Tri-axial deformation characteristics of Si-based particulate assemblies: a comparative study using DEM and atomistic simulations

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Abstract

In this paper, we investigate the macroscopic and micromechnical behavior of Si based particulate systems subjected to tri-axial compression loading using the Discrete Element Method (DEM). We considered four types of Si based three-dimensional particulate assemblies: Si, SiC, Si_3N_4 and SiO_2. The evolution of macroscopic mean strength of the assemblies and microscopic sliding characteristics of the assemblies are presented here. For the case of Si assembly, we compare the mean strength predicted from the current DEM simulations with the results obtained from Molecular Dynamics (MD) simulations reported by Mylvaganam and Zha [1] and a good qualitative agreement is obtained between the DEM and MD simulations at small strains. However, at large strains, the mean strength predicted from MD simulations does not scale-up with the DEM results. This discrepancy could be due to that MD simulations are only valid for particle contacts, which are independent of one another. They do not consider the inherent 'discrete' nature of particulates and induced anisotropy at bulk scale. The behavior of particulate assemblies at macroscopic scale strongly depends on the inherent discrete nature of the particles, their single-particle properties and induced anisotropy during mechanical loading.

Keywords: Tri-axial compression; Granular materials; Powder mechanics; DEM; MD simulations

1. Introduction

Silicon based particles are an important part of several engineering applications of technological importance. They can be used in many biological, optical, mechanical and electronic applications, offering significant advantages over existing technologies. The application of computer simulations for the design and optimization of powder processing is now becoming a more widely employed procedure. An optimum power process design would require a clear understanding on the macroscopic and internal behaviour of particulate materials at different loading conditions and length scales.

At first, we investigate the micromechanical compaction characteristics of selected Si-based particulate materials using DEM. The particulate materials were subjected to tri-axial compression loading ($\sigma_1 = \sigma_2 = \sigma_3 = \sigma$). We considered four different cases of Si-based three-dimensional particulate assemblies: Si, SiO_2, Si_3N_4 and SiC, in poly-dispersed phase. At the second stage, we perform a comparative study for the mean strength developed in Si assembly subjected to tri-axial compression using DEM and MD simulations.

2. Macroscopic and micromechnical characteristics

In particulate materials, the transmission of force occurs only through the inter-particle contacts, but the nature of contact force distribution is highly sensitive to the local arrangement of the particles and their properties at single particle level [e.g. 2,3,4,5]. Recent studies show a strong correlation between the macroscopic strength characteristics and the fabric anisotropy of force transmission pathways in particulate materials under mechanical loading [6,7,8]. The macroscopic behaviour of the assemblies depends on the collective behaviour of particle contacts under mechanical loading.

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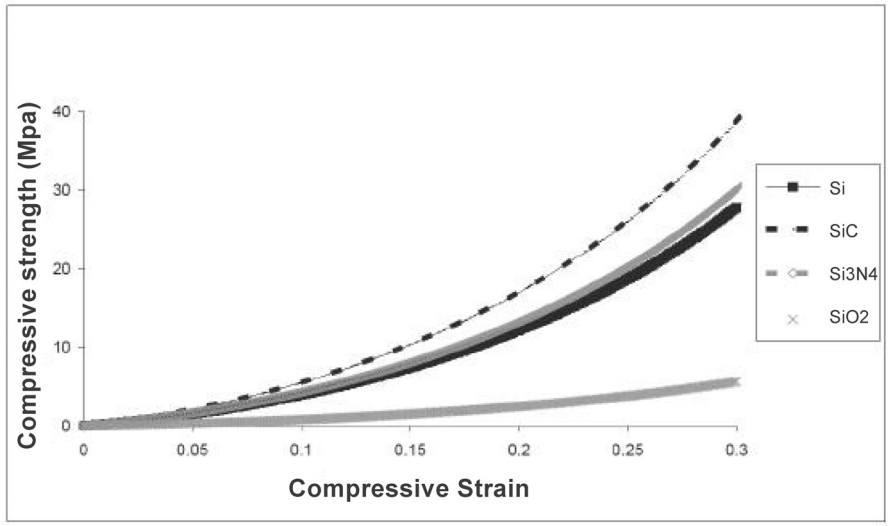

Fig. 1. Compressive strain vs compressive strength.

2.1. Simulations and results

In DEM, the interaction between contiguous particles are modeled as dynamic process and the time evolution of the particles is advanced using and explicit finite difference scheme [9]. A simple force mechanism was employed between contacting particles: linear normal (k_n) and tangential (k_t) spring stiffnesses were assigned. Slipping between particles would occur whenever the contact friction coefficient exceeds the specified value. The input parameters to the DEM modelling depend on the type of material under study [10]. Inter particle friction coefficient used for SiC was 0.78 and friction coefficient of 0.2 was used for Si, Si_3N_4 and SiO_2 particles. The normal spring stiffness is obtained from the normal spring stiffness equation of Hertzian springs, which is non-linear as:

$$K_n = 2E_{eq}\sqrt{R_{eq}\delta} \quad (1)$$

in which, E_{eq} is the equivalent Young's modulus, R_{eq} is the equivalent radius and δ is the indentation depth, calculated at $\delta^{max}/2$. The normal spring stiffness (k_n) used for SiO_2, Si, Si_3N_4 and SiC assemblies are 3500, 17,200, 18,600 and 24,000 kN/m respectively. All the assemblies were having the same value of stiffness ratio k_t/k_n equal to 0.9. Silicon-based particle assemblies studied here had identical initial packing fraction, and the shape of the particles was spherical. The assemblies each contained about 8000 particles with dense packing (packing fraction 0.645). Particles in each assembly ranged from between 0.5 and 1.35 of the mean size. The particle assemblies were initially random, isotropic and homogenous. During tri-axial compression, equal amount of axial strain was applied along the three axes in small increments of 1×10^{-6}, and several relaxation steps were performed within each increment.

Although we conducted a detailed investigation on several macroscopic and micromechnical features of the assemblies under mechanical loading, we present only selective results here. Figure 1 shows the variations of compressive strength (principal compressive stress) versus axial (compressive) strain. The compressive strength of the assemblies increases as a non-linear function of the compressive strain. It is an evident that the compressive strength of the Si-based assemblies significantly depends on the single particle properties of the assemblies. For the systems under study, SiC system presented the highest value of compressive strength while SiO_2 assembly presented the lowest value. The compressive strength of Si and Si_3N_4 assemblies were fairly identical. In general, the macroscopic compressive strength of the assemblies was proportional to the normal spring stiffness of the assemblies.

Figure 2 shows the proportion of sliding contacts (ratio between the number of contacts sliding and the total number of contacts) during compression. Except for SiC, all the assemblies presented a decreasing trend in proportion of sliding contacts as the compression progressed. Beyond a strain level of about 0.15, the sliding of the contacts in the assemblies ceased and beyond this strain level, the systems seem to have attained stable network of contacts to bear further compressive strength. However, the proportion of sliding of contacts for the SiC assembly was nearly negligible as SiC particles present a significantly higher value of inter-particle friction. The energy dissipated due to sliding of the contacts (per unit stiffness of the

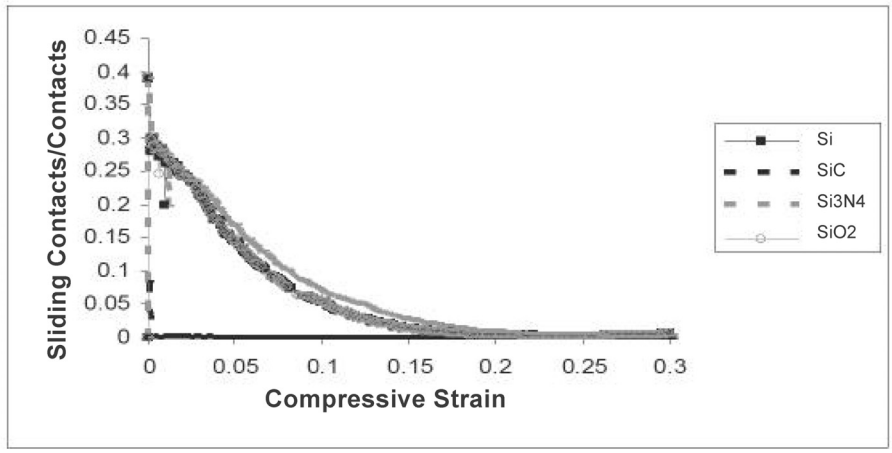

Fig. 2. Compressive strain vs proportion of sliding contacts.

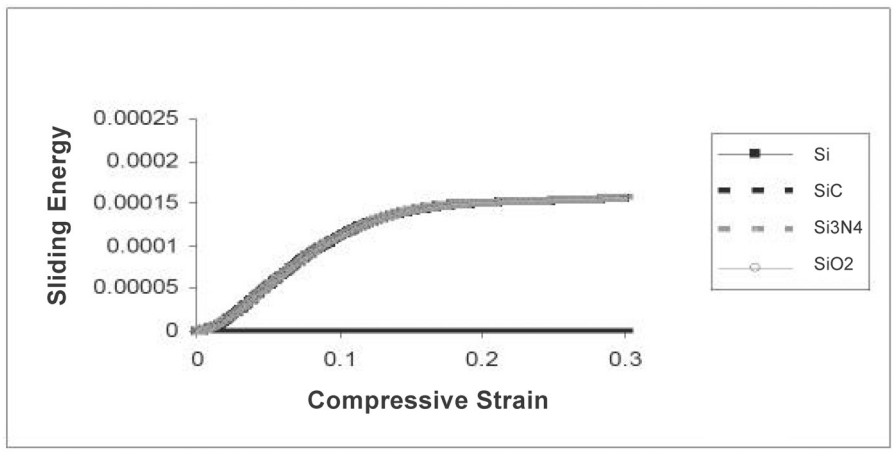

Fig. 3. Compressive strain vs energy dissipated due to the sliding.

particles) is presented in Figure 3. This further confirms that the SiC system behaved nearly like a solid block with no energy spent on sliding the contacts under mechanical loading. From a structural viewpoint, particle beds are composed of mutually contacting solid particles, or structural units. The existence of friction restricts the freedom of motion of the individual particles, and thus, conditions the strength and the rigidity of the bed. Due to the comparatively low strength of the friction bonds between the particles in systems other than SiC considered here, the structure of the particle bed changes, i.e. irreversible deformations take place even at low values of stress.

3. Comparison of mean strength predicted between DEM and atomistic (MD) simulations

In this section, we investigate the extent to which the mean strength predicted for materials at atomistic scale (for example, using MD simulations) differ from predictions using DEM at particulate level, qualitatively. For this, we performed DEM simulations for the tri-axial compressive strength of three dimensional Si assembly consisting about 8000 spherical particles (mono-dispersed phase) under periodic boundary conditions. We compared the results with predictions based on MD simulations for Si system subjected to tri-axial loading, reported recently by Mylvaganam and Zhang [1]. The atomistic simulation considered a cubic assembly of 34,353 silicon atoms (mono crystal) and a three-body Tersoff inter-atomic potential was assigned to

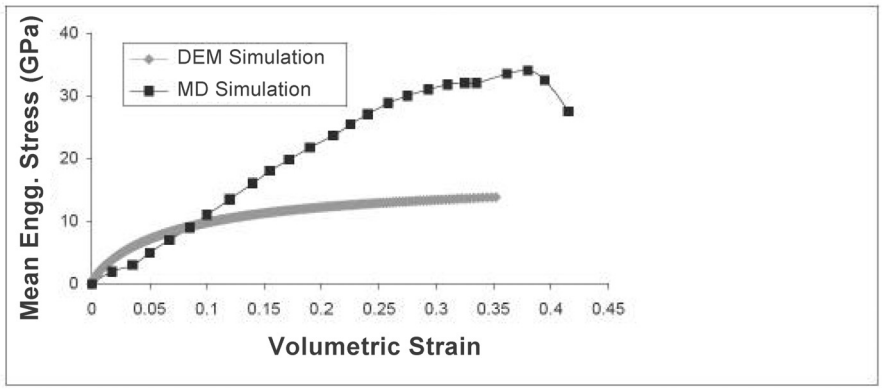

Fig. 4. Mean strength of Si assembly during tri-axial compression.

account the directionality of bonding between the Si-Si interactions. The system was subjected to tri-axial compression and the normal stresses were calculated by summing forces across the outermost planes of the assembly, divided by their cross-sectional area. Figure 4 shows the mean engineering stress, plotted against the volumetric strain during loading. For strain levels up to about 0.1, the predictions between DEM and MD simulations agreed fairly well, at least qualitatively. However, beyond this strain level, the predictions differed significantly. At high strain levels, the mean strength predicted from atomistic simulations were about three times higher than DEM results. This trend agrees with the general perception that the strength of particle assemblies predicted from MD simulation does not scale-up for particulate assemblies (as predicted, using the DEM simulation). MD simulations are only valid for particle contacts, which are independent of one another. In large particulate assemblies the macroscopic strength characteristics would depend on the discreteness of the particulates and several non-homogenous distributions of parameters (such as non-homogenous force distribution, fabric alignment and local voidage, etc.).

4. Conclusions

We conducted a comparative study for the macroscopic and microscopic deformation of selected Si-based particulate systems under tri-axial loading using DEM simulations. The macroscopic and microscopic behaviour of assemblies strongly depend on the individual properties of the particles. The comparison of results between DEM and MD simulations for the mean strength of the Si particulate assembly present a qualitatively good comparison at low strain levels, but does not scale up at high strain levels. The macroscopic behaviour of the particulate assemblies depends on the collective behaviour of inter-particle contacts under mechanical loading.

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