Chapter 1

Introduction

In geotechnical engineering, many problems involve local interaction between soil materials and a solid boundary. The interphase shown in Figure 1.1 is a localized region near a solid manufactured inclusion or natural surface that consists of granular soil and the inclusion surface. The interface, as normally discussed in geotechnical literature, is the boundary between the interphase soil and the inclusion or natural surface. The problem of determining how the interphase governs the overall behavior of a composite system during quasi-static shear is of considerable significance to civil engineering, material science, geophysics and granular physics.

Whether the inclusion is geosynthetic, steel, concrete, or a new material yet to be developed, the interactions between construction materials and soil particles must be governed by underlying physical principles that are related to measurable surface and soil properties. While interface characterization and design is well developed in rock mechanics, it is an emerging technology in soil mechanics practice. Unfortunately, to date there is little understanding of the physical principles governing the interphase behavior, and thereby, a lack of predictive relationships for interfaces available to the practice community that account for surface and soil properties. This deficiency in current practice is important because innovative applications are arising which require close control over the interface friction, and have operational strength less than the maximum values.

This dissertation presents new and fundamental contributions to our knowledge regarding interphase behavior. A discrete element model of an interphase system was developed and implemented in two dimensions. The nature of shear banding within the interphase is shown to be greatly influenced by the interface topography, or roughness. A theory was developed that permits interpretation of discrete information by traditional continuum methods. Using that framework, the mechanism governing interphase strength is shown to be contact between the first layer of particles and the solid surface. This fundamental result is used to develop a failure
criterion for interphase systems composed of spherical particles. The criterion can be extended to subrounded particle assemblages.

1.1. Dilative and Non-dilative Surfaces

The state of the interphase soil differs from the state of the matrix soil due to the presence of the inclusion. State differences can be due to geochemical reactions, differences between the fabric and void ratio of the matrix soil and interphase soil, presence of wear surfaces on the inclusion, or other effects. A number of past researches (Desai 1981; Yoshimi and Kishida 1982; Kishida and Uesugi 1987; Irsyam and Hryciw 1991; Hryciw and Irsyam 1993; Tejchman and Wu 1995; Ebling et al. 1997; Day and Potts 1998; Dove and Jarrett 1999; Gomez 2000; Esterhuizen et al. 2001; Dove and Jarrett 2002) have shown that surface topography and the degree of surface roughness is important in controlling soil-structure interaction. There are two end-member states for the interphase behavior and resulting interface strength: dilative and non-dilative.

For non-dilative surfaces, the relative grain to surface roughness is so low that no volume change takes place. Mechanisms of the interface friction for these surfaces are different from those for dilative surfaces. Experimental studies by Dove 1996 and Dove et al. 2006 show that 1) the peak state is controlled by elastic contact with weak adhesion at relatively low normal stresses and sliding plus a plastic deformation component at higher normal loads; and 2) the steady state is dominated by the relative material hardness and interaction of the particle with wear debris. Research on the mechanisms for non-dilative interface behavior is not the main focus of this thesis, but its strength behavior will be included in the formulated failure criterion, accounting for the full range from non-dilative to fully dilative.

For dilative surfaces, the relative grain to surface roughness is high and surface asperities will cause volume increase (dilation) to occur during shear. Variables that will influence the interface strength include grain shape, relative grain to surface geometry, normal stress, relative hardness, initial density of soil, grain to surface friction coefficient, etc. The effect of grain shape and relative hardness is outside of the scope of this work. The remaining variable with the largest influence is the relative grain to surface geometry, which will be the major objective of the current thesis. At present, the micromechanical processes controlling strength and
deformation behavior of the dilative interface are known incompletely. Failure criteria that account for the relative grain to surface geometry do not exist.

Unification of dilative and non-dilative behavior can be achieved through quantification of surfaces using normalized geometric parameters (Dove and Jarrett 1999), which can be used to systematically describe the surface geometry spanning from non-dilative to full dilative. In addition, the normalized Efficiency ($E$) parameter defined by Koerner 1990 as $E = \tan \delta / \tan \phi$, can be used to eliminate the variation due to soil properties, where $\delta$ is the effective stress interface friction angle and $\phi$ is the effective stress friction angle of the soil alone.

1.2. Basic Hypothesis and Approach

The basic hypothesis for this research is that the relative grain to surface geometry of an inclusion controls the degree to which soil shear resistance is mobilized. By determining how the surface geometry controls the micromechanical behavior of the system, a new failure criterion based on easily measured surface and soil properties can be developed that accounts for the presence of an inclusion. Publications resulting from this research are expected to be significant and original contributions to the geoengineering literature.

The research was accomplished using Discrete Element Method (DEM) simulations of dilative interphase systems. Discrete element modeling provides unique insights for understanding the strength and dilatancy behavior inside the shear zone very close to the construction material. It is also a powerful tool for revealing shearing mechanisms at the microscopic level, and relating the macroscopic mechanical behavior to the microscopic internal variables. The simulations were conducted in a systematic manner such that the influence of geometry can be determined. Simulation results were used to extend a relatively large experimental data set conducted on actual interphase systems similar to those used in the simulations.

1.3. Review of Previous Work

1.3.1. Shear Behavior of Granular Soils

In the literature, there are many significant contributions focusing on shear behavior of granular soils from both macro and micromechanical point of view. The physical mechanisms underlying the evolution of shear bands and the associated strain localization inside the shear
band during shear is considered important for this project. Major contributions to the understanding of shear banding and strain localization behavior include Roscoe et al. 1958; Morgenstern and Tchalenko 1967; Arthur et al. 1977; Nemat-Nasser 1980; Scarpelli and Wood 1982; Arthur and Dunstan 1982; Lade 1982; Vermeer 1990; Alshibli and Sture 2000; Gutierrez and Ishihara 2000; and Masson and Martinez 2001. Major solutions to the orientation of shear band include Mohr-Coulomb solution, Roscoe solution, Vardoulakis’ bifurcation solution and Arthur solution based on different assumptions:

1. Mohr-Coulomb solution which assumes a shear band forms in the direction of the planes on which maximum mobilized angle of friction occurs:

\[
\eta = \pm \left( \frac{\pi}{4} - \frac{\phi}{2} \right)
\]  

where \(\eta\) is the angle between the orientation of shear band and the major principal stress direction \(\sigma_1\), and \(\phi\) is the friction angle of the soil.

2. Roscoe solution which treats the shear band as a layer of intensely shearing material which coincides with the zero extension direction. By assuming coaxiality of principal stress and principal plastic strain increment directions, Roscoe obtained:

\[
\eta = \pm \left( \frac{\pi}{4} - \frac{\nu}{2} \right)
\]  

where \(\nu\) is the dilation angle.

3. Vardoulakis solution which treats shear band formation as an instability phenomenon using bifurcation theory, provides a more comprehensive form of solution for shear band orientation with the assistance of hardening modulus \(h\):

\[
\eta = \pm \left( \frac{\pi}{4} - \frac{\zeta}{2} \right)
\]

and

\[
\sin \zeta = \frac{\sin (\phi_p + \psi_p)/2}{\cos (\phi_p - \psi_p)/2}
\]  

where \(\phi_p\) is the maximum mobilized angle of friction (plane strain friction angle) and \(\psi_p\) is the peak dilation angle. Eqs. (1-3) and (1-4) represent the general bifurcation solution in case of
higher positive values of $h$, bounded by the Mohr-Coulomb and Roscoe solution in case of zero and small positive values of $h$, respectively.

(4) Arthur solution which assumes a series of local shear bands distributed approximately along the direction of bisector between the maximum stress obliquity and zero extension directions, can be deduced from Vardoulakis solution when the difference between $\phi_\rho$ and $\psi_\rho$ is small:

$$\eta = \pm \frac{\pi}{4} \left( \frac{\phi_\rho + \psi_\rho}{4} \right)$$  \hspace{1cm} (1-5)

The real orientation of the shear band in the soil will be influenced by the boundary conditions applied to the particular soil element (Scarpelli and Wood 1982). Despite these important contributions, very limited experimental work has been done on the shear deformation of interphase soils. Uesugi et al. 1988 observed the behavior of sand particles in sand-steel friction in simple shear apparatus and described qualitatively their deformation characteristics due to interface roughness. But in general, the shape, thickness of the shear band, and the particle movement at the microscopic level in the interphase region remain unknown.

The emergence of the Discrete Element Method (DEM) (Cundall 1971; Cundall and Strack 1979) and its numerical simulation provide a powerful tool for studying particulate media and greatly facilitate the understanding of granular micromechanics. Contributions to understanding microdeformation mechanisms controlling the strength and dilatancy behavior of granular material include Oda et al. 1982; Bathurst and Rothenburg 1990; Bardet and Proubet 1991 and 1992; Bardet 1994; Iwashita and Oda 1998; Kruyt and Rothenburg 2004. Among others, Oda et al. 1982 and Iwashita and Oda 1998 showed the important role of particle rolling in the strength and dilatancy behavior inside the shear band. Bathurst and Rothenburg 1990 found the macroscopic strength of the granular material is closely related to the shear-induced anisotropy of the contact normal and contact forces inside the granular assembly, which is essential for understanding the strength and deformation behavior of the granular material from the microscopic point of view. All this information have proven vital for the current project.

1.3.2. Failure Criteria in Rock Mechanics

In the soil mechanics literature, there are currently no general predictive relationships for interphase systems composed of coarse-grained soil and solid counterfaces. Relatively little work
has been conducted to understand interphase strength. However, the rock mechanics literature is rich in detailed studies.

Patton 1966 proposed a simple saw tooth model which explains how roughness or dilatancy adds to the shear strength of two serrated surfaces. The main contributors to the development of peak shear strength of rock joint in the low normal effective stress range are Landanyi and Archambault 1969 and 1980, Barton 1973 and Kulatilake 1995. Barton introduced Joint Roughness Coefficient (JRC) to quantify surface roughness and Joint Wall Compressive Strength (JCS) in one dimension, and proposed the well-known Barton’s shear strength equation based on JRC and JCS:

\[
\tau_{\text{max}} = \sigma_n \cdot \tan \left[ JRC \cdot \log \left( \frac{JCS}{\sigma_n} \right) + \phi_r \right]
\]

where \( \sigma_n \) = normal stress; \( \phi_r \) = residual friction angle. He suggested two methods for determining an appropriate value for JRC: (1) method of visual comparison of the roughness profile of a natural joint with 10 standard profiles, (2) method of tilt and pull tests performed on natural discontinuities. Besides JRC, some other parameters have been proposed for roughness quantification, like statistical parameters (Maerz et al. 1983; Wu and Ali 1978; Tse and Cruden 1979; Krahn and Morgenstern 1979; Dight and Chiu 1981; Reeves 1990), and fractal dimensions (Mandelbrot, 1983; McWilliams, Kerkering and Miller 1993; Huang et al. 1992; Brown and Scholz, 1985; Aviles et al. 1987; Lee et al. 1990). Kulatilake 1995, on the basis of Barton’s equation, developed new peak shear strength criteria for anisotropic rock joints which account for shear strength in different directions and take the following general form:

\[
\tau_{\text{max}} = \sigma_n \cdot \tan \left[ \phi + a(SRP) \left\{ \log_{10} \left( \frac{\sigma_j}{\sigma} \right) \right\}^c + I \right]
\]

where \( SRP \) is the stationary roughness parameter, \( I \) is another roughness parameter and the coefficients \( a, c \) and \( d \) can be determined by performing regression analysis on experimental shear strength data. \( SRP \) can be represented by four different kinds of parameters in four different approaches of roughness quantification such as conventional statistical parameters, fractal parameters, spectral/fractal parameters, and variogram/fractal parameters.

### 1.3.3. Correlations for Interface Friction in Soil Mechanics

The limited work in the soil mechanics literature generally offers simple and incomplete forms of correlations between interface friction coefficient and statistically based roughness
parameters. For example, Uesugi and Kishida 1986 proposed the following equation for the friction coefficient of sand-steel non-dilative interfaces:

\[ \mu_y = \frac{1}{\bar{R}} (A + B \cdot R_n) \]  

(1-8)

where \( \bar{R} \) is the modified roundness parameter of particles proposed by Oda 1971 to evaluate the particle angularity, and \( A, B \) are constants related to minerals of sand and type of steel. Paikowsky and Xi 1997 performed an extensive laboratory study on the micro and macro mechanical interfacial behavior of discrete material using photoelastic method and proposed S.G model for rough solid interface strength based on particular packing geometry. Frost and Han 1999 investigated various factors influencing the interface behavior between fiber-reinforced polymers and sands, and gave simple equations relating peak friction coefficient with each individual variable. Dove and Jarrett 2002 investigated the influence of surface topography on the shear stress and volume change behavior of dilative granular material-geomembrane interface systems. Valuable but incomplete discussions on certain aspects of interface behavior are found in Kishida and Uesugi 1986, 1987, and 1988; Irsyam and Hryciw 1991; Desai et al. 1985; and Jensen et al. 1999.

### 1.3.4. Constitutive modeling for Interface behavior in Soil Mechanics

In spite of the deficiency of research work regarding interphase strength criteria in the soil mechanics field, significant work has been done on constitutive modeling of the interphase behavior. The hyperbolic model for soil behavior developed by Duncan and Chang 1970 was extended to interphase by Clough and Duncan 1969 and 1971. Gomez, Filz and Ebeling 2000 extended the Duncan-Chang model to model a variety of stress path, where normal and shear stresses change simultaneously. The Gomez-Filz-Ebeling model provides good estimates of the response of a variety of soil/concrete interphases subjected to complex stress paths. In the aspect of constitutive modeling of large-deformation interface behavior, Esterhuizen, Filz and Duncan 2001 proposed a new displacement-softening model for geosynthetic interfaces, which in essence applies a hyperbolic formulation on the residual factor versus displacement ratio relationship and shows good prediction of interface behavior under constant normal stress. In the same paper, another new work-softening model was suggested for use in the case of increasing normal stress.
and was shown to perform better than the displacement-softening model. Both of two models are full elasto-plastic constitutive models.

1.4. Discrete Element Method

The Discrete Element Method (DEM) developed by Cundall 1971 and later improved by Cundall and Strack 1979, will be used for micromechanical modeling of the interphase system. The commercial software package, PFC2D, from Itasca Consultants used herein is based on Cundall's work (Itasca 2002). DEM models the movement and interaction of stressed assembly of rigid particles. In the DEM, the interaction of rigid particles is treated as a dynamic process with overall equilibrium achieved whenever internal forces balance. Movements of particles result from propagation of disturbance through the particle assembly caused by specified boundary wall, particle motion or body forces. Contact forces and total displacement of the assembly can be found by tracing the movements of individual particles.

DEM simulates the dynamic process represented numerically by an explicit time stepping algorithm. A small enough time step can always be selected so that during a single time step, disturbance can not propagate from any particle further than its neighboring particles. Therefore, at any time, forces acting on any single particle can be determined exclusively by its interaction with the particles in contact with itself.

Newton’s second law and the so-called “force-displacement” law are alternatively applied in every time step. Newton’s second law determines the motion of the particles due to the contact and body forces acting on them, while the “force-displacement” law determines the interaction forces at the contacts due to the relative motion of the particles. The calculation cycle in each time step is illustrated in Figure 1.2. It begins with updating all the contact forces from the known positions of particles and walls at the start of each time step. Then the force-displacement law is applied to each contact to update the contact forces based on relative motion between the two particles and the contact constitutive model. Next, the law of motion (Newton’s second law) is applied to each particle to update its velocity and position. Meanwhile, the wall positions are updated based on the specified wall velocities. The section below provides a brief overview of the algorithms used in PFC2D.
1.4.1. Law of Motion

The interaction of rigid particles is treated as a dynamic process with overall equilibrium achieved whenever internal forces balance. The translational motion of the center of a particle is described by its position $x_i$, velocity $\dot{x}_i$, and acceleration $\ddot{x}_i$. The rotational motion of the particle is described by its angular velocity $\omega_i$ and angular acceleration $\ddot{\omega}_i$.

The equation of translational motion can be written as

$$ F_i = m(\dot{x}_i - g_i) $$

where $m$ is the total mass of the particle and $g_i$ is the body force acceleration vector.

In a local system which is oriented such that it lies along the principal axes of inertia of the particle, the equation for rotational motion can be written as

$$ M_3 = I \ddot{\omega}_3 = (\beta m R^2) \ddot{\omega}_3 $$

where

$$ \beta = \begin{cases} 2/5, & \text{(spherical particle)} \\ 1/2, & \text{(disk - shaped particle)} \end{cases} $$

The equations of motion are integrated using a centered finite-difference procedure involving a time step of $\Delta t$. The values of $F_i^{(t+\Delta t)}$ and $M_3^{(t+\Delta t)}$, to be used in the next cycle, are obtained using the force-displacement law.

1.4.2. Force-displacement Law

The contact force vector $\bar{F}_i$ can be resolved into the normal and shear components with respect to the contact plane as

$$ \bar{F}_i = F_i^n + F_i^s $$

where $F_i^n$ and $F_i^s$ denote the normal and shear component vectors, respectively.

The magnitude of normal contact force is calculated by

$$ F^n = K^n \cdot U^n $$

where $K^n$ is the normal stiffness at the contact, and $U^n$ is the overlap between two entities (ball-ball or ball-wall) at the contact, where a ball is a particle and the wall is a boundary. The magnitude of shear contact force increment is calculated by

$$ \Delta F^s = -K^s \cdot \Delta U^s $$
where $K^s$ is the shear stiffness at the contact, and $\Delta U^s$ is the shear component of the contact displacement increment occurring over a time step of $\Delta t$. The new shear contact force is found by adding the shear contact force increment $\Delta F^s$ to the old shear contact force existing at the start of the time step:

$$F_{new}^s = F_{old}^s + \Delta F^s \leq \mu \cdot F^n \quad (1-15)$$

The new shear contact force should be checked to not be greater than the contact shear strength which is equal to $\mu \cdot F^n$, and $\mu$ is the friction coefficient at the contact.

After the normal and shear contact force are determined by Eqs. (1-13) and (1-15), they are added to the existing resultant force and moment on the two entities in contact.

### 1.5. Proposed Research Objectives

The objectives of the current research include:

1. Develop an appropriate micromechanical model (with PFC2D) to perform numerical simulations of the direct interface shear test. Determine parameters used in the discrete element model to provide realistic mechanical behavior by calibrating the model with laboratory interface shear test data;

2. Modify the model by incorporating particle rolling resistance. Verify the importance of particle rolling resistance by comparing the macroscopic stress-strain behavior to the lab test data;

3. Quantify strain localization and shear banding behavior using “saw-tooth” models with varying surface geometry by examining internal particle-level state variables such as particle positions, velocities, displacements and calculating shear strain distributions inside the shear box. Determine the microscopic origins of macroscopic interphase deformation and strength behavior, and the stress-dilatancy relationships;

4. Perform parametric studies to quantify the effects of grain to surface relative geometry, grain size distribution and particle to surface friction coefficient on the peak strength ratios of the interphase system;

5. Formulate a strength criterion for the model interphase system based on the results of the available laboratory test data and numerical parametric studies.

To achieve these objectives, we conducted DEM simulations of interface direct shear test in a systematic manner such that the effects of relative particle to surface geometry can be
quantified. Simulation results have been used to extend a relatively large experimental data set conducted on actual interphase systems similar to those used in the simulations.

1.6. **Dissertation Organization**

This dissertation reports the extensive numerical simulation program conducted to explore the physical principles underlying the interphase behavior and develop a practical failure criterion accounting for surface and material properties. The dissertation is organized as follows:

Chapter 2 describes the development of DEM model of interface shear box test through determination of multiple variables and incorporation of particle rolling resistance into the model, which is necessary for the realistic simulation of macro and micro mechanical interphase behavior. Calibration of the model is performed by comparing the model behavior with the laboratory data.

Chapter 3 investigates the micromechanical behavior of interphase soils by studying microscopic quantities extracted from DEM simulations and analyzes the influential factors of shear banding behavior. Effects of surface geometry on strain localization are presented.

Chapter 4 presents a theoretical framework of discrete-continuum analysis of granular media based on shear-induced anisotropy and homogenization theory. The framework is applied in a direct shear simulation to demonstrate how the discrete data can be used to interpret the macromechanical behavior in a continuum sense. New constitutive relationships considering the effects of non-coaxiality and non-horizontal zero extension direction are also presented.

Chapter 5 explores the physical principles governing the particulate-solid interaction and quantifies the effects of relative particle to surface geometry, particle size distribution and particle to surface friction coefficient on interphase strength.

Chapter 6 presents a practical failure criterion for particulate-solid interphases based on particle to surface contact. The criterion is validated using laboratory interface shear test data. A Fortran program is complied to put the failure criterion into practical use.

Chapter 7 provides a discussion of the results and conclusions.

Three appendixes which are referenced throughout the dissertation are attached.
Notation

*The following symbols are used in this chapter:*

- $A$, $B$ = constants related to minerals of sand and type of steel
- $E$ = efficiency parameter
- $F$ = resultant force vector acting on a particle
- $\vec{F}$ = contact force vector
- $\vec{F}''$ = contact normal force vector
- $\vec{F}'$ = contact shear force vector
- $g$ = body force acceleration vector
- $h$ = hardening modulus
- $I$ = moment of inertia of a particle
- $\text{JCS} = \text{Joint Wall Compressive Strength}$
- $\text{JRC} = \text{Joint Roughness Coefficient}$
- $K''$ = contact normal stiffness
- $K'$ = contact shear stiffness
- $m$ = total mass of a particle
- $M$ = moment vector acting on a particle
- $R$ = particle radius
- $\bar{R}$ = modified roundness parameter of particles
- $R_n$ = normalized roughness parameter
- $\text{SRP} = \text{stationary roughness parameter}$
- $U''$ = overlap between two entities (ball-ball or ball-wall) at the contact
- $x$ = particle position vector
- $\dot{x}$ = particle velocity vector
- $\ddot{x}$ = particle acceleration vector
- $\delta$ = effective stress interface friction angle (degrees)
- $\Delta t$ = time step
- $\Delta U'$ = shear component of the contact displacement increment occurring over a time step of $\Delta t$
\( \phi \) = effective stress friction angle of granular soil (degrees)
\( \phi_p \) = maximum mobilized angle of friction (plane strain friction angle)
\( \phi_r \) = residual friction angle
\( \eta \) = angle between the orientation of shear band and the major principal stress direction
\( \mu \) = friction coefficient at the contact
\( \mu_y \) = sand-steel interface friction
\( \nu \) = dilation angle
\( \sigma_i \) = major principal stress
\( \sigma_n \) = normal stress
\( \tau_{\text{max}} \) = maximum shear stress
\( \omega_i \) = particle angular velocity vector
\( \omega_i \) = particle angular acceleration vector
\( \psi_p \) = peak dilation angle

References
Bardet, J. P., and Huang, Q (1993), “Rotational Stiffness of Cylindrical Particle Contacts,”


Model for Interfaces: Parameter Values and Model Performance for the Contact between Concrete and Coarse Sand,” EREDICTL TR-00-7, US Army Corps of Engineers.


Figure 1.1. The interphase region.
Figure 1.2. Calculation cycle in DEM.