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SAND--93-0887C 1
Conf. 9311214-18

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A THERMODYNAMIC THEORY OF DYNAMIC FRAGMENTATION**Ching H. Yew**
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ABSTRACT

We present a theory of dynamic fragmentation of brittle materials based on thermodynamic arguments. We recover the expressions for average fragment size and number as originally derived by Grady. We extend the previous work by obtaining descriptions of fragment size distribution and compressibility change due to the fragmentation process. The size distribution is assumed to be proportional to the spectral power of the strain history and a sample distribution is presented for a fragmentation process corresponding to a constant rate strain history. The description of compressibility change should be useful in computational studies of fragmentation. These results should provide insight into the process of fragmentation of brittle materials from hypervelocity impact.

INTRODUCTION

Upon hypervelocity impact, shock waves are generated at the contact surface, propagate outward, and set the media into a state of compression. It is intuitively clear that the fragmentation process will not take place until the stress state in the media becomes tensile due to the reflected waves from the boundary or scattered waves from internal flaws or structure. A large amount of expansion energy is thus imparted to the material in a very short time period. When the tensile stresses exceed the fracture limit, a catastrophic break-down of the material occurs and a debris cloud is formed. However, there is a lack of rigorous analysis of this observed phenomenon. The major difficulty has been that the material, upon hypervelocity impact, will break down forming a debris cloud, yet the theories used in the analysis have always treated the material as a continuum. The catastrophic failure of material is not a well understood process. In a series of papers, a catastrophic failure theory based on local energy inequality and minimum fracture time requirement was developed by Grady (1982, 1985, 1988). The theory is however not completed because the evolution process that leads to the catastrophic failure of the material was not considered by Grady. This presents a difficulty in implementing the theory to computation simulation of the problem.

In this paper, we present a different approach to the problem by treating the fragmentation event as a thermodynamic process controlling energy and entropy distributions throughout the entire volume. We argue that since a large amount of expansion energy is imparted to the material by the reflected tensile waves, the body is not in a state of thermodynamic equilibrium, and the body tends to reach a state of equilibrium by breaking-down or by undergoing phase changes such as fluidizing or vaporizing or both. The dynamic fragmentation process can therefore be described by applying the thermodynamic theory. Since Grady's fragmentation theory will be employed extensively in the development of our theory, a brief recount of that theory will be presented in section II. A catastrophic

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fragmentation theory based on thermodynamic theory will then be developed in section III. Based on Grady's horizon condition, it will be shown in section IV that the particle size distribution is proportional to the spectral power of the reflected tensile strain history in the body. Assuming that the process that leads to the catastrophic fragmentation of the material is the rapid growth of internal cracks in the material, a quantitative description of material property degradation caused by the growth of internal cracks is developed in section V. The results are then used to derive the evolution equation for describing the material behavior during the period of internal crack-growth-to-failure of the material. Finally, a brief recount of the results developed in this study is presented in the concluding section -- section VI.

GRADY'S FRAGMENTATION THEORY

Consider a small body of material of volume V as shown in Fig. 1, which was previously compressed, is now in a state of rapidly diverging expansion under the action of a uniformly

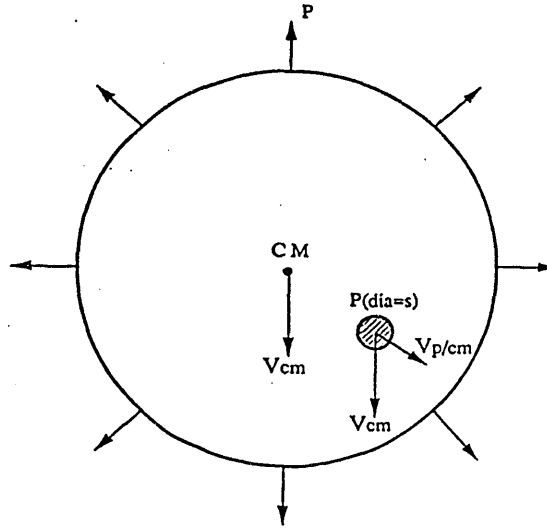


Fig.1: Formation of Fragments by Rapid Expansion

distributed tension P . Assume that, prior to break-down, the instantaneous kinematic state of the material is provided by the strain ϵ , strain rate $\dot{\epsilon}$, and temperature θ . Follow Grady (1982,1988) and consider, prior to fragmentation, an element of mass within the expanding material which will constitute the mass of an average fragment after the breakage process is completed. This mass element is illustrated by the spherical region of diameter "s" shown in Fig. 1. With reference to the position of mass-center, the kinetic energy of the mass element can be decomposed into a center-of-mass kinetic energy, T_{cm} , and a kinetic energy relative to the mass center, dT .

To obtain an explicit expression for the local kinetic energy (dT), consider a spherical mass element of diameter, s , expanding uniformly from the center due to a strain rate $\dot{\epsilon}$. The expansion kinetic energy density with respect to the mass center can be shown to be

$$dT = \frac{1}{120} \rho \dot{\epsilon}^2 s^2 \quad (1)$$

where ρ is the current mass density.

In addition, a strain energy density

$$dU = \frac{1}{2} \frac{P^2}{B} = \frac{1}{2} B (\dot{\epsilon} t)^2 \quad (2)$$

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is also present as the element is carried into tension.

In Eq. (2), $B = \rho c^2$ is the bulk modulus, ρ is the density, and c is the dilatational wave speed of the material. Grady argued that if the body is to undergo macroscopic failure by fracture at a time t , it is necessary for each and every volume of size $(ct)^3$ to failure independently. Since, at time t , the communication horizon is no great than (ct) , the size of each individual fragment should be governed by the inequality,

$$s \leq 2ct, \quad (3)$$

Substitution of Eq. (3) into Eq. (2) gives

$$dU \geq \frac{1}{2} B \left(\frac{\dot{\epsilon} s}{2c} \right)^2 \quad (4)$$

When the mass breaks down into "n" fragments of an average diameter "s", a fracture surface energy per unit volume approximately

$$d\Gamma = \frac{3K_c^2}{\rho c^2 s} \quad (5)$$

must be dissipated in the fragmentation process.

Grady (1988) postulated that, for brittle spall to be energetically permissible within the element δM , the following inequality must be satisfied:

$$dT + dU \geq d\Gamma, \quad (6)$$

Assuming that $dT \ll dU$ and the term dT can be neglected, the minimum time requirement of Eq. (6) gives the average size of fragments:

$$s = 2 \left[\frac{\sqrt{3} K_c}{\rho c \dot{\epsilon}} \right]^{2/3} \quad (7)$$

THERMODYNAMIC FORMULATION OF DYNAMIC FRAGMENTATION

Assume that the global volume shown in Fig. 1 is sufficiently small that the expanding strain rate $\dot{\epsilon}$ is uniform throughout the volume, and that the volume breaks down into "n" small spheres of an average diameter "s". Geometrical consideration gives

$$s = \left(\frac{6V}{\pi n} \right)^{1/3} \quad (8)$$

By multiplying Eqs. 1, 4, and 5 by the total volume V and substituting Eq. (8) into them, the equivalent energy terms in the volume can be written as:

Total expansion kinetic energy:

$$T = \frac{1}{120} \left(\frac{6}{\pi} \right)^{2/3} \rho \dot{\epsilon}^2 n^{-2/3} V^{5/3} \quad (9)$$

Total strain energy:

$$U \geq \frac{B}{8} \left(\frac{\dot{\epsilon}}{c} \right)^2 \left(\frac{6}{\pi} \right)^{2/3} n^{-2/3} V^{5/3} \quad (10)$$



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Total fracture dissipation energy:

$$\Gamma = \left(\frac{\pi}{6}\right)^{1/3} \left(\frac{3K_c^2}{\rho c^2}\right) n^{1/3} V^{2/3} \quad (11)$$

The above equations will be used in the derivation of Gibbs thermodynamic function G defined as (Sears and Salinger, 1975):

$$G = H - \theta S_c, \quad (12)$$

where H is the enthalpy, S_c is the configuration entropy, and θ is the absolute temperature of the system.

As mentioned earlier, since a large amount of expansion energy is imparted to the body by the expansion waves, the body V is not in a state of thermodynamic equilibrium, but tends to reach a state of equilibrium by breaking-down. Since the state of deformation of the body is described by the strain energy, it seems reasonable to assume that the strain energy and the heat energy generated by the impact are the internal energy in the body that contributes to the break-down of the material, while the kinetic energy in the body gives the expansional velocity within the fragment particles. In this study, we consider only the case that the body breaks down according to a K_c -controlled fracturing process. The energy necessary to fracture the body is governed by the internal energy imparted by the impact and by the surface energy dissipated in the fracturing process. Note also that the fracture surface energy is not recoverable, it contributes to the entropy increase of the system. The fragmentation of the body is assumed to occur under an isothermal condition.

The Gibbs function for a body that breaks into n spheres can be written as

$$G = G^0 + ng^f - \theta S_c \quad (13)$$

where ng^f is the contribution from the fracturing process, and S_c is the configuration entropy.

The above form of Gibbs function has been used in the study of void generation in perfect crystals (Varotsos and Alexopoulos, 1986). The function G^0 is defined under the assumption that the perfect crystal is so near to equilibrium that thermodynamic functions can be defined. For the present case, one can thus relate the function G^0 to the expanding strain energy in the body immediately prior to fragmentation, i.e.,

$$G^0 = \frac{B}{8} \left(\frac{\dot{\epsilon}}{c}\right)^2 \left(\frac{6}{\pi}\right)^{2/3} n^{-2/3} V^{5/3} \quad (14)$$

By replacing the term ng^f with Eq. (13), the Gibbs function (Eq. 13) for the fragmented body can be written as:

$$G = \frac{B}{8} \left(\frac{6}{\pi}\right)^{2/3} \left(\frac{\dot{\epsilon}}{c}\right)^2 n^{-2/3} V^{5/3} + \left(\frac{\pi}{6}\right)^{1/3} \left(\frac{3K_c^2}{\rho c^2}\right) n^{1/3} V^{2/3} - \theta S_c \quad (15)$$

Following Varotsos and Alexopoulos (1986), the configuration entropy of n cracks that could occupy $N+n$ sites in the volume V is

$$S_c = k \ln \left(\frac{(N+n)!}{N!n!} \right) \quad (16)$$

where k is Boltzmann's constant.

Under a constant P and θ , the Gibbs function is a minimum in the equilibrium state. The number of fragments can be found from

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$$\left(\frac{\partial G}{\partial n}\right)_{\theta, P} = 0 \quad (17)$$

to give (note that $B = \rho c^2$)

$$-\frac{\rho c^2}{8} \left(\frac{6}{\pi}\right)^{2/3} \left(\frac{\dot{\epsilon}}{c}\right)^2 \left(\frac{2}{3}\right) n^{-5/3} V^{5/3} + \left(\frac{\pi}{6}\right)^{1/3} \left(\frac{3K_c^2}{\rho c^2}\right) \left(\frac{1}{3}\right) n^{-2/3} V^{2/3} = k\theta \ln\left(\frac{n+N}{n}\right) \quad (18)$$

Making use of Eq. (8), the above equation becomes

$$-\left(\frac{\pi \rho \dot{\epsilon}^2}{72}\right) s^5 + \left(\frac{\pi K_c^2}{6 \rho c^2}\right) s^2 = k\theta \ln\left(\frac{n+N}{n}\right) \quad (19)$$

Using the following data:

TABLE 1: Material Properties (Aluminum) Used In Computation

ρ (density)	$= 2,800 \text{ Kg/m}^3$
K_c (stress intensity factor)	$= 29.13 \times 10^6 \text{ N/m}^{3/2}$
c (wave speed)	$= 6,300 \text{ m/s}$
k (Boltzmann constant)	$= 1.39 \times 10^{-23} \text{ N-m}^\circ\text{K}$
θ (temperature)	$= 1,273 \text{ }^\circ\text{K}$

the number of particles n and the average particle size s can be calculated from Eqs. 8 and 19, respectively.

However, based on the values in Table 1, the coefficient $k\theta$ in Eqs. (18) and (19) is negligibly small in comparison with the coefficients on the left-hand side of the equation. The expressions for number of particles and average particle size s can be derived by dropping the right-hand term in Eqs. (18) and (19) to give

the number of particles:

$$n = \frac{1}{2\pi} \left(\frac{c \rho \dot{\epsilon}}{K_c}\right)^2 V \quad (20)$$

and the average particle size:

$$s_o = 2 \left(\frac{\sqrt{3} K_c}{\sqrt{2} \rho c \dot{\epsilon}}\right)^{2/3} \quad (21)$$

The above equation differs with the Grady's equation (Eq. 7) by a factor $1/(2)^{1/3}$. It should be mentioned that, despite the closeness of results, the approach used in this derivation is very different from that used by Grady. In our derivation, the number of fragments in a volume V is calculated by minimizing the Gibbs function (i.e., $U + \Gamma$) in the volume with respect to the number of fragments. While, in Grady's derivation, the number of fragments is calculated by imposing a minimum time requirement to the local energy inequality (Eq. 6).

The average size of particles and particle densities for strain rates of 10^4 , 10^5 , and 10^6 are calculated from Eqs. (20) and (21) and are tabulated as follows:

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TABLE 2: Average Particle Size And Particle Density At Different Strain-Rates

$\dot{\epsilon} = 10^4$,	$s_0 = 6.89 \text{ mm}$,	$n/V = 5.84 / \text{cm}^3$
$\dot{\epsilon} = 10^5$,	$s_0 = 1.48 \text{ mm}$,	$n/V = 584 / \text{cm}^3$
$\dot{\epsilon} = 10^6$,	$s_0 = 0.32 \text{ mm}$,	$n/V = 58400 / \text{cm}^3$

Consider, for an example, an aluminum sphere of radius 1 cm expanding at a velocity of 6 km/sec. The average strain rate is $\dot{\epsilon}_0 = u/r = 6 \times 10^5$. One thus expects the sphere would break down into fragment particles of an average size less than 1 mm.

Substitution of Eq. (21) into Eqs. (2) and (3) give the other corresponding expressions derived by Grady as follows:

Time to break-down:

$$t_f = \frac{1}{c} \left(\frac{\sqrt{3} K_c}{\sqrt{2} \rho c \dot{\epsilon}} \right)^{2/3}, \quad (22)$$

and the strength of tensile wave at break-down:

$$P_t = \left(\frac{3}{2} \rho c K_c^2 \dot{\epsilon} \right)^{1/3} \quad (23)$$

PARTICLE SIZE DISTRIBUTION

The horizon condition, Eq. (3), has an important implication in particle size distribution. Observe that the wave length (λ) is related to the frequency (ω) and wave speed (c) by

$$\lambda \omega = c. \quad (24)$$

Replacing c in Eq. (3) by the above equation and ω by $1/t$, the horizon condition becomes

$$s \leq 2t\lambda\omega = 2\lambda. \quad (25)$$

The above equation suggests that the particle size can not be larger than two-times the corresponding wavelength of the tensile wave in the expanding body. Furthermore, if the tensile wave in the body is composed of waves of different wavelength, Eq. (25) appears to imply that the distribution of fragment size depends upon the spectral power of the tensile wave in the body.

Since a material sample of volume V is assumed to be subjected to a hydrostatic expansion at a constant strain rate $\dot{\epsilon}$, the expansion wave can be represented by the strain history

$$\epsilon(t) = \begin{cases} \dot{\epsilon}t, & 0 \leq t \leq t_f \\ 0, & \text{otherwise} \end{cases}, \quad (26)$$

where t_f is the time to fracture. The assumption of size distribution being proportional to the frequency spectrum of the expansion wave suggests the following relation:

$$s(\omega) = \beta |\epsilon(\omega)|^2, \quad (27)$$

where $|\epsilon(\omega)|^2$ is spectral power of the strain history, $s(\omega)$ is the size distribution, and β is a proportionality constant. Since the strain $\epsilon(t)$ is produced by the reflected waves, it is reasonable to

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assume that the spectral distribution of $\epsilon(\omega)$ is a banded distribution with a central frequency ω_0 .

The quantity $|\epsilon(\omega)|$ is determined by using the Fourier transform, giving

$$|\epsilon(\omega)|^2 = \left| \frac{1}{2\pi} \int_{-\infty}^{\infty} \epsilon(t) e^{-i\omega t} dt \right|^2 \quad (28)$$

Equations (26) and (28) give the result

$$|\epsilon(\omega)|^2 = \left(\frac{\dot{\epsilon} t_f^2}{2\pi} \right)^2 \frac{[\eta^2 - 2(\cos \eta + \eta \sin \eta - 1)]}{\eta^4} \quad (29)$$

with $\eta = (\omega - \omega_0)t_f$.

Equations (27) and (29) give the size distribution once the constant β is known. We can determine this constant by using Eqs. (27) and (29) to define an average particle size and equate the result to the definition of average particle size derived in the last section as represented in Eq. (21). We can define an average particle size in terms of the size distribution in Eq. (27) as follows:

$$s_{ave} = \frac{\int_{-\infty}^{\infty} s(\eta)^2 d\eta}{\int_{-\infty}^{\infty} s(\eta) d\eta} \quad (30)$$

Substituting Eq. (27) and (29) into the above equation yields

$$s_{ave} = \beta \left(\frac{\dot{\epsilon} t_f^2}{2\pi} \right)^2 R \quad (31)$$

where R is defined as

$$R = \frac{\int_{-\infty}^{\infty} f(\eta)^2 d\eta}{\int_{-\infty}^{\infty} f(\eta) d\eta}, \quad (32)$$

with

$$f(\eta) = [\eta^2 - 2(\cos \eta + \eta \sin \eta - 1)] / \eta^4$$

Evaluation of the integrals in Eq. (32) gives $R = 0.1578968$. Equating the definitions of the average particle size as they appear in Eqs. (21) and (31) leads to the result

$$\beta = \frac{1}{R} \left(\frac{2\pi}{\dot{\epsilon} t_f^2} \right)^2 s_0 \quad (33)$$

where s_0 is defined in Eq. (21).

Equations (27), (29), and (33) yield the particle size distribution

$$s(\eta) = \frac{s_0}{R} [\eta^2 - 2(\cos \eta + \eta \sin \eta - 1)] / \eta^4 \quad (34)$$



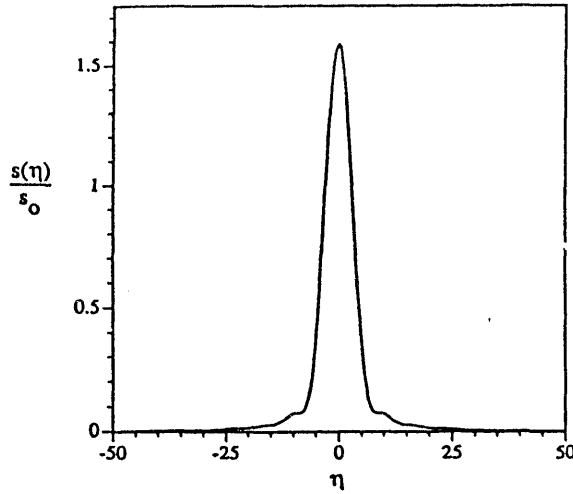


Fig. 2: Particle Size versus Dimensionless Frequency

A plot of this distribution as a function of the dimensionless frequency parameter η is displayed in Fig. 2. The figure suggests that the low frequency components give rise to the larger fragment sizes whereas, the higher frequency components yield the smaller sizes. It is interesting to note that the largest fragment sizes are roughly 60% larger than the average size. If one replots the size distribution with the vertical scale modified to enhance the details at the shoulder of the peak, one will notice a number of plateaus suggesting that certain sizes are generated by wave components in compact frequency domains. Recall that $\eta = \omega t_f$, where t_f denotes the time to fracture. If one acknowledges the "horizon condition", and assumes that fracture occurs in minimum time, then t_f can be represented by the Grady relation (1988)

$$t_f = (t_f)_{\min} = \frac{1}{c} \left(\frac{\sqrt{3} K_{\epsilon}}{\rho c \epsilon} \right)^{2/3} \quad (35)$$

It should be emphasized that the above observations result from the postulation of a horizontal condition. Experimental evidence is needed for its verification.

EQUATION OF STATE DURING BREAKING DOWN

Equations (20), (22) and (23) give a description of the body at its final stage of breaking down. At this instant, the body is at a state of equilibrium again. In order to describe the behavior of material during its fracture growth-to-failure stage, a model is needed. The study of constitutive models for dynamic failure of materials has been undertaken by many authors (Carroll and Holt, 1972; Cochran and Banner, 1977; Seaman, Curran and Shockey, 1976; Asay and Kerley, 1987). In their studies, the material was modelled as a porous medium, and the failure (or loss of integrity) of material was characterized by the increase of pore size (or void volume) in the material. In this study, a different approach is taken. We argue that since the hypervelocity impact produces a very large stress in the material in a very short time period, the material is not expected to experience a significant amount of void growth during the period of internal crack nucleation and growth. Therefore, it seems reasonable to assume that, during this period, the material behaves as an elastic material with degrading moduli which are caused by the growth of internal cracks in the material.

The size of fragments, in an approximate manner, can be considered to be determined by the intersecting crack network in the volume. If one models the fragments as spheres as described in section II, when there is one crack (i.e. $n_c = 1$), the body can be considered to break-down eventually

into two spheres ($n = 2$); and when $n_c = 2$, $n = 4$, and so on. The relationship between the number of cracks and the number of spherical fragments is $n = 2n_c$. Thus, the amount of energy dissipated, when the number of cracks in the volume grows, can be expressed by replacing n in Eq. (11) by $2n_c$ to give

$$\Gamma = (9\pi)^{1/3} \left(\frac{K_c^2}{\rho c^2} \right) n_c^{1/3} V^{2/3} \quad (36)$$

Assuming that the effect of internal cracks on the material behavior is reflected in the bulk modulus B_c of the cracked material, the change of strain energy in the material when the body cracks under the action of a constant expansion pressure P (or tensile stress σ) must be equal to the energy dissipated by the cracking process, i.e.,

$$\frac{1}{2} \sigma^2 \left(\frac{1}{B_c} - \frac{1}{B} \right) V = (9\pi)^{1/3} \left(\frac{K_c^2}{\rho c^2} \right) n_c^{1/3} V^{2/3} \quad (37)$$

Replacing the bulk modulus B in the above equation by compressibility $C (= 1/B)$, and making use of relation $n = 2n_c$ and Eq. (20), the equation which relates the change of compressibility (ΔC) [or the degradation of material property during the process of breaking down] can be written as:

$$\Delta C = \left(\frac{18K_c^4}{\rho c^4} \right)^{1/3} \frac{\dot{\epsilon}^{2/3}}{\sigma^2} \quad (38)$$

Equation (38) describes the degradation of material compressibility resulting from the growth of internal cracks during the fragmentation process. When the number of internal cracks equals

$$n_c = \frac{1}{4\pi} \left(\frac{c\rho\dot{\epsilon}}{K_c} \right)^2 V \quad (39)$$

the internal cracking process is completed, and the body breaks down catastrophically into " n " fragments, and the tensile stress in the body drops to zero abruptly.

CONCLUDING REMARKS

A theory for dynamic fragmentation of brittle materials, based on thermodynamic arguments, has been presented. The expressions for average fragment size and number of fragments are identical to those derived by Grady. We have extended the previous work by obtaining descriptions of fragment size distribution and compressibility change due to the fragmentation process. The size distribution is assumed to be proportional to the spectral power of the strain history and a sample distribution has been presented for a fragmentation process corresponding to a constant rate strain history. These results should provide insight into the process of fragmentation of brittle materials from hypervelocity impact. Furthermore, the description of compressibility change should be useful in computational studies of fragmentation.

ACKNOWLEDGEMENT

The work has been supported in part by a grant NAG9-114 from the Johnson Space Center - NASA to the first author (CHY). The reported study was developed when the first author was with Sandia National Laboratories as a summer faculty member (1992). The hospitality of SNL is gratefully acknowledged.

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