Quantifying microstructure and fabric chains in granular materials through X-ray CT experiments

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Abstract. The evolution of the contact network in granular materials plays a key role in stress transmission. This study investigates the evolution of fabric chains—pathways formed by maximally aligned inter-particle contacts—in an assembly of quartz particles subjected to one-dimensional compression. High-resolution synchrotron-based XRCT imaging captures the 3D microstructure at multiple loading stages. Fabric chains are extracted by iteratively tracking maximally aligned neighbors, and their network characteristics are quantified using fabric chain length, tortuosity coefficient, and participation index. The results reveal that chain lengths initially increase with loading, indicating the formation of more extensive pathways due to particle rearrangement. The tortuosity coefficient rises, reflecting the increasing curvature of chains as the contact network becomes more tortuous. The participation index highlights the degree of chain merging, with higher values indicating particles participating in multiple overlapping chains, signifying the emergence of an interconnected fabric chain network. These findings offer insights into the evolution of microstructure in granular materials under compressive loading conditions.

1 Introduction

Granular materials exhibit complex mechanical response due to their discrete nature. Among other macroscale influences, the mechanical response of granular materials is controlled by the spatial arrangement of the particles (i.e., the orientation and spatial distribution of particles, inter-particle contacts, and voids). When a granular ensemble is sheared, the deformation stems from the particles rearranging - in other words, the fabric evolves during deformation. Within these evolving network of particles, force propagation primarily occurs through inter-particle frictional contacts. This is often explained as a network of force-bearing structures, often referred to as "force chains"[1]. This network of frictional inter-particle contacts is considered the primary conduit for stress transmission. Direct measurement of inter-granular stresses is challenging, requiring high-fidelity experimental techniques such as photoelasticity[2] or a combination of 3D X-ray diffraction and X-ray computed tomography (XRCT) imaging[3].

Recent studies on frictional granular materials suggest that metrics derived from contact networks and adjacency information serve as effective indicators for analyzing force transmission within granular assemblies [4, 5]. "Fabric chains" are defined as paths formed by maximally aligned inter-particle contacts, and they offer a complementary perspective to stress transmission pathways. We conjecture that these fabric chains correspond to regions of maximum stiffness, making them potential indicators of preferred load transfer directions [6]. In this study, we compute quantitative metrics related to the evolution of fabric chains. When analyzed alongside particle-scale features such as packing rearrangement and breakage mechanisms, these metrics offer meaningful insights into the evolving microstructural signatures of the granular assembly under uniaxial loading. The fabric chain length represents the number of particles in the chain, and the tortuosity coefficient captures the curvature of these chains. The participation index is a measure of the degree of merging and connectivity within the contact network, and is a measure of the interconnectivity of the network of fabric chains [7].

The objective of this work is to characterize the evolution of fabric chains in a confined quartz particle assembly under uniaxial compression using in-situ high-resolution XRCT imaging. The fabric chains are computed by tracking maximally aligned contacts, and their evolution is characterized by measures such as chain length, tortuosity, and participation index. Particle breakage, contact network evolution, and particle rearrangement in granular materials are also discussed.

2 Experimental details

The sample used in this study consists of single-crystal angular quartz particles obtained by ball milling hydrothermally grown single-crystal α-quartz particles (Sawyer Technical Materials, LLC). Approximately 2000 sieved particles, with sizes ranging from 150 μm to 180 μm, are poured into an aluminum cylinder with an inner diameter of 1.80 mm and a height of 3.6 mm, forming an ensemble

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with an initial packing fraction (ϕ) of 0.58. The cylinder is placed on a bottom platen of 1.8 mm diameter. The confined sample is uniaxially compressed using the Rotation and Axial Motion Stage (RAMS) at the Cornell High Energy Synchrotron Source (CHESS). The loading assembly is presented in Fig. 1a. The sample is loaded in five stages, and at each stage of loading, tomography scans are made. The axial strain value for the sample during the final stage of loading is 4.33%. The stress-strain curve for the sample is shown in Fig. 1c. The images captured during the tomography scans are analysed. The XRCT data analysis begins with the segmentation of the data where the individual particles are uniquely labeled. The rendering of the segmented 3D sample is presented in Fig. 1b.

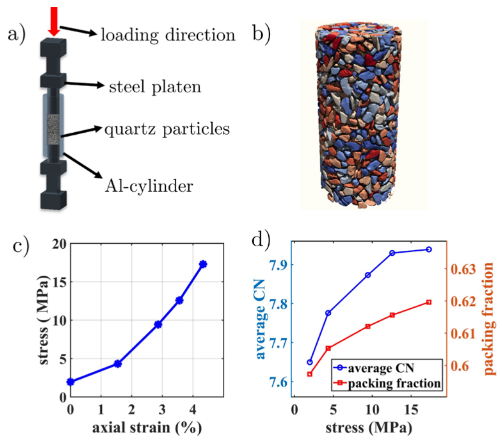

Figure 1. (a) Schematic of the loading assembly. (b) 3D rendering of the segmented cylindrical quartz specimen (c) stress-strain curve d) evolution of packing fraction and average coordination number (CN) as loading progresses.

3 Quantitative analysis of fabric chains

The segmentation process delineates the particle morphology and, in effect, identifies the inter-particle contacts, centroids of the particles, and volume of particles. In addition, the principal axes of orientation of the particles and the orientation of contacts are also obtained by performing principal component analysis (PCA). A micro-fabric tensor is computed for each particle and is given by:

$$F_{\text{micro}} = \frac{1}{N_c^p} \sum_{i=1}^{N_c^p} \vec{n}_i \otimes \vec{n}_i$$

where N_c^p is the number of bonds passing through the pth particle, and $\vec{n}_i$ is the ith contact normal of the particle.The major principal eigenvector of this tensor indicates the direction of the highest contact density for a given particle. The contact normals, the principal vector of the micro-fabric tensor (F_{micro}), and the spatial coordinates of the particle centroids are used to construct fabric chains.
The fabric chain is constructed by seeding a particle from the top layer of the specimen and iteratively identifying its maximally aligned neighbors. The scalar dot product of the branch vector (vector joining the centers of the seed & neighbor particle) with the major eigenvector of F_{micro} of the seed particle is computed. The neighboring particle yielding the maximum dot product is identified as the maximally aligned neighbor. This neighboring particle then becomes the new seed, and the process is repeated iteratively until no further maximally aligned neighbors are found, thereby completing the fabric chain. The fabric chains are propagated vertically downward, since the confined sample is compressed uniaxially in the downward direction. At each step in constructing the fabric chain, only those neighboring particles are considered whose centroids lie below the current seed particle. Hence, the fabric chain terminates when a particle has no neighbors with centroids located below it—that is, when the bottom boundary of the specimen is reached.

When all particles in the top layer are seeded and the corresponding fabric chains are evaluated, we observe that many chains merge as they propagate downward, resulting in fewer chains percolating all the way to the bottom. In the first loading stage, only 10% of the seeded particles form chains that reach the bottom, indicating that most chains merge along the way. Fig. 2a presents a representative fabric chain, and Fig. 2b highlights the merging chains. To characterize the behavior and evolution of

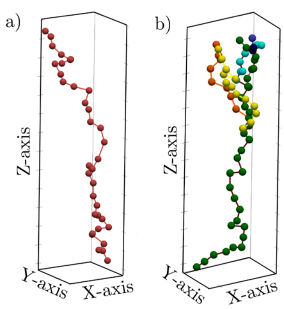

Figure 2. (a) Representative single fabric chain, which is obtained by seeding a top layer particle. (b) Different fabric chains that emerge from the top layer merge into a single chain that percolates through the bottom of the sample.

fabric chains, we quantify their properties using three key measures: fabric chain length, tortuosity coefficient, and participation index. A detailed description of each measure is presented below.

3.1 Fabric Chain Length

Fabric chain length refers to the number of particles in each chain.

3.2 Tortuosity Coefficient

The tortuosity coefficient captures the geometric structure of fabric chains by measuring their curvature. It is defined as the ratio of the sum of individual link lengths (branch vectors) to the magnitude of the end-to-end vector connecting the first and last particle in the chain. The tortuosity coefficient is computed using the following expression:

$$\text{Tortuosity coefficient} = \frac{\sum_{i=1}^{n} L_i}{L} = \frac{\sum_{i=1}^{n} \|(x,y,z)_{i+1} - (x,y,z)_i\|}{\|(x,y,z)_n - (x,y,z)_1\|} \quad (1)$$

where n is the number of particles in the chain (chain length), [x,y,z] represents the position of particle i, L_i represents the magnitude of each branch vector, also called link length, and L is the magnitude of the end-to-end vector. A model chain, along with its constituent link lengths and the end-to-end vector, is shown in Fig.3a. A tortuosity coefficient of unity indicates a perfectly linear chain, while more curved (tortuous) chains exhibit tortuosity coefficients greater than one. Fig.3b and Fig. 3c display two representative fabric chains: one with a lower tortuosity coefficient (more linear) and the other with a higher tortuosity coefficient (more curved), respectively.

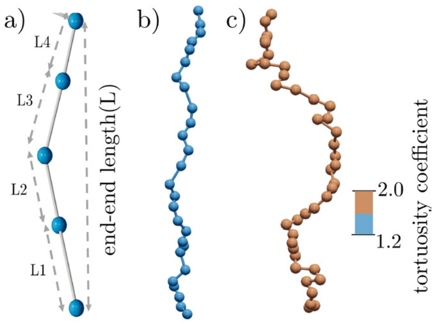

Figure 3. (a) A model chain showing link lengths and end-to-end length (b) fabric chain with a lower value of tortuosity coefficient (c) fabric chain with higher value of tortuosity coefficient

3.3 Participation Index

The participation index quantifies the degree of merging among fabric chains by measuring the likelihood of individual particles being part of multiple chains.

In the absence of merging, when seeding about a hundred particles at the top of the specimen, around a hundred distinct fabric chains would typically emerge and percolate through the sample. However, in the sample of quartz particles, merging occurs, resulting in fewer chains propagating to the bottom. The participation index is defined for each particle in the chain using the following expression:

$$\text{Participation index (\%)} = \frac{\sum_{i=1}^{N} p_i}{N} \times 100 \qquad (2)$$

where N is the total number of chains seeded and

$$p_i = \begin{cases} 1, & \text{if the particle is part of } i^{th} \text{ chain.} \\ 0, & \text{otherwise.} \end{cases} \qquad (3)$$

The participation index (expressed as a percentage) reflects the degree of chain merging. A lower participation index indicates particles that belong to distinct, non-merged chains. A higher participation index signifies particles that are part of multiple merged chains. While fabric chain length and tortuosity coefficient are defined on a chain; the participation index is defined for each particle in the chain.

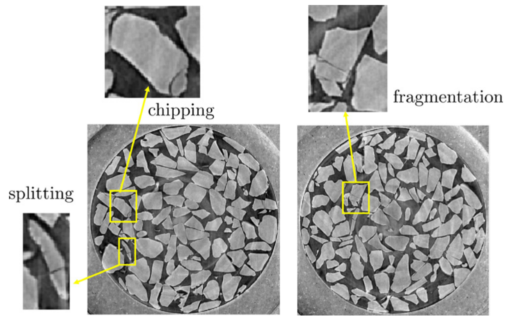

Figure 4. Cross-sectional XRCT images showing chipping, splitting, and fragmentation of particles

4 Results and discussions

During uniaxial loading of the confined quartz sample, particle breakage is observed. At the initial stage of loading, breakage predominantly occurs through chipping as small fragments detach from particle edges, causing minor surface changes. With continued loading, particles begin to split into multiple fragments. With significant straining, extensive fragmentation of particles occurs, breaking particles into many smaller pieces. Fig.4 presents the chipping, splitting, and extensive fragmentation of particles. Fig.5a shows the initial and final grain size distribution curves. The curve shifts leftwards, indicating an increase in the cumulative density of smaller particles due to breakage. Fig.5b shows the number of particles segmented. With progressive loading, the packing fraction of the ensemble follows an increasing trend as shown in Fig.1d. We also observe that with continued loading, the ensemble progresses towards a packing where larger particles are surrounded and cushioned by many small particles. The average coordination number shows an increasing trend (from 7.6 to 7.9). During the final stages of loading, numerous small fragments fill the voids and surround the larger particles, increasing their coordination numbers; however, the fragments themselves have low coordination, keeping the overall average relatively constant.

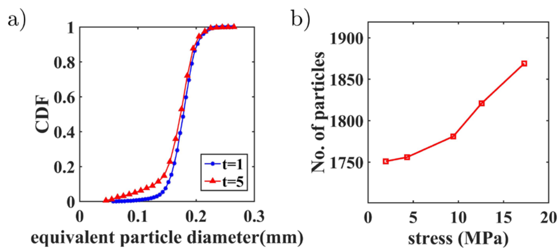

Figure 5. a) Cumulative distribution function (CDF) of particle sizes for initial and final loading stages. b) Number of particles segmented for various loading stages.

The evolution of mean fabric chain length is presented in Fig.6a. During the second loading stage, where chipping-dominated breakage occurs, the mean fabric chain length slightly decreases from 29 to 28 particles per chain. In the third and fourth stages, characterized by splitting-dominated breakage, the mean chain length increases as newly formed fragments also participate in the network, creating chains with more particles. It is inter-

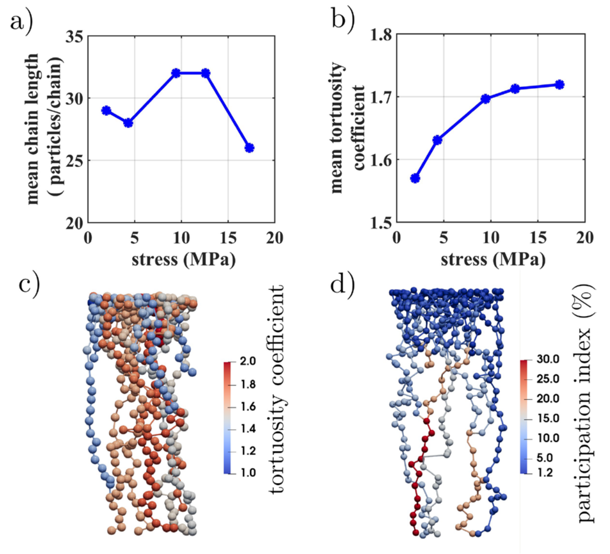

Figure 6. (a) Evolution of mean fabric chain length with stress. (b) evolution of mean tortuosity coefficient. (c) fabric chains from the initial loading stage, colored based on their tortuosity values. (d) fabric chains with participation index of particles.

esting to note that during the final stage, despite increased fragmentation generating a larger number of particles in the ensemble, it leads to a sharp decrease in chain length. Since the sample height also decreases due to compaction, fewer particles are needed to span from top to bottom, so the chain length decreases. Chain length is affected by both breakage and height reduction due to compaction.

The mean tortuosity coefficient exhibits a progressive increase with loading, indicating that the fabric chains become increasingly tortuous, as shown in Fig.6b. The process of breakage changes the morphology of particles, which in turn affects the contact network and particle neighborhood. As a result, the set of maximally aligned neighbors changes significantly. At the same time, rearrangement during loading changes the local contact directions and fabric orientation. Hence, the progressive particle breakage and rearrangement concomitantly make the fabric chains more tortuous. In addition, we also plot a scatter plot of the tortuosity coefficients to visualize the spatial variations in the tortuosity of chains as seen in Fig.6c. We observe that the chains seeded near the periphery of the cylinder are less tortuous due to the boundary constraints, while the particles seeded near the middle have more tortuous chains.

The participation index, while attributed to single particles, is a measure of the degree of coalescence of the fabric chains and, in effect, an indicator of the formation of strong, interconnected networks within the granular assembly. The scatter plot of the participation index shown in Fig.6d reveals that some particles exhibit values around 20–30%, indicating that they are part of multiple fabric chains. These particles effectively serve as bridging nodes, connecting several chains.

5 Summary

This study investigates the evolution of fabric chains and microstructural features in a confined assembly of uncemented quartz particles subjected to uniaxial compression using synchrotron XRCT imaging. As loading progresses, the material exhibits increasing particle breakage—ranging from chipping and splitting to fragmentation—which contributes to the reorganization of the contact network and alters the fabric chain configurations. The average coordination number increases with progressive loading but saturates at the final stage of loading due to extensive fragmentation. Results from fabric chains show that with increasing breakage and densification, fabric chains exhibit greater tortuosity, particularly during the final loading stage when fragmentation becomes dominant. The participation index reveals that chain merging occurs, where few particles become part of multiple chains, forming a strong interconnected network. Further studies using Discrete Element Method (DEM) simulations are currently underway to assess the extent to which fabric chains can serve as reliable surrogates for force chains.

6 Acknowledgments

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