confining pressure [Peacock and Sanderson, 1994; Childs et al., 1996; Patton et al., 1998]. Numerical modeling and outcrop studies of normal faults, for example, have shown that faults initiate as steep/vertical extension fractures in the strong layers which are linked via shallow dipping faults within the weak layers [e.g., Peacock and Sanderson, 1994; Crider and Peacock, 2004; Micarelli et al., 2005; Schöpfer et al., 2006]. These dramatic fault dip variations are generally attributed to different modes of fracturing within the different lithologies of high strength contrast sequences at relatively low effective confining pressures [Gross, 1995; Sibson, 1998; Ferrill and Morris, 2003]. Fault dip variations (often referred to as fault refraction) are less dramatic if all the layers comprising the sequence fail via Coulomb shears. In the case of Coulomb shear failure, the difference in fault dip between layers is theoretically half the difference in friction angle of the two different materials, though slightly larger refraction angles can be obtained if shear stress acts on the interface between layers [Mandl, 2000]. Relatively small (5-10 degrees) normal fault dip variations are therefore typically observed either within poorly lithified sequences or at high confining pressures.

The fault surface characteristics described above are defined from outcrop observations, interpretation of reflection seismic data, laboratory experiments and empirical failure criteria. Outcrop studies can give insights into fault geometry but only provide a snapshot in time. In the case of syn-sedimentary faulting it is possible, in principle, to reconstruct the growth of certain elements of fault zones (e.g. fault segmentation/relay zones; [e.g., Childs et al., 2003; Walsh et al., 2003]), but such
studies are relatively rare and, in any case, provide few constraints on either the
effective confining pressure and the mechanical properties of the faulted sequence at
the time of faulting. Although these deformation parameters can be controlled in the
rock deformation laboratory, only finite stages can be investigated, i.e. the growth
sequence has to be inferred from different samples that experienced different finite
strain [Patton et al., 1998], though acoustic emissions can be used to determine
aspects of the growth sequence in the case of brittle fracture. Analogue modeling can
give valuable insights into the growth of faults, but the scaling of experiments,
especially in the natural gravity field, will never be perfect [Mandl, 2000].

An alternative approach for investigating the impact of strength contrast and
confining pressure on fault geometry and growth is the Distinct Element Method
(DEM), a relatively new numerical method in structural geology [e.g. Morgan and
Boettcher, 1999; Hazzard et al., 2000; Burbridge and Braun, 2002; Strayer and
Suppe, 2002]. In DEMs rock is modeled as an assembly of particles (e.g. discs in 2D,
spheres in 3D) that interact with each other via their contacts. Particles can be bonded
with each other and these bonds can break if their strength is exceeded, which
corresponds to fracture. Using the Distinct Element Method, the aim of this paper is to
investigate the impact of confining pressure and of strength contrast of layering on
fault geometry and growth. A detailed description of the methodology, model
calibration and boundary conditions, which underpin the modeling results presented in
this paper, are given in the companion paper (Schöpfer et al., Part 1). Analyzing the
models from both a geometrical and mechanical perspective we describe the transition
from tensile to shear failure with increasing confining pressure and decreasing
strength contrast and discuss its impact on fault zone geometry and evolution.
2 The Transition From Extension to Shear Fracture: Definition and State of the Art

As stated in the previous section, outcrop studies on normal faults suggest that faults within layered sequences often exhibit dramatic dip refraction at low effective stress, where one lithology has sufficient cohesion to fail in tension [e.g. Ferril and Morris, 2003; Crider and Peacock, 2004]. Dip variations are less pronounced at high confining pressure where all lithologies comprising the sequence fail in shear. Fault dip variations observed in outcrop are therefore attributed to differences in either the modes of failure or the angles of internal friction of the interbedded lithologies. In the rock mechanics laboratory, two end-members of brittle fracture are typically distinguished: extension fractures formed in tension parallel to $\sigma_1$ and shear fractures (faults) formed in compression, with an inclination of 20-40° to $\sigma_1$. Ramsey and Chester [2004] performed a series of direct tension experiments on dog bone shaped samples of Carrara marble at various confining pressures and have shown, for the first time, that there is a continuous transition from extension to shear fracture. These ‘transitional fractures’ are known by a variety of names in the literature (Engelder, 1999); we follow the terminology used by Ramsey and Chester [2004] throughout this paper and call them hybrid fractures. Since we observed a similar transition in our DEM models described below, it is worth summarizing their findings. The stress data from the Ramsey and Chester [2004] experiments are plotted on both a Mohr diagram and a principal stress graph in Figure 1, where different symbols were used for the three different fracture morphologies observed (extension, hybrid and shear fracture). Extension fracture surfaces are characterized by discrete, highly reflective intragranular cleavages, whereas shear fracture surfaces are covered with a powder of comminuted grains and contain short grooves parallel to the direction of maximum
shear traction. Hybrid fractures display transitional surface characteristics and exhibit patches of discrete, reflective, cleaved crystals between areas of comminuted material with slip lineations. The fracture morphologies show a strong correlation to confining pressure insofar as the total area of cleaved crystals decreases with increasing confining pressures. Ramsey and Chester [2004] have pointed out that neither the two-, nor the three-dimensional Griffith criterion, which for clarity are not plotted on Figure 1, fit the stress data. Additionally the fracture angles observed for hybrid and shear fracture are systematically lower than predicted from the slope of the failure envelope (Figure 1a). It appears, however, that a Coulomb-Mohr criterion with tension cut-off [Paul, 1961] fits the stress data satisfactorily (Figure 1b). This criterion, however, predicts only two different fracture orientations, whereas the lab data clearly show a gradual increase in fracture angle with increasing confining pressure. This discrepancy between stress state at failure and fracture angle can be seen in the Mohr diagram (Figure 1a), where lines joining the mean stress points \(((\sigma_1 + \sigma_3)/2)\) and their corresponding points that represents the normal and shear traction \((\sigma_n and \tau)\) acting on the failure plane are not normal to the failure envelope as would be the case for the Coulomb-Mohr hypothesis (see dashed lines in Figure 1a).

The Coulomb-Mohr criterion expressed in terms of principal stress can be written as

\[ \sigma_1 = \sigma_{uc} + q \sigma_3, \]  

where \(\sigma_{uc}\) is the unconfined compressive strength and

\[ q = \left[ (\mu^2 + 1)^{1/2} + \mu \right]^2 = \tan^2(\pi / 4 + \phi / 2), \]  

(1b)
where \( \mu \) is the coefficient of internal friction equivalent to \( \tan \phi \). Although the Coulomb-Mohr criterion with tension cut-off fails to predict the observed macroscopic fracture orientations, it is capable of predicting the stress states at which the transitions from extension to hybrid and hybrid to shear fracture occur (Figure 1b). Extension fractures develop when the minimum principal stress, \( \sigma_3 \), is equal to the tensile strength of the material, \(-T\), shear fracture occurs if \( \sigma_3 \) is equal or greater than zero, and hybrid fractures form if \(-T < \sigma_3 < 0\). Expressed in terms of the maximum principal stress, \( \sigma_1 \), shear fractures develop if \( \sigma_1 \) is equal to or greater than the unconfined compressive strength of the material, \( \sigma_{uc} \). Consequently the transition from hybrid to shear fracture occurs where the failure envelope crosses the \( \sigma_3 \) axis in a principal stress plot (Figure 1b). The transition from extension to hybrid fracture occurs (approximately) where the two straight lines comprising the failure envelope cross; the \( \sigma_1 \) value at which this transition occurs is obtained by substituting \(-T\) for \( \sigma_3 \) in equation (1). This stress-based definition of the three types of fracture (extension, hybrid and shear) is an approximation to the experimental results of Ramsey and Chester [2004] and will be used throughout this paper.

3 Methods

We used the Discrete Element Method (DEM), as implemented in commercially available Particle Flow Code (PFC2D; Itasca Consulting Group [1999]), for modeling the growth of faults through multilayer sequences. The methodology and boundary conditions used in this study are described in detail in a companion paper (Schöpfer et al., Part 1). Each multilayer model is comprised of >23,000 cylindrical particles with an average diameter of ~10 cm. The models contain four 1 m thick strong layers...
alternating with four 1.5 m thick weak layers. A 3 m layer, the primary function of
which is model confinement, overlies this 10m thick sequence. Four different
calibrated bonded materials formed the strong layers within the models with average
unconfined compressive strengths of 128, 106, 83 and 64 MPa. The weak layers
(including the top layer) in each model consist of non-bonded particles. Calibration of
rock materials involved both unconfined and confined biaxial tests and direct tension
tests, together with the construction of associated failure envelopes (Coulomb-Mohr
with tension cut-off; see Schöpfer et al., Part 1). Material properties of the strong
layers are comparable with those of limestones, whilst the weak layers have no tensile
strength and are comparable to some shales.

The models were deformed at four different overburden pressures of
approximately 23, 46, 74 and 100 MPa, which, assuming lithostatic conditions and an
overburden density of 2500 kg m⁻³, correspond to depths of faulting of approximately
1, 2, 3 and 4 km. Localization of a single through-going fault is achieved by
introducing a pre-cut 60° dipping ‘fault’ at the base of the 15-m-wide times 13-m-high
multilayer sequence (defined by >23,000 particles), and by moving the L-shaped
hangingwall downward at a constant velocity (figure 8 in Schöpfer et al., Part 1); this
boundary condition ensures that a single fault rather than several faults is localized
within the model. Each of the models was recorded at increments of throw of 0.5 m
up to a maximum fault throw of 2 m.

To ensure that fault zone structural variability is a function of confining
pressure and strength contrast and is not influenced by particle distribution (see
Schöpfer et al., Part 1), the initial distribution of particles is the same for a suite of 16
models, which together provide a matrix of four confining pressures and four strength
contrasts (Figure 2). Similarly, the distribution of bond strengths is the same for each
confining pressure. Since the bonds between particles were installed following sample confinement and the coordination number (number of contacts per particle) of particles is a function of confining pressure there is a slight (3%) increase in the number of bonds from the lowest to highest confining pressure models.

4 Geometries of Modeled Fault Zones

The results of the 16 models with varying strength contrast and confining pressure are shown in Figure 2 at 0.5 m throw intervals. The positions of main faults are highlighted by separation lines which join initially adjacent particles that are now more than 10 cm apart; the positions of broken bonds and smaller (< 10 cm) faults are more pervasive and are not individually shown. The models highlight a variety of important features about both the geometry and growth of fault zones. Fault zones are highly segmented at low confining pressure and high strength contrast and, in these circumstances, are often characterized by the presence of paired, and sometimes multiple, slip surfaces between which displacement is partitioned. As a consequence, the fault zone width, across which most of the displacement is accommodated, is generally wider at low confining pressure and high strength contrast. These wide fault zones are generated by localization of steeply dipping faults within the strong layers which are later linked via shallower dipping faults in the weak layers. Asperities arising from fault refraction and segmentation are progressively removed, giving rise to fault-bounded blocks that rotate within the fault zone as displacement accumulates. Despite the increased fault zone width associated with the combination of low confining pressure and high strength contrast, these conditions provide for the best localization of >10 cm displacement faults. At a throw of 0.5 m, for example, only a few >10 cm offsets exist within the high confining pressure and low strength contrast
models, with deformation occurring by dilational shearing or folding within zones of widespread bond breakage. The strong layers within these zones lose their cohesion and behave like a homogeneous, weak (non-bonded) material to form a cataclastic shear zone.

The difference in localization at different confining pressures and strength contrasts is highlighted by the micro-response of the strong layers. For models with throws of 2m, Figure 3 presents contour diagrams showing (a) the percentage of bonds broken (either in tension or shear), (b) the percentage of tensile bond failures and (c) the percentage of broken bonds with separations greater than 10 cm. Figure 3a reveals that the number of broken bonds increases as the strength of the strong layers decreases and confining pressure increases. Evidently, despite the less segmented nature of faults in these circumstances, there is a great deal more associated damage and ductile deformation. Whatever the conditions, on the microscale tensile failure is the dominant mode of deformation (Figure 3b), despite the fact that the shear bond strength is half the normal bond strength (see Schöpfer et al., Part 1). There is, however, a slight proportional decrease in tensile failure, and therefore, increase in shear failure at high overburden pressures and low strength contrasts, a feature which is consistent with the theoretical considerations of confining pressure-dependent failure referred to above. This slight change in microscale behavior shows some similarity with that of macroscale deformation of the strong layers in which fractures show the full range of extension, hybrid and shear failure, as will be discussed later.

The degree of localization and the amount of related damage is highlighted by Figure 3c, which shows that at low confining pressure and high strength contrast almost 50% of the broken bonds have separations >10 cm, meaning that most of the material outside, and the blocks within, the fault zone are intact. In contrast the ‘damage‘ at
high confining pressure and low strength contrast is considerable (only 5% of the
broken bonds have separations >10 cm) such that there is hardly any intact material
within the fault zone and there are abundant fractures immediately outside the fault
zone. This relationship again highlights the fact that in these circumstances,
deformation associated with the fault appears to be more ductile than that of the better
localized, albeit more segmented, faults at lower confining pressures and higher
strength contrast.

5 Fault Mechanics

Geometrical analysis of faults within DEM multilayer models has revealed several
characteristics of both the geometry and growth of faults, which can be related to both
the confining pressure during faulting and to the properties of the faulted sequence. In
this section details of the mechanics of localization of faults within multilayers are
explored, by reference to the stresses and strains associated with the suite of 16
models at fault throws of 10 cm. The relatively low throw value chosen permits both
the nature and mode of fracture to be investigated, together with a comparison to
theoretical considerations, without the introduction of complications arising from
progressive displacement accumulation and fault zone growth. Both stress and strain
concepts are used to demonstrate the principal controls on extension, hybrid and shear
failure, followed by a brief analysis of the control on fault and fracture orientations of
tensile strength and confining pressure.

5.1 Stress State at the Onset of Faulting

Stress is a continuum concept, whereas a Distinct Element model is a discontinuum.
Although the stress tensor can be obtained for each particle, the state of stress at this
point (i.e. the center of the particle) is meaningless on a macroscale. Therefore a stress homogenization approach, which averages the state of stress within a circle (2D) or sphere (3D), is implemented in PFC (measurement circle logic; (see Potyondy and Cundall, [2004] for details). Because the thickness of the strong layers in our models is always 1m and because calibration of their strength was performed on samples of 1m in diameter (Schöpfer et al., Part 1), a measurement circle diameter of 1m was chosen. With measurement circles, containing on average 92 particles, located at the center of the layers and with a horizontal spacing of 0.5 m, the magnitudes of the principal stresses were obtained at 116 points for each material within the models. Because the stress analysis is performed on models with only 10 cm throw, the state of stress close to the onset of faulting can be computed in both the strong and weak layers.

The stress states in the strong and weak layers within each of the 16 models are shown in principal stress plots in Figures 4a and b, respectively. For the strong layers, the best-fit Coulomb-Mohr envelopes with tension cut-off were determined from tests on unconfined and confined dog-bone shaped samples (Figure 4a; see Schöpfer et al., Part 1). For the weak layers, the Coulomb-Mohr criterion is plotted using $\mu = 0.45 \pm 0.05$ (one stdev), which was obtained from confined biaxial compression tests, and zero tensile strength (Figure 4b).

As a prelude to a detailed consideration of the model stress data, we construct a plot of unconfined compressive strength against vertical stress (= confining pressure) showing the dominant mode of failure expected in each of the 16 models (Figure 5). The unconfined compressive strength data in Figure 5 are derived from biaxial tests and include both the mean and one standard deviation for each of the four strong model materials. The vertical stress $\sigma_1$ is derived from the stress
measurements shown in Figure 4b using the \( \sigma_1 \) values of the weakest models and can be related to the depth of faulting assuming lithostatic conditions. Using the definitions given in section 2, the stress states of possible tensile, hybrid and shear fracture as a function of unconfined compressive strength, \( \sigma_{uc} \), and maximum principal stress, \( \sigma_1 \), which is equal to the overburden pressure in our models, can be distinguished (Figure 5). The fields of shear and hybrid failure are simply separated by the line

\[
\sigma_1 = \sigma_{uc} \quad (2a)
\]

and the fields of hybrid and extension failure are divided by the line

\[
\sigma_1 = \sigma_{uc} \left(1 - \frac{\left(\sqrt{\mu^2 + 1} + \mu\right)^2}{R}\right), \quad (2b)
\]

where \( \mu \) is the friction coefficient (set to 0.5, which is the approximate average value for the strong layers; see table 2 in companion paper) and \( R \) is the ratio of unconfined compressive strength to tensile strength (positive value), which for the model materials in this study is approximately 3.5. The plot shown in Figure 5 predicts those models that should predominantly show shear failure (three models – low strength and high overburden pressure), those which should be dominated by tensile failure (two models – high strength and low overburden pressure) and those remaining models characterized by hybrid failure. Since the ratio of unconfined compressive strength to tensile strength of our model material is low compared to
natural rock (Figure 1b), the field of hybrid fracture is broader in our models than predicted for rocks.

The theoretical fields for extension, hybrid and shear failure for the models are derived from the best-fit failure envelopes shown in the principal stress plots (Figure 4a; fields separated by dash and dash-dot lines) and using equation (2). The predictions derived from Figure 5 can then be compared with the independently derived principal stress states sampled within individual models (Figure 4). The predictions and measured states of stress within the strong layers of the models show a remarkable level of consistency. The two strongest models at low confining pressure (23 MPa) are characterized, as predicted, by tensile failure, with even the occasional indications of hybrid failure being consistent with the predictions for strengths towards the weaker end of the range of values derived from biaxial tests. The two weaker models at a confining pressure of 23 MPa show a transition from tensile to hybrid failure. At greater confining pressure (46 MPa), predominantly hybrid failure is observed in all the models. At a confining pressure of 74 MPa, the two strongest models are dominated by, as predicted, hybrid failure, whilst at lower strengths the models show the transition from hybrid to shear failure. At the greatest confining pressure (100 MPa), the strongest model is still characterized by hybrid failure, the second strongest has an approximately equal proportion of hybrid and shear failure, whereas the two weakest models are dominated, as predicted, by shear failure. It is important to recall, however, that at the particle bond scale, tensile failure is the predominant failure mode (Figure 3b); the different types of macrofracture described here are therefore the result of linking predominantly tensile microfractures. Although the close correspondence between stress states derived from calibration and the stress states for the strong layers within the multilayer models provides support for the
application of this modeling approach, the models also highlight the heterogeneous
nature of stress distributions within faulted multilayer sequences, the characteristics of
which could not have been predicted from theory alone. For the weak layers, theory
would predict entirely shear failure within these zero tensile strength materials. As
expected, the stress data for the weak layers therefore plot close to the Coulomb-Mohr
failure envelope, with higher principal stresses at increasing confining pressures
(Figure 4b). Indeed, the majority of the stress data for the weak material appear to be
close to the critical state of shearing, a feature which is attributed to the fact that
monoclinal folding of the strong layers is accommodated by ductile flow in the weak
ones as will be discussed in detail below. That some data points plot above the failure
envelope, i.e. in the unstable stress field, suggests that the friction coefficient is
locally higher than the mean value, possibly arising from local packing variations.

5.2 Strain Distribution at the Onset of Faulting

The preceding section shows that the stress states close to the onset of faulting, i.e. at
10 cm throw, reveal a great deal about the nature of failure at different confining
pressures and for multilayers with different properties. In this section the strain
distributions at the onset of faulting are examined for two principal reasons. Firstly,
strain distributions within models, and particularly within weak layers, provide a more
accessible and potentially more useful representation of localization associated with
faulting. Secondly, strain distributions reflect the finite strain history up to 10 cm
throw, rather than representing, as stress states do, infinitesimal strains at a particular
time. As such, strain distributions and measures are a complement to equivalent stress
measurements. Strain, like stress, is a continuum concept and, as a consequence,
homogenization procedures are required for studying strain in discontinua [O’Sullivan
In this study we determine strain for each particle for a circular, 0.3 m diameter, homogenisation area containing, on average, eight particles [see Schöpfer et al., 2006]. These relatively small homogenization areas were used for obtaining strain distribution details within the multilayer models that would not be seen if larger areas would be used. For each circular region the relative displacements of particles surrounding the central particle are calculated in order to remove the translational component of deformation. Once this translation has been removed the best-fit displacement gradient tensor can be calculated using a least-squares method, enabling the deformation tensor and the Lagrangian strain tensor to be obtained. It is important to note that particle rotations are not used for calculating strain. Alternative methods that take rotations into account and are not restricted to particle center displacements, are described and compared in O’Sullivan et al. [2003]. Using our simple method the maximum shear strain distributions were computed at 10 cm of throw for the 16 models.

The strain distributions at 10 cm throws for the suite of 16 models reveals many features (Figure 6; see Plate 1 for a color version of this figure) not seen in the geometric representations of DEM models shown before (Figure 2). At this early stage of faulting, the increased segmentation and fault zone width at low confining pressures and high strength contrasts has yet to fully emerge, but is nevertheless reflected in the generally relatively poor continuity of faults between strong and weak layers. For these conditions the origin of fault refraction by initiation in strong layers is clearly demonstrated in the strain contours. At high confining pressure fault refraction is less pronounced and deformation becomes more distributed in the strong layers. The real advantage of examining strain distributions is, however, illustrated by deformations observed within the weak layers. At low confining pressure, low angle
antithetic deformation zones develop in the weak layers within the hangingwall of the incipient fault. These zones accommodate low amplitude monoclinal folding of the strong layers and link the fold-related outer arc stretching at the top of one layer with that at the base of the overlying layer [Schöpfer et al., 2006]. As one would expect the width of these monoclinal zones increases with decreasing confining pressure and increasing strength contrast. It is clear therefore from inspection of maximum shear strain distributions that although a through-going fault may localize later within the weaker layer than in the strong layer its geometry is controlled to a significant extent by the geometry and scale of the pre-cursory monocline and associated fracturing within the stronger layers.

In an attempt to characterize and quantify the strains associated with the models, the principal quadratic elongations, $\lambda_1$ and $\lambda_3$, for the suite of 16 were calculated. The principal strains were determined at the same locations as the stress data described in the previous section, i.e. for 1 m diameter circular areas, containing on average 92 particles, with a spacing of 0.5 m located in the center of each layer; these larger areas were used in order to minimize noise. The data obtained are plotted in a principal quadratic elongation graph (PQEG; Figure 7), which can be used for plotting the full range of possible strain ellipses in 2D [Ramsay, 1967]. Strain analysis of naturally deformed rocks typically only allows determination of the ratio of the principal strains, whereas the principal quadratic elongation graph (PQEG) requires knowledge of the absolute values of strain and is therefore often of limited practical use. Because absolute strain values can be recorded in the models, the PQEG provides a very useful means of plotting and rationalizing the strains associated with 2D DEM models.
The PQEG is divided into areas of compactional and dilational strain separated by the hyperbola $\lambda_1 = 1/\lambda_3$ representing constant area deformation (Figure 7). The strain data for the 16 models lie almost entirely within the dilational field (Figure 8) with some minor compaction at low strains; these strains are expected for deformation of a granular medium. The data for the strong and weak layers in each model occur within distinct trends that define characteristic strain paths for a particular model. The strain paths for the weak layers are the same in all models but there is a systematic change in the strain paths for the strong layers, with progressively less dilation with increasing confining pressure and decreasing unconfined compressive strength. The PQEG cannot distinguish between coaxial and non-coaxial strain [Ramsay, 1967] and it is therefore not possible, on the basis of the data in Figure 8 alone, to separate simple and pure shear components of deformation. However, because our imposed boundary condition results in faulting, we can assume that the higher strains within each model are characterized by both a simple shear and a dilational component of strain. Schöpfer et al. [2006] present detailed descriptions of strain paths for individual locations for the model with an unconfined compressive strength of 106 MPa at a confining pressure of 23 MPa which confirm this assumption. It is therefore useful to interpret the strain paths in Figure 8 in terms of dilational simple shear.

The kinematics of an idealized shear zone in 2D that exhibits dilations (transtension/transpression) can be described with the deformation tensor [e.g., Krantz, 1995]

$$D = \begin{pmatrix} 1 & \alpha^{-1} \gamma \\ 0 & \alpha^{-1} \end{pmatrix},$$ (3)
where $\alpha^{-1}$ is the stretch normal to the shear zone boundary and $\gamma$ is the shear strain, which is equivalent to $\tan \psi$ (where $\psi$ is the angular shear). If no lengthening or shortening occurs normal to the shear zone boundary ($\alpha^{-1} = 1$), the displacement vectors are parallel to the shear zone boundary and the deformation is simple shear, which is by definition constant area. The strain path of progressive simple shear therefore plots on the curve $\lambda_1 = 1/\lambda_3$ in the PQEG (Figure 7; inset iii). If the displacement vector is not parallel to the shear zone boundary, deformation is characterized by area changes. The angle between the displacement vector and the shear zone boundary is the angle of divergence/convergence, $\beta$ (see inset in Figure 7), and is related to the stretch and shear strain by [Krantz, 1995]

$$\tan \beta = \frac{1 - \alpha^{-1}}{\alpha^{-1} \gamma}. \quad (4)$$

Strain paths for various $\beta$-values (positive denotes convergence) are plotted in the PQEG, together with examples of deformed unit squares in Figure 7. The two end-member deformations that can be defined using equation (3) and (4) are simple compaction ($\gamma = 0$, $\alpha^{-1} < 1$ and $\beta = 90^\circ$; example i) and simple extension ($\gamma = 0$, $\alpha^{-1} > 1$ and $\beta = -90^\circ$; example v) and plot in the PQEG along lines given by $\lambda_1 = 1$ and $\lambda_3 = 1$, respectively. Convergent shear paths ($\gamma \neq 0$, $\alpha^{-1} < 1$ and $0 < \beta < 90^\circ$; example ii) plot in the field bound by the line $\lambda_1 = 1$ and curve $\lambda_1 = 1/\lambda_3$, whereas divergent shear paths ($\gamma \neq 0$, $\alpha^{-1} > 1$ and $0 > \beta > -90^\circ$; example iv) plot in the field bound by the line $\lambda_3 = 1$ and curve $\lambda_1 = 1/\lambda_3$ (Figure 7).
Using a least-square method we determined the best-fit $\beta$-value for the strains within each model (Figure 8). The best-fit strain paths within the weak layers (i.e. non-bonded particles) are independent of confining pressure and have divergent angles ranging from $-10^\circ$ to $-13^\circ$ (dashed lines in the PQEGs in Figure 8).

Deformation within the strong layers is, as expected from our stress analysis, strongly dependent on confining pressure, with best-fit $\beta$-values $<-50^\circ$ for models that are expected to fail in tension (Figure 5). This style of deformation is expected in layers that fail via extension fractures that, with increasing displacement, lead to the formation of pull-aparts. The $\beta$-values gradually increase with both decreasing strength and increasing confining pressure (i.e. from the top left diagram to the bottom right one in Figure 8) until, in the ‘weakest and deepest’ model, the $\beta$-values for the strong and weak layers are almost the same. This gradual decrease in divergence with increasing confining pressure is interpreted to reflect the transition from extension fracture to shear failure, which is accompanied by a decrease in fault dip in the strong layers, details of which are given in the next section. In summary, strain within our multilayer models is highly partitioned at low confining pressure, whereas, as confining pressure increases, the style of deformation within the strong layers becomes gradually more similar to the deformation style within the intervening weaker layers.

5.3 Fault and Fracture Orientations

The stress and strain analysis of our DEM models presented above has shown that the brittle layers in the multilayer models exhibit a transition from extension to shear failure with increasing confining pressure; the weak, cohesionless layers can fail in shear only. Since extension fractures develop parallel to maximum principal stress,
\(\sigma_1\), and shear fractures at an inclination of 20-40º, (inclination angle of \(45º - \phi/2\) according to Mohr’s hypothesis) confining pressure dependent normal fault dip variations within the strong layers are expected, with steeply dipping faults at low confining pressure and 50-70º dipping faults at high confining pressure. In order to quantify these variations we measured the fault dips within the upper two strong layers from the maximum shear strain contour plots shown in Figure 6. The fault dips obtained from our DEM models are plotted against normalized confining pressure together with the fracture orientations observed in direct tension tests on Carrara marble [Ramsey and Chester, 2004, Table 1] in Figure 9. The fracture dip in both DEM models and Carrara marble decreases with increasing confining pressure, though the dips in our DEM models show a much greater variability than those obtained for marble. The large variability in the models arises for two reasons, firstly the model material is heterogeneous at the scale of the thickness of the strong layers (Schöpfer et al., Part 1) and secondly, because of the boundary conditions and the bedded nature of the model sequence, the fractures form in a heterogeneous stress field. Less variability in fracture orientation, though not necessarily fault zone complexity, would be expected in higher resolution models. Although the marble data plot within the range of DEM model data points, the majority of the latter plot below marble fracture dips, which might be due to the difference in friction coefficient between model (\(\mu = 0.5\)) and marble (\(\mu = 0.97\)).

The main conclusion arising from this study is that, although stress based predictions of the mode of failure are generally consistent with stress-derived measurements from the multilayer models (Figure 4 and 5), the localization of faults is strongly controlled by complex interactions developed within heterogeneous multilayers. The weak correlation between fracture dip and confining pressure
suggests, nevertheless, that fault surface irregularities, and related asperity sizes,
should increase with decreasing confining pressure and increasing strength (Figure
10) as the fracture dips within the strong layers become closer to those of the weak
layers. This conclusion is generally in line with the results of larger throw models,
which suggest that there are concomitant broad increases in the degree of fault
refraction and segmentation and in fault zone width.

Discussion

Faults contained in layered sequences are often segmented and it has been suggested
that the degree of segmentation is partly a function of strength contrast and confining
pressure. Using the Distinct Element Method (DEM), a relatively new approach for
fault mechanics, we show that faults within multilayer models are highly segmented at
low confining pressure and high strength contrast, with fault bound blocks that are
progressively rotated and incorporated into the fault zone. As the confining pressure
increases, or the strength contrast decreases, faults become less segmented and
resemble the geometries of cataclastic shear zones. Our results are therefore consistent
with the experiments by Patton et al. [1998], who have shown that the bulk ductility
and the area of microfracturing increase with increasing confining pressure.

The models show the full range of fracture modes and transitions between
extension, hybrid, and shear fracturing of the strong layers are observed. Although the
full range of fracture types is defined at the macroscale, i.e. on the scale of the layers,
microscale fracturing (= bond failure) within the models is either in tension or in
shear, with tensile bond failure being the predominant mechanism at all confining
pressures applied in this study (Figure 3b). This is consistent with existing theories
that suggest that hybrid and shear fractures arise from the linkage of stepped (Mode I) cracks [Reches and Lockner, 1994; Engelder, 1999].

The fracture dips within the strong layers decrease with increasing vertical stress, $\sigma_1$, and decreasing strength (Figure 9), but due to the heterogeneous nature of the model material and layering the dip data are highly variable. Therefore we did not attempt to quantify the relationships between dip and strength/stress but suggest that future DEM modeling with particular emphasis on the transition from extension to shear failure may provide insights into this highly topical area of fracture mechanics. Nevertheless, these model observations have direct implications for the dimensions of fault asperities that become incorporated into fault zones (Figure 10). Fault dip variations are a function of both strength contrast and confining pressure. The greater the fault dip variations, the greater the space problems that arise during fault growth which cause additional fault zone complexities, such as splaying and the development of antithetic faults.

The modeling in this study clearly demonstrates the importance of mechanical layering on fault segmentation. In isotropic materials fault segmentation is typically attributed to (often) non-plane stress fields at the tips of faults [e.g., Mandl, 1987; Cox and Scholz, 1988; Treagus and Lisle, 1997]. Layering, however, introduces heterogeneous stress and strain distributions that may play a more important role in determining fault propagation mechanisms and initial fault geometry than those which occur in isotropic rock. DEM modelling provides a mechanical basis for the growth of fault zones, and for their inherent complexity of structure, despite the operation of a small number of processes. DEM is a promising avenue for future fault mechanics research.
Conclusions

• Distinct Element modeling of fault growth in layered sequences has shown that fault zone complexities are a function of strength contrast and confining pressure.

• Model faults at low confining pressure and high strength contrast are characterized by multiple zones of high strain enclosing zones of rigid body rotation. Models at high confining pressure and low strength contrast tend to form individual wider zones of more distributed shear.

• More complex fault zone structure at low confining pressure and high strength contrast results from the more segmented and irregular fault geometries associated with fault initiation under these conditions.

• The modeling demonstrates the transition from extensional, through hybrid, to shear fracture with increasing confining pressure, which is observed in rock deformation experiments.

• The mode of fracture, which is active in the strong layers of a mechanical multilayer at a particular confining pressure, determines the fracture dip in the strong layer and therefore exerts an important control on fault geometry.

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**Figure Captions**

**Figure 1.** Transition from extension to shear fracture in Carrara Marble. The stress states at failure in the experiments by Ramsey and Chester [2004; their table 1] are plotted in a (a) Mohr diagram and (b) principal stress graph. The dashed lines in (a) have acute angles with the $\sigma_n$-axis of $2\theta$, where $\theta$ is the inclination of the fracture to the $\sigma_1$-axis. Different symbols are used for different fracture morphologies: triangles are extension, squares are hybrid and circles are shear fractures. A least square fit (by minimizing the $\sigma_3$-deviations numerically) was fitted to the data using a Coulomb-Mohr criterion with tension cut-off; best-fit parameters are provided, where $T = \text{tensile strength}$, $\sigma_{uc} = \text{unconfined compressive strength}$, and $\mu = \text{coefficient of internal friction}$. In this study the intercept of this failure envelope with the $\sigma_1$-axis is taken as the transition from hybrid to shear fracture and the ‘kink’ is the transition from extension to hybrid fracture. The latter transition does not exactly match the experimental data but, for simplicity, will be used throughout this study. Although this failure criterion provides a reasonable fit to the stress data, it cannot predict the failure angles observed in experiment, as highlighted in the Mohr diagram (a).

**Figure 2.** Multilayer model results at throws of 0.5, 1, 1.5 and 2.0 m. White layers are strong (thickness is 1 m) and gray layers are weak (thickness is 1.5 m). Black lines are particle separations that are greater than 10 cm, i.e. lines joining particles that where initially neighbors and are now separated by a distance greater than 10 cm. The strength decreases to the right and confining pressure increases towards the bottom.
Figure 3. Contour diagrams of bond breakage vs. confining pressure for strong layers within the model matrix shown in Figure 2 at a throw of 2 m. (a) Percentage of broken bonds, i.e. total number of broken bonds at a throw of 2 m / initial number of intact bonds. (b) Percentage of tensile failure, i.e. number of bonds failed in tension / total number of broken bonds. (c) Percentage of broken bonds with separations > 10 cm, i.e. separations of particles exceeding a distance of 10 cm / total number of broken bonds.

Figure 4. Principal stress diagrams illustrating the state of stress within (a) the strong layers and (b) the weak layers of the 16 models (Figure 2) at a throw of 10 cm; the arrangement of the diagrams is the same as in Figure 2. In each diagram the experimentally derived failure envelopes (see Schöpfer et al., Part 1) are plotted. In (a) the bold lines are the best-fit failure envelopes obtained from confined tension tests, and the thin failure envelopes are the 0.01/0.99 probability curves. The theoretical fields of extension, hybrid and shear failure are shown (dashed horizontal lines). The dashed line separates diagrams where extension and hybrid failure of the strong layers is expected and the dash-dot line separates fields of hybrid and shear failure based on Figure 5. In (b) the Coulomb-Mohr criterion ($\mu = 0.45 \pm$ two standard deviations) is plotted in each diagram.

Figure 5. Brittle failure mode plot of unconfined compressive strength vs. vertical stress illustrating the fields of extension, hybrid and shear failure according to the experimentally derived Coulomb-Mohr envelopes with tension cut-off. This plot is for the strong layers only, since the weak, incohesive layers fail in shear at all confining pressures. The fracture mode transitions expected for the DEM model material are
plotted as bold dashed lines and are determined using equation (3) (using a friction
coefficient of 0.5 and a ratio of unconfined compressive strength to tensile strength of
3.5). The extension to hybrid fracture transition for Carrara marble using the best-fit
parameters given in Figure 1b and equation (3b) is also shown as thin dotted line. The
two stars represent the kink and the $\sigma_3$-intercept of the failure criterion plotted in
Figure 1. Vertical dashed lines are average unconfined compressive strength of strong
layers obtained from 30 biaxial tests (see Schöpfer et al., Part 1) and horizontal
dashed lines are average $\sigma_1$ with ranges calculated using the stress data shown in
Figure 4b for $\sigma_{uc} = 64.0$ MPa models; the error bars ($\pm$ one standard deviation)
indicate the range of these parameters. The intersections of thin dashed lines relate to
the model matrix shown in Figure 2 and different open symbols are used for models
where the strong layers are expected to fail via extension (triangles), hybrid (squares)
and shear fractures (circles). This partitioning of the diagram is a guideline, since both
the model material strength and the stress distribution within the multilayer sequences
are heterogeneous.

**Figure 6.** Maximum finite shear strain contour diagrams (contour interval 0.025) of
the models shown in Figure 2 at a throw of 10 cm (white layers are strong). Following
the predictions of Figure 5, the bold dashed line separates models of extension and
hybrid failure and the dash-dot line separates fields of hybrid and shear failure.

**Figure 7.** The principal quadratic elongation plot in the context of dilational shear; $\lambda_1$
and $\lambda_3$ are defined as the squares of the maximum and minimum stretches,
respectively (stretch = finite length / initial length). Some representative finite strain
ellipses together with undeformed circles are shown. Because, by definition $\lambda_1 \geq \lambda_3$,
all data points that represent strain fall on or below a line of unit slope, where the
point (1,1) represents the undeformed state. The dotted labeled curves are constant
area change defined by \( (\lambda_1,\lambda_3)^{1/2} = A \); the curve \( A = 1 \) separates the regions of area
increase (dilation) and decrease (compaction). The solid labeled curves are strain
paths for constant divergence/convergence angle \( \beta \), which is defined in the inset (\( \psi \) is
the angular shear and \( \alpha^{-1} \) is the shear zone normal stretch). The labeled examples
illustrate: (i) Simple compaction. (ii) Transpression. (iii) Simple shear. (iv)
Transtension. (v) Simple extension. The 'slip vector' (arrows) in the five examples is
0.5 units long and a 0.5 slip contour is plotted in the graph as dash-dot line, together
with the points that represent the finite strain of the examples given.

Figure 8. Principal quadratic elongation graphs illustrating finite strain within the
strong layers (solid squares) and the weak layers (open circles) of the 16 models
(Figure 2) at a throw of 10 cm; the arrangement of the diagrams is the same as in
Figure 2. The labeled solid and dashed curves are best-fit strain paths for constant
divergence angle \( \beta \) for the strong and weak layers, respectively (the \( \beta = 0 \), i.e.
constant area, curve is shown in each diagram; see Figure 7 and text for further
explanation).

Figure 9. Fracture dips vs. normalized confining pressure \( (P_c = \sigma_1) \) for the upper two
strong layers of the DEM models shown in Figure 6 (filled symbols) and Carrara
marble (open symbols; [Ramsey and Chester, 2004, Table 1]). The key for the filled
symbols refers to different unconfined compressive strengths of the DEM model
materials. For Carrara marble data different open symbols are used for different
fracture morphologies: triangles are extension, squares are hybrid and circles are shear fractures. The dashed areas denote the limit of the data. The theoretical orientations of shear fractures according to Coulomb-Mohr hypothesis are shown as horizontal dashed lines using friction coefficients of 0.5 (DEM) and 0.97 (marble). Additionally, the transitions for extension to hybrid and from hybrid to shear fracture according to equation (3) are shown as vertical lines.

Figure 10. Schematic diagram illustrating the effects of confining pressure and strength contrast on fault dip variations within a multilayer sequence and consequently the dimensions of fault asperities (shaded regions; HWA and FWA = hangingwall and footwall asperity, respectively).
Schöpfer et al., Fig. 1
<table>
<thead>
<tr>
<th>Unconfined Compressive Strength [MPa]</th>
<th>Throw = 0.5 m</th>
<th>Throw = 1.0 m</th>
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<td>128.4 ± 16.1</td>
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<td>106.4 ± 13.0</td>
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<td>64.0 ± 8.0</td>
<td><img src="image7" alt="Graph" /></td>
<td><img src="image8" alt="Graph" /></td>
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*Schöpfer et al., Fig. 2*
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<th>Confining Pressure [MPa]</th>
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</thead>
<tbody>
<tr>
<td>128.4 ± 16.1</td>
<td>23.3 ± 8.0</td>
</tr>
<tr>
<td>106.4 ± 13.0</td>
<td>45.9 ± 11.5</td>
</tr>
<tr>
<td>83.1 ± 11.8</td>
<td>73.9 ± 18.9</td>
</tr>
<tr>
<td>64.0 ± 8.0</td>
<td>99.5 ± 20.0</td>
</tr>
</tbody>
</table>

*Throw = 1.5 m*

*Throw = 2.0 m*
average unconfined compressive strength [MPa]

(a) Percentage of broken bonds
(b) Percentage of tensile bond failure
(c) Percentage of broken bonds with separations > 10 cm
unconfined compressive strength [MPa]

128.4 ± 16.1
106.4 ± 13.0
83.1 ± 11.8
64.0 ± 8.0

shear
hybrid
extension

confining pressure [MPa]
23.3 ± 8.0
45.9 ± 11.5
73.9 ± 18.9
99.5 ± 20.0

σ₁ [MPa]
σ₁ [MPa]
σ₁ [MPa]
σ₁ [MPa]

Schöpfer et al., Fig. 4a
unconfined compressive strength [MPa]

128.4 ± 16.1
106.4 ± 13.0
83.1 ± 11.8
64.0 ± 8.0

confining pressure [MPa]

23.3 ± 8.0
45.9 ± 11.5
73.9 ± 18.9
99.5 ± 20.0
unconfined compressive strength [MPa]

23.3 ± 8.0
45.9 ± 11.5
73.9 ± 18.9
99.5 ± 20.0

confining pressure [MPa]

128.4 ± 16.1
106.4 ± 13.0
83.1 ± 11.8
64.0 ± 8.0

maximum shear strain
contour interval = 0.025

10 m

Schöpfer et al., Fig. 6
Schöpfer et al., Fig. 8
fracture dip [°] vs confining pressure / unconfined compressive strength

- Carrara Marble
- DEM models
- Hybrid - shear transition (Eq. 2a)
- Hybrid - shear transition (Eq. 2b)
- Extension - hybrid transition (Eq. 2b)

Schöpfer et al., Fig. 9
Schöpfer et al., Fig. 10

- confining pressure
- strength
- asperity size

HWA

strong

weak

FWA