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Single Particle Impact Crushing Simulation and Establishment of Specific Fracture Energy Model

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Abstract: Based on the JH-2 constitutive model, a UFLC particle collision simulation model was established, the dynamic collision process of two particles on the UFLC platform was analyzed, and the failure forms of particles with different diameters under different impact velocities were analyzed. On this basis, based on the impact velocity model and the force-displacement model, an empirical expression for the specific fracture energy of different particle sizes was established, which provided a method for determining the undetermined coefficients of the statistical model of the specific fracture energy during the collision of titanium dioxide particles. The study found that the law of the change of the specific fracture energy with the particle diameter given by the established ultrafine particle collision finite element simulation model during collision is consistent with the law given by Tavares' experimental model, which verifies the accuracy of the model.

Keywords: Impact Crushing; Finite Element Simulation; Contact Model; Strain Energy; Fracture Energy.

1. Introduction

Ultrafine grinding technology is a high-tech technology that has developed rapidly in the past 20 years. It is widely used in many fields at home and abroad, such as material preparation, medicine, chemical industry, energy and environmental protection, electronic optics, etc., including the preparation of nanomaterials, nano drug carriers, coating fillers, electronic devices, optical materials, etc. Ultrafine grinding technology can improve material properties, increase drug bioavailability, prepare high-performance catalysts, improve energy conversion efficiency, prepare high-precision optical materials, etc., so it has attracted many scholars to conduct in-depth research. With the development of nanotechnology and the increase in application demand, the research on ultrafine grinding technology has also received more and more attention and has become one of the hot spots in the field of high-performance material preparation.

At present, wet grinding technology is one of the most commonly used methods for mechanical preparation of ultrafine particles. During the grinding process, the coupling effect between particles and liquid media, as well as the collision and crushing between particles, can effectively reduce the particle size of the powder and improve the quality of the product. In ultrafine grinding experiments, by controlling grinding parameters such as the type of grinding media, the nature and concentration of the liquid medium, and the grinding time, the size of the product particles can be adjusted, thereby affecting the performance and application characteristics of the product [1]. When studying the wet grinding process, numerical calculation methods can be used for discrete element simulation to simulate the interaction between particles and particles, and between particles and liquid media, and then analyze the movement and loading of grinding media and materials in different areas of the mill [2]. At the same time, statistical distribution models such as population balance and stress intensity-stress number [3] are combined to evaluate the crushing of materials at various positions in the mill. However, with the development of mathematical models of different mills, crushers, and processing systems, it is necessary to further study the crushing mechanism of single particle crushing in the process of mechanical preparation of ultrafine particles when combined with discrete element simulation.

Tavares [4] studied the single-particle collision and crushing behavior of granulite and other materials using the UFLC impact crushing platform, revealing the influence of particle size on particle specific fracture energy. However, there are three unknown coefficients in the expression of Tavares' specific fracture energy model, and a large number of collision experiments are required when applying the model to titanium dioxide particles. This chapter uses the finite element simulation platform to establish a corresponding simulation model, uses the JH-2 constitutive model to model granulite, and simulates the dynamic process of particle collision on the UFLC platform. The statistical model of specific fracture energy under different particle sizes is fitted by the impact velocity model and the force-displacement model, and then compared with the experimental model made by Tavares to verify the consistency of the simulation model and the experimental model. This provides a method for determining the unknown coefficients in the statistical model of specific fracture energy, and analyzes the crushing form of granulite under impact load.

2. Introduction to the UFLC Experimental Model

UFLC [4] (Ultra-Fast Load Cell) is an abbreviation for Ultra-Fast Load Cell, which was developed by Weichert at the Utah Comminution Center. The technology is the result of the combination of a simple drop weight device and a Hopkinson bar developed by Weichert and Herbst in 1986. It consists of a long steel bar equipped with strain gauges, on which a single particle or a bed of particles is placed and impacted, as shown in Figure 1.

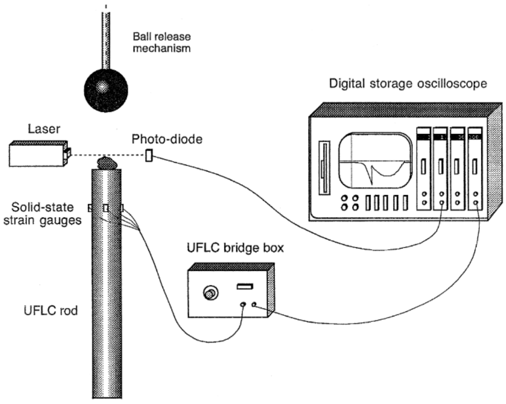


Figure 1. Schematic diagram of ultrafast load cell

When the steel ball falls and impacts, a compression wave is generated within the rod, which propagates down the rod and is sensed by a solid-state strain gauge. This causes a change in voltage in the Wheatstone bridge, which is then recorded as a function of time using a digital oscilloscope. Combining the mechanical and physical properties of the rod and the bridge and gauge coefficients, the individually measured outputs can be converted into a time history of force and further statistically calculated for the required fracture energy during the particle collision.

3. Establishment of the Finite Element Simulation Model of Particle Collision on the UFLC Platform

3.1. Basic Assumptions of Finite Element Simulation

For the convenience of calculation, this chapter makes the following assumptions in the simulation process: 1. The workpiece material is isotropic, that is, the properties are the same in all directions, which helps to simplify the mechanical model and reduce the complexity of calculation; 2. The workpiece is in a natural state, that is, there is no stress inside the workpiece before the collision occurs.

3.2. Establishment of Material Constitutive Model

Combined with the UFLC collision platform, the target to be impacted is assumed to be a sphere, the material is granulite, the material of the ball and the UFLC rod is structural steel, the UFLC rod is simplified into a square and set as a rigid body, the main physical properties parameters of granulite and structural steel are shown in Table 3.

Table 1. Main physical properties of granulite and structural steel

	Density (Kg/m^3)	Elastic Modulus(GPa)	Poisson's ratio
Granulite	2660	50-80	0.2-0.3
Structural Steel	7850	200	0.3

The constitutive relationship adopted in the finite element simulation is the JH-2 constitutive model, which was originally used to simulate the behavior of brittle materials, especially ceramics.

Figure 2 describes the strength curve of brittle materials from three aspects: intact state, damaged state and fracture state. Different states have their own strength equations, which give the relationship between normalized equivalent stress and normalized pressure. The analytical function in the damaged state can be regarded as a general form of the three states, and its normalized equivalent stress is expressed as

$$\sigma^* = \sigma_i^* - D\left(\sigma_i^* - \sigma_f^*\right) = \sigma/\sigma_{HEL} \quad (1)$$

Where, σ^* is the normalized complete equivalent stress, σ_f^* is the normalized fracture stress, D is the damage factor, σ_{HEL} is the equivalent stress at HEL-Hugoniot elastic limit, represents the net compressive stress (including hydrostatic pressure and deviatoric stress components) when a one-dimensional shock wave with uniaxial strain exceeds the elastic limit of the material. Among them, σ is the actual equivalent stress, calculated by the von Mises stress formula:

$$\sigma = \sqrt{\frac{1}{2}\left[\left(\sigma_x - \sigma_y\right)^2 + (\sigma_x - \sigma_z)^2 + \left(\sigma_y - \sigma_z\right)^2 + 6\left(\tau_{xy}^2 + \tau_{xz}^2 + \tau_{yz}^2\right)\right]} \quad (2)$$

Where, σ_x, σ_y, σ_z are the normal stress components in three directions, τ_{xy}, τ_{xz}, τ_{yz} are the shear stress components in three directions.

The normalized full intensity is given by:

$$\sigma_i^* = A(P^* + T^*)(1 + C \cdot In\dot{\varepsilon}^*) \quad (3)$$

The normalized breaking strength is given by:

$$\sigma_f^* = B(P^*)^M(1 + C \cdot In\dot{\varepsilon}^*) \quad (4)$$

Where, A, B, C, M, N are material constants, normalized pressure $P^* = P/P_{HEL}$, where P is the hydrostatic pressure, P_{HEL} is the net water pressure at HEL, and the standardized maximum tensile hydrostatic pressure is $T^* = T/P_{HEL}$, where T is the maximum tensile hydrostatic pressure that the material can withstand. The dimensionless strain rate $\dot{\varepsilon}^* = \dot{\varepsilon}/\dot{\varepsilon}_0$ is $\dot{\varepsilon}$ the actual equivalent strain rate, and $\dot{\varepsilon}_0$ is the strain $\varepsilon = 1.0s^{-1}$ rate reference strain rate. The actual equivalent strain rate is similar to the equivalent stress and is expressed as:

$$\dot{\varepsilon} = \sqrt{\frac{2}{9}\left[\left(\dot{\varepsilon}_x - \dot{\varepsilon}_y\right)^2 + (\dot{\varepsilon}_x - \dot{\varepsilon}_z)^2 + \left(\dot{\varepsilon}_y - \dot{\varepsilon}_z\right)^2 + \frac{3}{2}\left(\gamma_{xy}^2 + \gamma_{xz}^2 + \gamma_{yz}^2\right)\right]} \quad (5)$$

Where, $\dot{\varepsilon}_x$, $\dot{\varepsilon}_y$, $\dot{\varepsilon}_z$ are the normal strain rate components in three directions, γ_{xy}, γ_{xz}, γ_{yz} are the shear strain rate components in three directions.

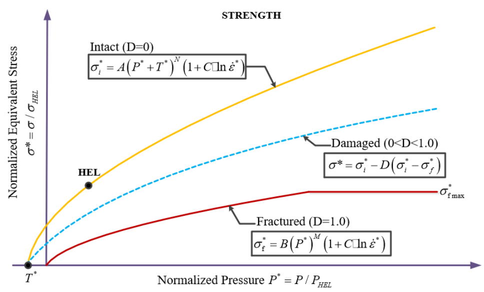


Figure 2. Strength model of JH-2 constitutive model

In the JH-2 constitutive model, the brittle material begins to soften when damage begins to accumulate (see the damage curve in Figure 2). The softening process can be represented by equation (1), which allows the material to gradually soften as the plastic strain increases, although softening does not continue when the material is completely damaged (D = 1).

The JK-2 constitutive parameters of granulite are shown in

Table 2.

Table 2. Constitutive parameters of granulite JK-2

constant	Granulite	constant	Granulite
Full Strength Factor$A$	1.248	Complete Strength Index$N$	0.676
Fracture strength factor$B$	0.0077	Maximum tensile strength$T(MPa)$	57
Strain rate coefficient$C$	0.0051	Hugoniot elastic limit$\sigma_{HEL}(GPa)$	4.5
Breaking strength index$M$	0.35	HEL pressure$P_{HEL}(GPa)$	2.93

3.3. Establishment of Material Failure Criteria

The damage shows a nonlinear increasing trend as shown in Figure 3. The expression of the cumulative damage caused by fracture is:

$$D = \sum \frac{\Delta\varepsilon^P}{\varepsilon_f^P} = \sum \frac{\Delta\varepsilon^P}{[D_1(P^* + T^*)]^{D_2}} \quad (6)$$

In the formula, $\Delta\varepsilon^P$is the plastic strain in the integration cycle, ε_f^P is the plastic strain of fracture under constant pressure P, $D_1$and $D_2$are $\varepsilon_f^P$the damage factors.

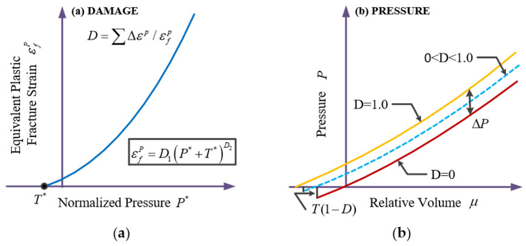


Figure 3. Damage model and EOS model of JH-2 constitutive model

The damage factors of granulite are shown in Table 3.

Table 3. JK-2 failure criterion parameters

Damage ConstantD_1	Damage ConstantD_2
0.008	0.435

3.4. Pressure Polynomial State Equation

In physics, when the plastic deformation or damage of a unit accumulates to a certain threshold, the material fails and loses strength. This is called fluid-like behavior, where the unit cannot withstand any stress, but the hydrostatic pressure and deviatoric stress are equal to zero. Here, the polynomial state equation (EOS) represents the relationship between the hydrostatic pressure P and the volume strain μ (Figure 3), which consists of a purely elastic stage and a plastic damage stage. The detailed expression is as follows:

$$P = \begin{cases} K1 \cdot \mu + K2 \cdot \mu^2 + K3 \cdot \mu^2 & D = 0 \\ K1 \cdot \mu + K2 \cdot \mu^2 + K3 \cdot \mu^2 + \Delta P & 0 < D \leq 1 \end{cases} \quad (7)$$

In the formula, $K1$, $K2$, $K3$are coefficients, $\mu = \frac{\rho}{\rho_0} - 1$, $\rho$are current density, $\rho_0$and are initial density. For tensile stress ($\mu < 0$), the equation can be replaced by $P = K1 \cdot \mu$. When the material breaks, the energy generated by expansion causes ΔPa change in the pressure increment.

The incremental internal elastic energy reduction is converted into potential internal energy through incremental increase ΔP. The shear stress and deviatoric stress decrease with increasing crack length due to the σ decrease in equivalent plastic flow stress. The elastic internal energy of shear stress and deviatoric stress is expressed as:

$$U = \sigma^2/6G \quad (8)$$

Where $G$is the shear modulus.

The incremental energy loss is:

$$\Delta U = U_{D(t)} - U_{D(t+\Delta t)} \quad (9)$$

Where, $U_{D(t)}$and $U_{D(t+\Delta t)}$are the elastic internal energies at different time steps.

The energy loss ΔU is mainly converted into fracturing energy ΔF. The approximate equation for this energy conservation is:

$$\Delta F = \beta \cdot \Delta U \quad (10)$$

Where $\beta(0 < \beta < 1)$ is the coefficient of converting elastic energy loss into fracturing energy.

The pressure polynomial state parameters of granulite are shown in Table 4.

Table 4. JK-2 pressure polynomial state parameters

constant	Granulite	constant	Granulite
Bulk modulus$K1(GPa)$	25.7	The third pressure coefficient$K3(GPa)$	12800
Second pressure coefficient$K2(GPa)$	-386	Volume coefficientβ	1.0

3.5. Geometric Model Establishment and Mesh Division

The finite element simulation mesh model of UFLC impact crushing is shown in Figure 4. The spherical particles No. 3 are granulite particles, the diameter of the sphere No. 1 is 4 mm, the size of the fixed support plate No. 2 is $6mm \times 6mm \times 2mm$, and the material is structural steel. The contact between the spheres is set to be frictionless, and the collision process of the particles is calculated using the Lagrangian method.

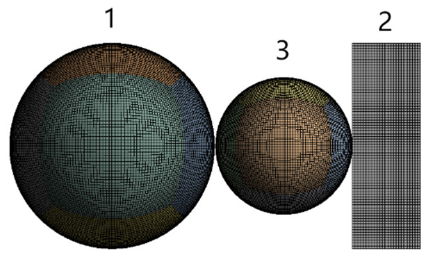


Figure 4. UFLC impact crushing finite element simulation mesh model

4. Finite Element Simulation Results and Analysis

4.1. Simulation Scheme of Finite Element Simulation

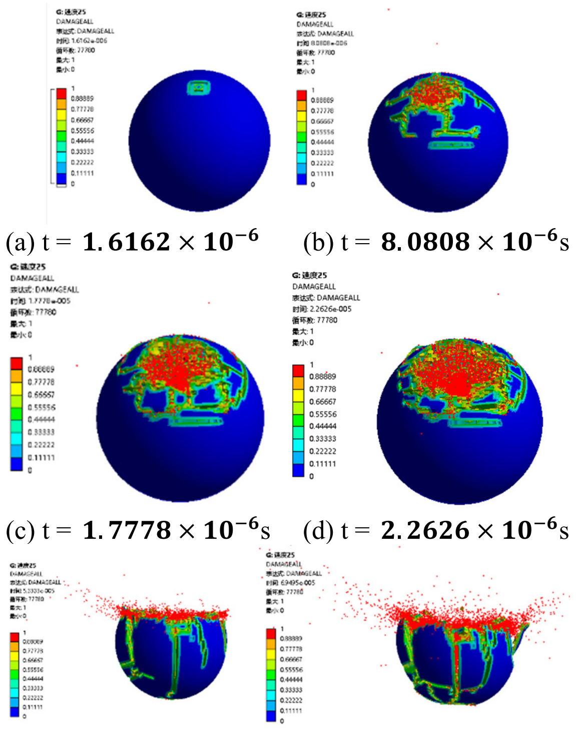
In order to deeply study the crushing damage forms of granulite particles with different particle diameters under impact loads, the simulation schemes listed in Table 5 were used for simulation and analysis. Through these simulation schemes, the response of particles with different diameters under different impact loads can be systematically observed, thereby revealing the microscopic behavior and crushing mechanism of granulite particles in the crushing process.

Table 5. Granulite particle collision simulation parameters

serial number	Particle diameter (mm)	Impact speed (m/s)
1	4	25, 20, 18, 17, 16
2	3	13, 14, 15, 16
3	2.5	10, 11, 12, 13
4	2.0	10, 11, 12
5	1.5	9, 10, 11
6	1.0	9, 10

4.2. Dynamic Crushing Analysis of Granulite Particles under Impact Load

According to Figure 5 (a), at time $t = 1.6262e^{-6}$s, the granulite particles first produce damage in the Hertz ring of the collision contact area, which leads to the destructive crushing of the outermost layer of the contact surface to form fine fragments, while the contact area inside the Hertz ring forms material densification under the action of compressive stress.



(a) t = $\mathbf{1.6162 \times 10^{-6}}$ (b) t = $\mathbf{8.0808 \times 10^{-6}}$s

(c) t = $\mathbf{1.7778 \times 10^{-6}}$s (d) t = $\mathbf{2.2626 \times 10^{-6}}$s

(e) t = $\mathbf{5.3333 \times 10^{-5}}$s (f)t = $\mathbf{6.9495 \times 10^{-5}}$s

Figure 5. Impact crushing diagram of 4 mm diameter granulite when impacted by a structural steel sphere at 25 m/s

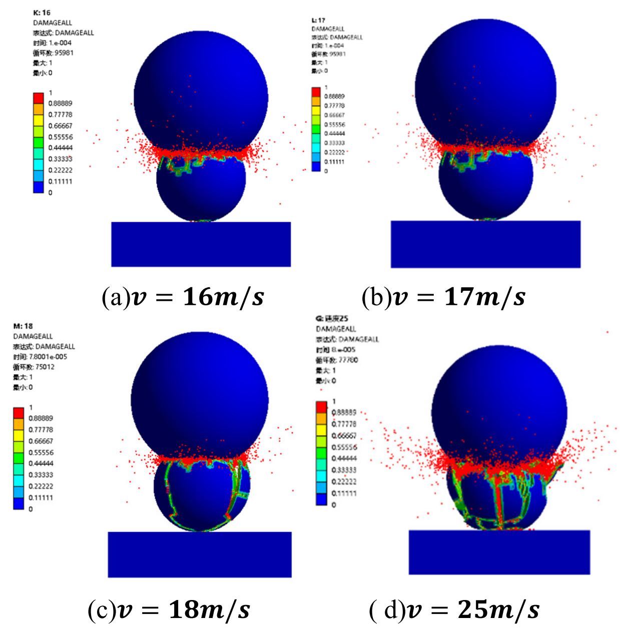
As the loading progresses, the fragments formed on the contact surface propagate from the contact area into radial cracks, as shown in Figure 5 (e). When the time is reached $t = 5.333e^{-5}$, radial cracks are also formed in the center of the granulite and extend along the meridian plane to form a central crack, while the cracks outside the particles gradually connect with the cracks inside to form leaf-shaped cracks and gradually fall off, which is the same as the damage form of brittle spherical particles under medium and high-speed impact loads summarized by SZ Wu et al., as shown in Figure 6. As can be seen from Figure 5 (f), the granulite particles will be broken into a large number of daughter particles when impacted by a structural steel sphere at a speed of 25 m/s.

Figure 6. 3D schematic diagram of the crack pattern inside the sphere under impact load

4.3. Effect of Impact Velocity on Granulite Particle Fragmentation

Figure 7 shows the crushing of 4 mm granulite at different impact velocities. Comparing Figure 7 (c) and Figure 7 (d), when the impact velocity of the structural steel sphere is 25 m/s, the daughter particles produced after the granulite is crushed are smaller. This is because the number of radial cracks in the particles is greater under high-speed collision. This shows that the size of the daughter particles produced by particle crushing decreases with the increase of impact velocity, while the number of daughter particles increases with the increase of impact velocity.

For Figure (a) and Figure (b), when the impact velocity is 17 m/s, the particles do not break, but only cracks are generated in the local area of the collision contact surface. This shows that the critical impact velocity for the breakage of 4 mm granulite is 18 m/s.



(a)$\boldsymbol{v = 16m/s}$ (b)$\boldsymbol{v = 17m/s}$

(c)$\boldsymbol{v = 18m/s}$ (d)$\boldsymbol{v = 25m/s}$

Figure 7. Impact crushing diagram of 4 mm diameter granulite at different impact velocities

4.4. Establishment of Specific Fracture Energy Model under Impact Velocity Model

Yashima [5]and Weichert et al. independently derived an exponential relationship between mass-specific particle fracture energy and particle size based on Hertzian contact theory and the Weibull weakest link criterion. However, the studies showed that as particle size increases, the measured energy tends to a constant value that is unique to each material. A model that describes the data well is:

$$E_{m_{50}} = E_{m,\infty}\left[1 + \left(d_{p,0}/d_p\right)\right]^{\emptyset} \quad (11)$$

Where, $E_{m,\infty}$, $d_{p,0}$, $\emptyset$are the model coefficients fitted by the least squares method; $E_{m,\infty}$represents the residual particle fracture energy of larger-sized materials, and $d_{p,0}$ is the characteristic size of the material microstructure.

Assuming that the initial kinetic energy of the structural steel particles during the collision is transferred to the granulite particles and applied to the particle crushing, the mass specific fracture energy of granulite particles with different diameters can be calculated by the following formula:

$$E'_{m_{50}} = m_1 v^2 / 2m_3 \quad (12)$$

Where, m_1, $m_3$represent the masses of the structural rigid sphere and granulite particles, respectively.

The critical impact velocity of granulite particles with different diameters during crushing is extracted from the finite element analysis results and substituted into equation (12) to solve the particle specific fracture energy. Using Python mathematical analysis software, the least squares method is used to fit the curve of the mass specific fracture energy required for crushing granulite particles as a function of particle diameter, thereby obtaining the fitting parameters.

This process is called regression analysis or data fitting in data analysis. If the mathematical model used is linear, it is called linear regression; conversely, if a nonlinear model is used, it is called nonlinear regression. Whether it is linear regression or nonlinear regression, the purpose is to minimize the total sum of squared errors. Python's NumPy library provides simple commands that make linear regression and nonlinear regression very convenient.

According to the distribution law of each point, it is judged that it obeys the change law of formula (11), so it is fitted, and the fitting result reaches 99.9% goodness of fit:

$$E_{m_{50}} = 457.22750188\left[1 + \left(2.47740746/d_p\right)\right]^{3.28244484} \quad (13)$$

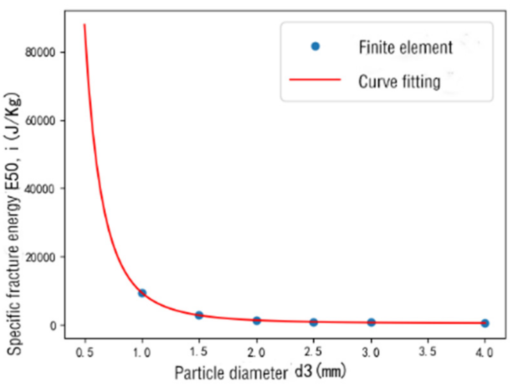


Figure 8. Relationship between specific fracture energy and particle diameter

It can be observed from Figure 8 that as the particle diameter decreases, the specific fracture energy gradually increases. It is observed that the mass specific fracture energy required for the crushing of granulite with a diameter of 1 mm is about 1000 J/Kg, but the results of experimental research show that the specific energy required for the crushing of 1 mm granulite is only 500 J/Kg. This conclusion fully demonstrates that during the collision process, the initial kinetic energy of the structural steel particles is not completely converted into the energy required for particle crushing, but is partially converted into the internal energy and kinetic energy of the daughter particles after crushing, and some kinetic energy is still stored in the structural steel particles.

4.5. Size Effect of Granulite Particle Crushing

According to Figure 9, when the granulite particles with a diameter of 2 mm are broken at the critical impact velocity, no radial cracks are formed on the outer surface, and cracks are only generated and extended along the central section, eventually causing the particles to break into two halves along the meridian plane. This phenomenon is similar to the failure form of brittle material particles under static load compression.

Arbiter and Chau et al. [6] observed the static compression failure mode of brittle materials and found two separated or almost separated cones and two or three orange slices below the contact area. One possible scenario for this phenomenon is that the two spherical caps under contact are crushed to form compression cones, which are then driven into the specimen to initiate tensile meridian cracks. Finally, whether the sphere splits into two or three slices depends on the pre-existing inhomogeneities in the sphere, as shown in Figure 10.

This shows that at the critical impact velocity, as the diameter of the granulite particles decreases, the cracks generated inside and on the outer surface of the particles gradually decrease, and the main failure mode of granulite particles with a diameter of less than 2 mm under low-speed impact load is meridian cracks.

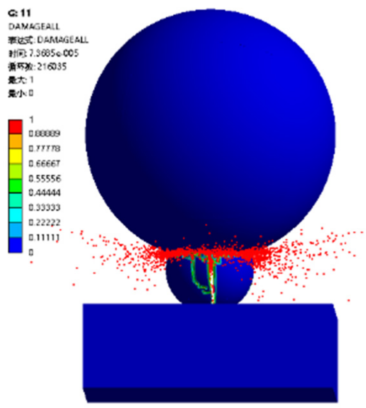


Figure 9. Failure diagram of granulite particles with a diameter of 2 mm at the critical impact velocity

Figure 10. modes of brittle material particles under static compression [6]

5. Chapter Summary

In this chapter, a dynamic simulation model of particle collision on the UFLC platform is established, and the crushing damage forms of granulite particles under different impact velocities are analyzed. Based on the impact velocity model and the force-displacement model, a specific fracture energy model of granulite particles is established, and the influence of particle diameter on specific fracture energy is studied. The following conclusions are drawn:

(1) A finite element simulation model of dynamic collision of granulite was established, and the failure mode of granulite particles under medium- and high-speed collision mode was studied. The results show that when a structural steel particle with a velocity of 25 m/s hits a granulite particle with a diameter of 4 mm, the failure mode of the granulite particle is similar to the failure mode of a brittle spherical particle under medium- and high-speed impact load. In this process, a large number of cracks are formed on the outer surface and inside of the granulite particle, and many daughter particles are generated.

(2) A specific fracture energy model of granulite particles under the critical impact velocity model was established. The comparison between the predicted and actual values of the specific fracture energy shows that in the actual collision process, the initial kinetic energy carried by the structural steel particles is not completely converted into the energy required for particle crushing. Instead, part of the energy is converted into the internal energy and kinetic energy of the daughter particles after crushing, while part of the kinetic energy is still retained in the structural steel particles.

(3) A finite element simulation model of dynamic impact of granulite was established, and the failure mode of granulite under critical impact velocity was analyzed. The results show that as the diameter of granulite particles decreases, the cracks generated inside and on the outer surface of the particles gradually decrease. Moreover, the main failure mode of small-diameter granulite particles under low-velocity impact loads is meridian cracks.

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