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Simulation of Microscale Features Effect on Mechanical Properties of PTFE-Al Composites

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Abstract. The compression behavior of polytetrafluoroethylene (PTFE)–aluminum (Al) is studied by the means of the two-dimensional finite element analysis of mesoscale model containing a random dispersion of particles. The results show that for composite materials with a single particle size the strength of the material increases first and then decreases with the increase of the content of metal particles. When the particle content is high the strength of the material can be improved by a reasonable particle gradation. The influence of particle content and size on the strength of particle composites is obtained and theoretical analysis is carried out from the perspective of the formation and evolution of force chains.

1. Introduction

Reactive materials fragment combines kinetic energy damage with explosion damage which greatly improves the terminal damage effectiveness of the ammunition warhead[1-2]. The mixture of polytetrafluoroethylene (PTFE) and aluminum (Al) is a typical reactive material and the strength is important for the application of this type of material. The mechanical and chemical properties of PTFE-Al particle composites can be optimized from meso-structures such as particle content and particle size[3, 4]. High strength particles(like tungsten) are added to the reactive material in order to increase the strength of the material[7-10]. Studies have shown that component ratio and relative size relationship between different kinds of metal particles has its mechanical strength has a significant effect on the strength and energy release of the active material[5]. However, there is no systematic study on the optimum content of metal particles and the proportion of particles in size and the coupling relationship between the particle content and the size of the particles is often ignored.

In this paper, the effect of particle content and particle size on the material strength is studied by means of mesoscopic numerical simulation. The finite element model of random distribution of metal particles is established and the compression process of the particle composite is numerically simulated. Further, the influence mechanism of particle composition on the mechanical behavior of PTFE-Al particle composites is analyzed.

2. Simulation

2.1. Simulation Model

A mesoscale distribution model is developed to analysis of the relationship between the macroscopic strength of the particle composite and the microscopic characteristics (content and size) of the particle and the formation process of the force chain during compressed is observed. The following simplifications are made in the establishment of a finite element model with randomly distributed particles:



- (1) The shape of the particles is simplified to an ideal sphere (circular in two dimensions);
- (2) Regardless of the particle size distribution the same size particles are considered to be equal diameters;
- (3) The particle position (center) distribution satisfies the random uniform distribution in the space and the particles do not overlap and voids are not considered.

The finite element software ANSYS /LS-DYNA is used to establish a finite element model of the two-dimensional particle random distribution of particle composites. The ANSYS command stream files is written by APDL, which can be directly imported into ANSYS /LS-DYNA.

In order to investigate the effect of particle content and particle size on the mechanical properties of the active material. The mesoscopic models of four different Al content are used for numerical simulation. The sample parameters are listed in Table 1 where N_A is the number of the particles of Al. The Al particles diameter of sample below is 21 μm . The overall size of the model is $200\mu\text{m} \times 200\mu\text{m}$ and the falling speed of the upper substrate is always 1 m/s.

Table 1. Formulations and related parameters of reactive materials

Sample	N_A	Al(v%)	Density (g/cm ³)	Sample	N_A	Al(v%)	Density (g/cm ³)
1	25	21	2.26	3	52	45	2.39
2	42	36	2.34	4	61	53	2.44

2.2. Material Model

The Johnson-Cook material model is used for Al particles and PTFE. The Gruneisen equation of state was used to define the pressure in compression and tension. The Johnson-Cook strength model can be expressed as

$$\sigma_y = \left(A + B\varepsilon_p^N \right) \left[1 + C \ln \left(\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right) \right] \left[1 - \left(\frac{T - T_0}{T_m - T_0} \right)^m \right] \quad (1)$$

The material model used for PTFE is the Johnson-Cook with Failure, based on the equation

$$\varepsilon_f = \left[D_1 + D_2 \exp(D_3 \sigma^*) \right] \left[1 + D_4 \ln \dot{\varepsilon}^* \right] \left[1 + D_5 T^* \right] \quad (2)$$

Table 2. Constitutive model and equation of state material parameters

	PTFE	Al
Johnson-cook		
ρ	2.14×10^{-9}	2.7×10^{-9}
A	11	265
B	44	426
N	1	0.34
C	0.12	0.015
Gruneisen		
c0	1.7×10^6	5.4×10^6
s	1.12	1.34
γ_0	0.59	1.97

The PTFE sample considers the failure behavior taking $D1 = 0.4$, $D2$, $D3$, $D4$, and $D5$ are approximately set to zero. The Johnson-Cook material model without failure is used for aluminum particles. In addition the Gruneisen equation of state can be expressed as

$$P = \frac{\rho_0 c_0^2 \eta}{(1 - s \eta)} \left(1 - \frac{\gamma_0 \eta}{2}\right) + \gamma_0 \rho_0 E_m \quad (3)$$

The parameters under the unit system of mg-ms- μm in the Johnson-cook material model and the Gruneisen equation of state are listed in the table 2.

3. Results and Discussion

The deformation and effective stress contours of Al-PTFE with vary volume fractions of Al at different global strain are shown in Figure 1. In general, mechanical properties of granular composites are closely related to the formation and change of the mesoscopic force chain of the metal particles. When subjected to a compressive load, the particles are displaced as the matrix is compressed and gradually form a contact network thereby forming a strong chain of the supporting material. But the formation of the force chain means the concentration of local stress which would cause the matrix of the stress concentrated portion to be destroyed. And then, the composites begin to fail. The formation and distribution of the strong chain is significantly affected by the geometric distribution of the particles and the toughness of the matrix.

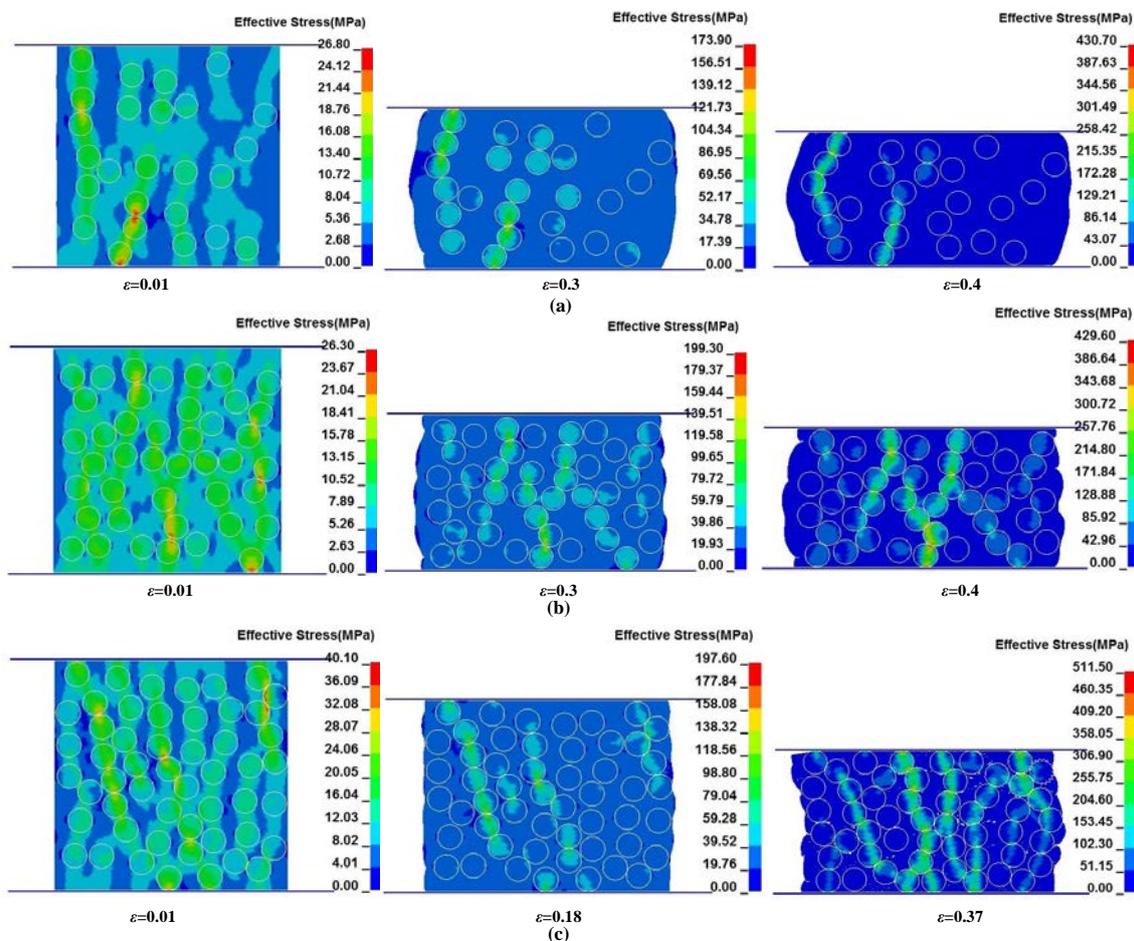


Figure 1. Contour of von Mises stress of PTFE-Al numerical sample with different Al content (a)Sample1 (b) Sample2 (c) Sample3

Both samples in figure 1 have formed force chain finally at different global strain. The contours of effective stress show great inhomogeneity of stress in granular composites. The force chains through whole sample form at different global strain. In the samples with more metal particle, force chains appear at a low global strain. There are two strong force chains formed in sample 1 at 0.4 global strain, while three chains in sample 2 at the same global strain. It means that increasing the particle content can get more force chains. For sample 3, four force chains appear at 0.37 global.

The strength of the metal particles in the active material is much higher than the PTFE matrix. The load is mainly distributed along the high-strength particles and the path along which the load is carried is called the force chain. The microscopic composition determines the distribution of the force chain and thus the overall strength of the material. When pressed, metal particles force chain mainly supports axial pressure, while the relatively weak poly matrix give a support to the high strength force chain. Increasing particle content can improve the strength and number of force chains when the material is compressed and then the strength of material is enhanced. However since the granular force chain can only bear less shearing force, the lateral force of the supporting force chain depends on the matrix constraint. The matrix can prevent the tangential sliding of the particles from slowing down the main chain bending and supporting the strong chain.

The relationship between the average stress at the top of the sample and the overall strain of the sample is shown in the figure 2(a). The numerical simulation results show the same rules as the experimental results. When the particle content is small, the material exhibits good toughness. As the particle content increases the material strength increases first and then decreases. At the same time the failure strain of the material decreases as the particle content increases. When the content of the particles is too much, the matrix content is insufficient to restrain the deformation of the force chain and the material strength begins to decrease at a low global strain. A reasonable ratio between the particles and the matrix can result in the best material strength.

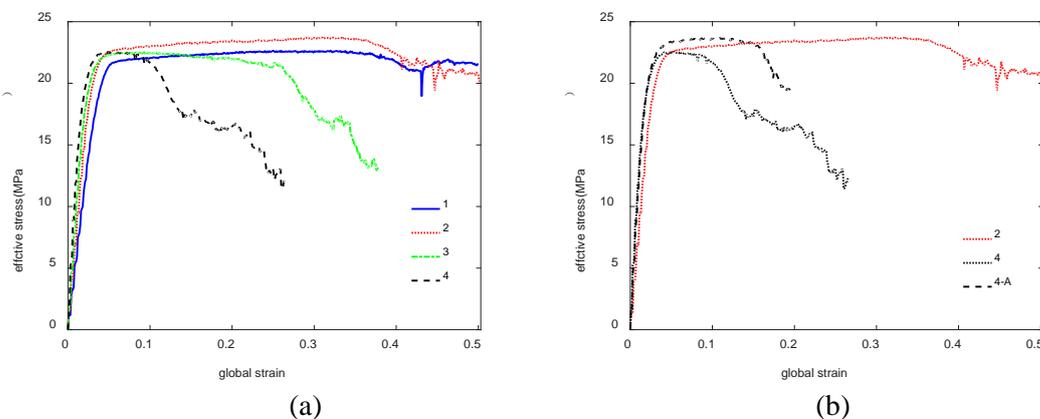


Figure 2. Average engineering stress at the top of the numerical sample plotted against the global strain

In accordance with the numerical simulation results, for a single particle size ($21\mu\text{m}$), when the particle content is increased to more than 36%, the matrix is insufficient to support metal particle force chain. It shows that excessive metal particles break the continuity of the matrix. But in some cases, we need to add more metal particles to the material. In order to maintain the continuity of the matrix at a high particle volume content in the sample 4 (particle volume content of 53%), more than 36% of the partial diameter is halved so that the extra particles are filled in the voids of the large particles and a numerical simulation sample 4-A is obtained. The relationship between the average stress at the top of the sample and the overall strain of the sample with the same Al content but different particle size is shown in the figure 2(b). It can be found that the compressive strength is significantly improved.

The deformation and effective stress contours of Al-PTFE with different Al particle size at different global strain are shown in Figure 3. It shows that during the forming of the force chain, the

size particle grading sample exhibits better uniformity. When most of the large particles become part of the strong chain, weak force chain are formed between smaller particles. Specially, replacing some large particles with small particles can effectively avoid stress concentration.

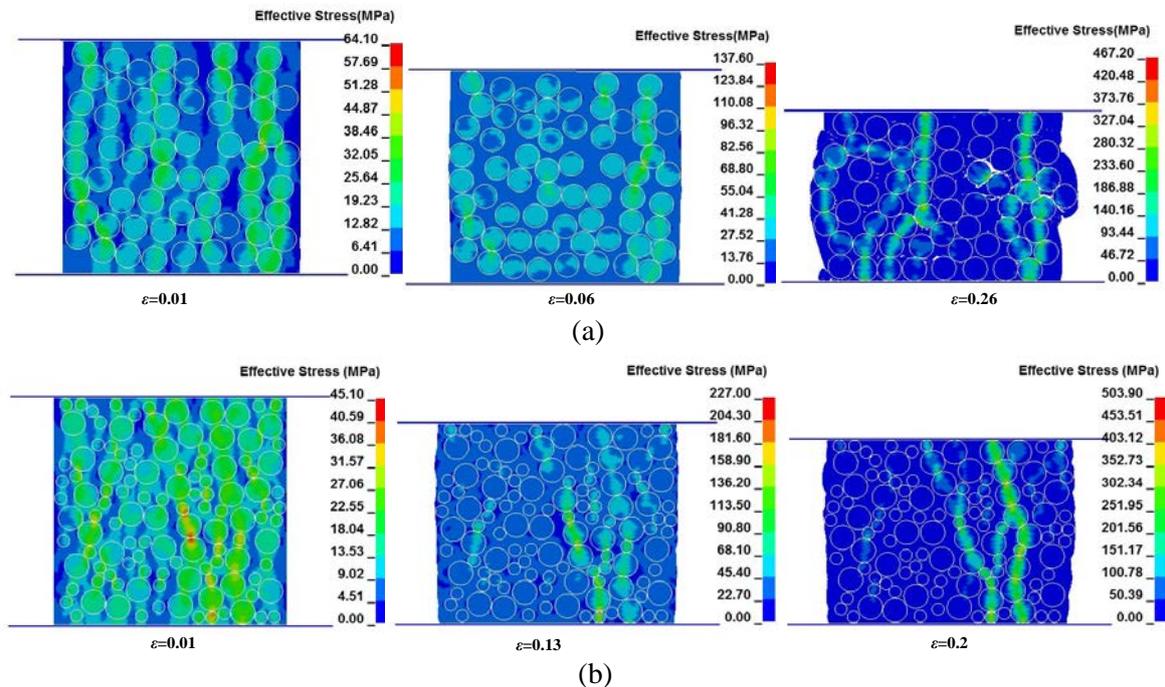


Figure 3. Contour of von Mises stress of PTFE-Al numerical sample with different Al particle size (a) Sample 4 (b) Sample 4-A

The contour of plastic strain of sample with different particle distribution are shown in figure 4. At the global strain of 0.2, significant stress concentration appears in the sample 4 (particle volume content of 53%, single particle size). But in the sample 4-A, strain concentration is clearly dispersed which increases the ultimate strain of the material and gives the material a higher compressive strength. The large particles beyond the capacity of the matrix are refined into small particles and filled into the voids so that the contact points between the particles increase. As a result, the overall compressive strength of the material is improved.

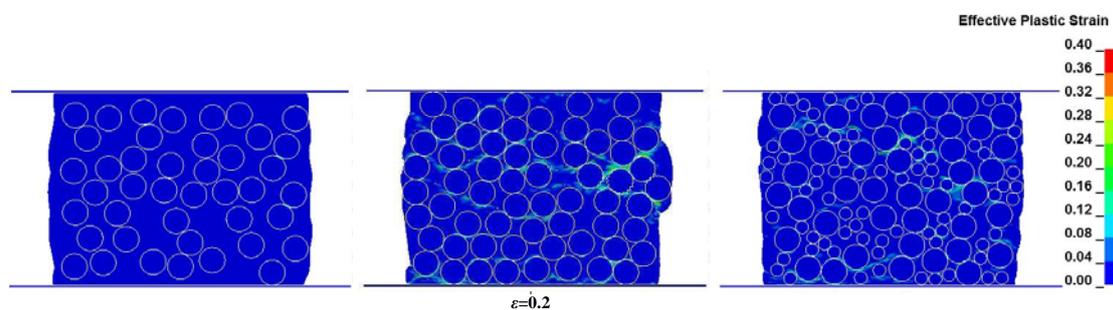


Figure 4. Strain distribution in sample 2, 4 and 4-A at 0.2 global strain

The two-dimensional calculations demonstrate that the geometric distribution of metal particles is very important for granule metal composites. Too many metal particles would cause excessive deformation of the matrix. When the metal composites need high content of metal particles, particle grading is a good choice. But it is difficult to determine the content of particles of different sizes.

4. Conclusions

The effects of mesoscale characteristic of Al-PTFE granule metal composites on their compression behavior have been analyzed in this paper. The major conclusions can be summarized as follows:

- (1) The strength and fracture mode of granule metal composites are mainly determined by the force chain of the metal particle group when compressed and the formation of the force chain is significantly affected by the geometric distribution of the particle;
- (2) The volume content of the particles significantly affects the formation of the metal particle force chain and the strength of granule metal composites. The strength of the material increases first and then decreases with the increase of the content of metal particles.
- (3) The strength of granule metal composites can be improved by a reasonable particle grading. When the particle content is higher than the best optimum ratio, replacing excess large particles with small particles can increase the strength of the material.

5. Acknowledgments

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