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Force chains behaviours of Al-PTFE granular composite under elevated strain rates

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Abstract. This study proposed a simulation method to characterize the influence of mesostructural force chains on the dynamic response of aluminum-polytetrafluoroethylene(Al-PTFE) granular composite under strain-controlled compression. The model was developed followed real Al particle size distribution. Based on the analysis of force chains, the global deformation, mechanical strength, and failure behaviour for the material were investigated. The results indicate that, with the increasing of strain rates, the yield strength of the Al-PTFE increases, but it is inversely proportional to the ultimate compressive strength. The stability of force chains accounts for the phenomenon that a higher strength is observed in the material under lower strain-rate impact. Particularly, an angle of force transmission is introduced to quantitatively explain the evolution mechanism of force chains.

Keywords: Al-PTFE; Mesoscale model; Mechanical response; Force chains; Strain rates

1. Introduction

Reactive materials (RMs) show great advantages in both military and engineering applications due to their dual properties of mechanical and energetic use [1]. Al-PTFE granular composite as the typical RMs is generally prepared by homogeneously mixing, cold pressing, and hot sintering of metal powders mixed into a fluoropolymer binder [2]. The shock sensitivity and the rate of energy releasing are tailored by chosen strain rates to accommodate low-strength samples, and the deformation magnitude can be modified. Moreover, one of the distinguishing features for such sub-stable material is that the mechanical response and even exothermic reaction driven by bulk disintegration have been ascribed to the behaviors of agglomerated metal granules known as force chains.

Force chains are major contributors to identify and quantitatively characterize the underpinning mechanisms for dense, cohesionless granular assemblies like rock or soil matter [3], and such material are of obvious strain rate effect. However, few research works on force transmission in fluoropolymer-based metal composite as highly complicated interparticle contacts and laterally cohesive supporting from matrix, that must be account for in order to gauge the strength enhancement performance of the material under elevated strain rates. Furthermore, research methods like theoretical or experimental analyses are confined to low visualized description for local deformation mechanisms and force chains changes, especially in resolving contact forces problems at temporal and spatial scales. For these two reasons, efforts devoted to developing mesoscale model to simulate the impact process of the RMs, and introducing force chains to elucidate unusual mechanical behaviors. Herbold [4] illustrated dynamic properties of Al-W-PTFE granular composites under shock loading by means of numerical modeling at grain level and force chains formation mechanisms. Chen [5] clarified the relationship between the contact forces and force chains in granular materials using digital image correlation. As a result, although there are many simulation methods on force chains researches, generally agreed-upon quantitative calculations to reveal the connection between bulking deformation and grains motions of the Al-PTFE material under dynamic loading requires further exploration.

This paper proposes a numerical method based on real microstructural characteristics to study the dynamic compressive mechanical behavior of Al-PTFE granular composite. The evolution process of force chains including activation, destruction and rearrangement are explored to reveal

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the strength and failure mechanism of the material under elevated strain rates compression. Moreover, an angle of contact forces transmission among force chains is particularly introduced and quantitatively calculated to explain the effects of force chains stability on the dynamic fracture process.

2. Simulation Method

2.1 Numerical Model

In this investigation simulations are performed in composites consisting of 26.5wt% Al (air atomized Al powder, type FLPA250) and 73.5 wt% PTFE (Dupont) but variation in Al sizes and strain-controlled compression conditions. Specifically, the effect of microvoids of the Al-PTFE composite on the mechanical properties is not considered in the modelling because of the PTFE material produced by a melting and recrystallizing process. Thus, the model uses a randomly distributed Al particles with circular shape packing in the compacted PTFE matrix to solve dynamic compaction behavior of the composite. Based on the statistics analysis, the probability density of diameter distribution for real Al particles are obtained as shown in the Figure 1, and a normal distribution with mean μd = 119 μm and standard deviation σd = 36 μm is derived to depict Al particles generations. However, the spatial arrangements of Al particles should meet the requirements of both fully random packing in the domain and there is no particles overlapping.

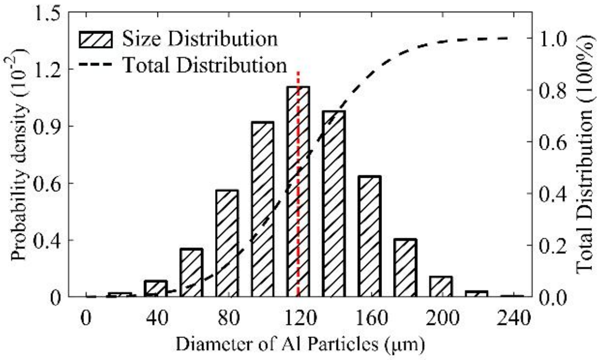

Figure 1. Diameter distribution of Al particles.

A two-dimensional model in the frame of the Lagrange approach covers an area of 3000 μm × 2000 μm as shown in Figure 2. Finite element analysis simulating a strain-controlled compressive process of drop-weight tests in real time is performed with ANSYS software. Additionally, the grid quality and solution efficiency is improved by using self-adaptive meshing, and the minimum grid length and area size of Al and PTFE material are 10 μm and 40 μm2. There are two modes of boundary conditions implemented to the model: (i) loading conditions with impact velocities of 2.5 m/s, 3.5 m/s, 5.0 m/s, and 7.5 m/s are imposed on the upper nodes to calculate stress and strain distribution, and the corresponding strain rates are approximately 1250 s-1, 1750 s-1, 2500 s-1, and 3750 s-1, respectively; and (ii) the bottom nodes are fixed in the y-direction to constrain the movement during compression. Particularly, the effectiveness of the model is proved by relevant experiments and the consistency of the model is also well verified in our previous work [6].

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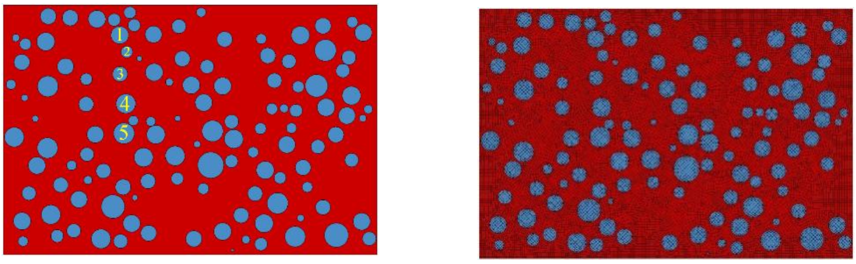

(a) Geometric model (b) Grid model

Figure 2. Mesoscale simulation model.

2.2 Material Model

The material models used for describing the physical and mechanical properties of Al and PTFE material under dynamic loading are Johnson-Cook (JC) strength model and Gruneisen equation of state (EOS). In the JC model, the equivalent plastic stress σ is written as:

$$\sigma = [A + B(\bar{\varepsilon}^{p})^{n}](1 + C\ln\dot{\varepsilon}^{*})(1 - T^{*m}) \tag{1}$$

where $\bar{\varepsilon}^{p}$ is the effective plastic strain, $\dot{\varepsilon}^{*}$ is the normalized effective plastic strain rate, T^{*} is the homologous temperature, A, B, C , n, and m are constants.

The soft PTFE matrix should take the structure damage in to account, and the failure criterion is written as:

$$\varepsilon_{\mathrm{f}} = \left[D_1 + D_2\exp\left(D_3\sigma^{*}\right)\right]\left[1 + D_4\ln\dot{\varepsilon}^{*}\right]\left[1 + D_5T^{*}\right] \tag{2}$$

where D1 is obtained from dynamic experiment data, D2, D3, D4, and D5 are assigned a value of zero as initial approximation. The material properties of Al and PTFE used for simulation are listed in Table I and Table II [7].

Table 1. Relevant constants of JC model [7].

Material	ρ_0 (g/cm^3)	A (GPa)	B (GPa)	n	C	m	T_{melt}(K)
PTFE	PTFE	2.20	0.011	0.044	1.00	0.12	1.0
Al	Al	2.71	0.265	0.426	0.34	0.015	1.0

Table 2. Relevant constants of EOS [7].

Material	c_0 (cm/μs)	S_1	S_2	S_3	γ_0
PTFE	0.168	1.12	3.983	-5.797	0.59
Al	0.520	1.40	0.0	0.0	1.97

3. Results and Discussion

The engineering stress versus engineering strain curves of the Al-PTFE granular composite subjected to four different impact velocities are shown in Figure 3. The curves show that global failure strains of each sample are 0.705, 0.679, 0.506, and 0.363, and the corresponding ultimate compressive strengths are 77.2 MPa, 71.0 MPa, 56.9 MPa, and 51.2 MPa, respectively. Results demonstrate that the Al-PTFE shows typical elastic-plastic mechanical characteristics under shock loading. The yield strength of the material increases as the strain rate increases, but it is inversely proportional to the ultimate compressive strength. Noticeable differences are observed in their elastic and plastic properties, which are dominated by the behaviours of agglomerated metal particles, and that is so-called mesoscale granular force chains. The Von Mises effective stress and deformation distributions of the samples during shock compressive process are shown in the Figure 4, which makes a significant contribution to the underlying mechanisms.

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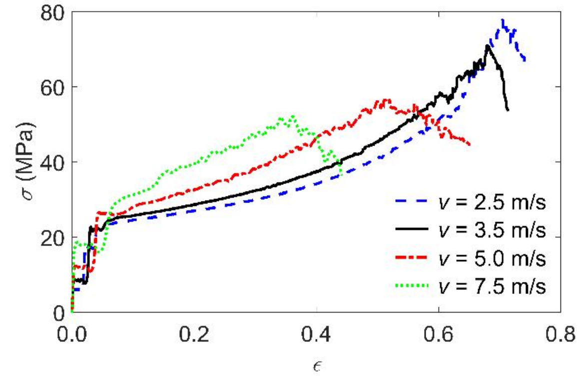

Figure 3. Stress-strain curves of the samples under elevated strain rates.

Three stages including nonlinear elastic deformation of the matrix, severe plastic deformation among particles and matrix, and surface crack in matrix following macrocracks propagation are described as dynamic response of the samples. The soft PTFE material mainly resists the impact loading in the primary stage, and the average stress rapidly increases with deformation continues. Elevated strain rates strengthen the yield strength to some extent, since the interacted squeeze between Al and PTFE material do not coincide with the bulk deformation spatially. Upon strain further increasing, features can be obtained from the comparison in the self-organization of metal particles. Several force chains are activated and interlinked across the samples from the top to the bottom. It demonstrates that the sample under lower strain rates is conductive to creating such skeletons to enhance the global strength, and this performance can also be explained from the stress increase shown in the Figure 3.

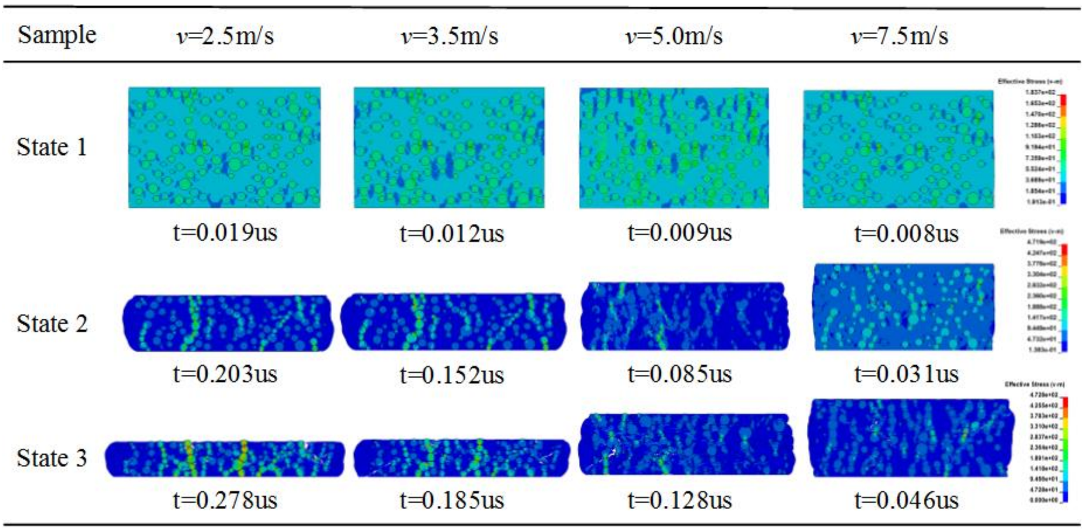

Figure 4. The effective stress distributions for the samples.

In contrast, when the impact velocity increases to 7.5 m/s, there are weaker friction among particles to provide a buildup for resisting further deformation, and the material shows more brittle mechanical properties. Force chains are created in the form of short clusters and these particle are found to be easily rearranged by shear forces, which resulting in localized strain accumulation and subsequent generation of the macrocracks. This suggests that the dependence of the critical failure strength should be sensitive to strain rates, and the formation and stability of force chains are an important mechanism affecting the strength behavior and macrocracks propagation. In this case, an angle of contact forces transmission among force chains α is introduced, and defined as the angle between normal direction of contacted surface for two particles among force chains and horizontal

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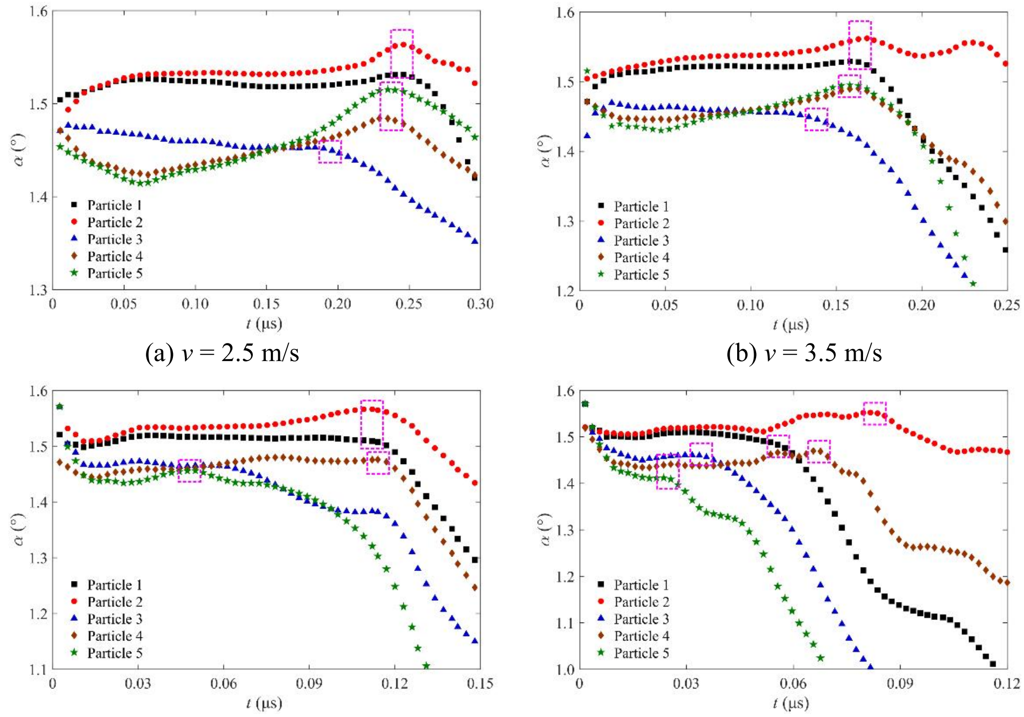
direction. Five particles each composed of a buckled force chains segment are quantitatively analyzed, and the location arrangements are shown in the Figure 2.



(a) v = 2.5 m/s (b) v = 3.5 m/s

(c) v = 5.0 m/s (d) v = 7.5 m/s

Figure 5. The variation of angle α changed with time.

The variation of angle α changed with time for such five particles are shown in the Figure 5, and particular attention is paid to the cracks and disintegration within such strong force chains of contacts. It is found that larger value of α accounts for the stability of force chains. With the increase of the α, the transition direction of contact forces among force chains particles are more close to the external loading direction. However, when there is abruptly changed in the slope of the α, which is referred as inflection points, it is a crucial signal of the cracks formation and possibly growth. This can be compared to the disintegration of the matrix due to unordered movement of spatial locations for Al particles shown in the Figure 4. When the α keeps decreasing, force chains begins to disintegrate and subsequently macrocracks propagate in the relatively weak matrix. The box in the Figure 5 is just where the force chains break. It demonstrates that the evolution of force chains crucially depends on elevated strain rates, and the sample under higher impact velocity are prone to be destroyed in the course of deformation and fracture.

4. Conclusion

It is demonstrated by simulation method that the effects of mesostructural force chains behaviors on the dynamic mechanical response of Al-PTFE granular composite under elevated strain rates compression. The major conclusions can be summarized as follows:

(1) With the increasing of strain rates, the yield strength of the Al-PTFE increases, but it is inversely proportional to the ultimate compressive strength.

(2) The stability of force chains affect the mechanical strength and macrocracks propagation. The sample under lower strain-rate compression is conductive to creating strong skeletons to enhance the global strength.

(3) Inflection points occurring on slope variation of the contact forces transmission is a crucial signal of the cracks generation in the matrix. Force chains disintegration and the fracture behavior are responsible for the sustained reduction in the angle.

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