Final Report for 4000136273

Modeling Dynamic Fracture of Cryogenic Pellets

June 30, 2016 by P. Parks

Introduction

This work is part of an investigation with the long-range objective of predicting the size distribution function and velocity dispersion of shattered pellet fragments after a large cryogenic pellet impacts a solid surface at high velocity. The study is vitally important for the shattered pellet injection (SPI) technique, one of the leading technologies being implemented at ORNL for the mitigation of disruption damage on current tokamaks and ITER. The report contains three parts that are somewhat interwoven. In Part I we formulated a self-similar model for the expansion dynamics and velocity dispersion of the debris cloud following pellet impact against a thick (rigid) target plate. Also presented in Part I is an analytical fracture model that predicts the nominal or mean size of the fragments in the debris cloud and agrees well with known SPI data. The aim of Part II is to gain an understanding of the pellet fracturing process when a pellet is shattered inside a miter tube with a sharp bend. Because miter tubes have a thin stainless steel (SS) wall a permanent deformation (dishing) of the wall is produced at the site of the impact. A review of the literature indicates that most projectile impact on thin plates are those for which the target is deformed and the projectile is perfectly rigid. Such impacts result in "projectile embedding" where the projectile speed is reduced to zero during the interaction so that all the kinetic energy (KE) of the projectile goes into the energy stored in plastic deformation. Much of the literature deals with perforation of the target. The problem here is quite different; the softer pellet easily undergoes complete material failure causing only a small transfer of KE to stored energy of wall deformation. For the real miter tube, we derived a strain energy function for the wall deflection using a non-linear (plastic) stress-strain relation for 304 SS. Using a dishing profile identical to the linear Kirchkoff-Love profile (for lack of a rigorously derived profile) we derived the strain energy associated with the deflection and applied a virtual work principle to find a relationship between the impact (load) pressure to the measured wall deflection depth. The inferred impact pressure was in good agreement with the expected pressure for oblique cryogenic pellet impacts where the pellet shear stress causing cleavage fracture is well above the yield stress for pure shear. The section is concluded with additional discussion on how this wall deformation data lends further support to the analytical fracture model presented in Part I. In Part III we present three different size distribution models. A summary, with a few brief suggestions for a follow on study, is provided at the end of this report.

Part I Expansion dynamics of debris cloud, energetics and nominal size of fragments

Ia. Debris plume velocity dispersion and expansion dynamics

In Shattered Pellet Injection (SPI) a large cryogenic pellet traveling at high velocity inside a "breaker tube" strikes the curved section of the tube at oblique angle. The impact causes the pellet to disintegrate, and generates a spray of smaller fragments called the "debris plume." The debris plume consists of a mixture of smaller chunky fragments with a considerable fraction of very finely divided particles or vaporous material, "fog". All SPI methods produce a range of fragment sizes, so in order to design the SPI system it is necessary to have a theory that can predict a mean size that in some way characterizes the total spray. A histogram of different sizes can be obtained experimentally and used to verify the mean size predicted from theory. Good plasma penetration is expected only for the solid fragment component, especially for fragment sizes exceeding > 0.1 mm. The evolution of the fragment swarm may be described from the standpoint of continuum mechanics, which assumes that around any point there exists a volume element which is both large enough in comparison with the microscopic structure of the debris material and at the same time small enough for the state of the material to be considered uniform throughout it. The 1-D continuity equation within the paraxial approximation describes the evolution of the mass density $\rho(s,t)$

$$\frac{\partial\rho}{\partial t}+\frac{1}{A(s)}\frac{\partial}{\partial s}\big(A(s)\rho(s,t)\upsilon(s,t)\big)=0\ , \tag{1}$$

where υ is the bulk longitudinal flow velocity of the fragment ensemble through the cross sectional area $A(s)$ and s is the longitudinal distance measured from the point $s=0$ where the large pellet impacts the bent section of the breaker tube and is completely shattered. The smaller pellet fragments, have a certain size and velocity distribution. Initially, the debris plume is quite dense (infinitely dense for an idealized point-like impact). However, because the fragments have different initial velocities, the plume becomes progressively more "stretched out" as time goes on. Inside the breaker tube, the debris plume undergoes a lengthwise elongation, since the walls of the tube limit lateral expansion. The diameter of the breaker tube for ITER is $D = 4$ cm and therefore A is a constant for $s < s_E$, where $s_E \approx 25$ cm is the location of the tube exit plane in ITER. Whatever residual velocity the fragments have in the lateral direction before they exit the tube will be manifest by a divergence of the fragment plume as it comes out of the tube into the free space and plasma regions, $s > s_E$. According to Larry Baylor, the full divergence angle of the fragment spray is observed to be about 20 degrees. Thus beyond the tube exit plane, A (s) could be assumed to vary with longitudinal distance $A = A(s)$ with no time dependence. In ITER the diameter of the plume at the plasma surface, $s_1 = 35 - 40$ cm, is estimated to be somewhere in the range $D_1 \in (7.6, 9.5)$ cm. A realistic description of the SPI neutral source inside the plasma requires the mass per unit length, $\Sigma(s,t) = \rho A$, velocity υ, and mass flow rate $\Sigma\upsilon$. Since A is not time-dependent, Σ satisfies a 1-D time-dependent equation of the form

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial}{\partial s}\big(\Sigma(s,t)\upsilon(s,t)\big) = 0 , \tag{2}$$

To solve this equation we transform to the CM coordinate system (z,t) defined by $z = s - \upsilon_{\rm cm} t$, where $\upsilon_{\rm cm}$ is the velocity of the center-of-mass of the whole debris plume. Since

$$\left.\frac{\partial \Sigma}{\partial t}\right)_s = \left.\frac{\partial \Sigma}{\partial z}\right)_t \frac{\partial z}{\partial t} + \left.\frac{\partial \Sigma}{\partial t}\right)_z , \tag{3}$$

we can transform Eq. (2) into a continuity equation involving the CM coordinates:

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial}{\partial z}\big(\Sigma(z,t)u(z,t)\big) = 0 , \tag{4}$$

where $u = \upsilon - \upsilon_{cm}$ is the velocity of the debris cloud in the CM system, responsible for the velocity dispersion and lengthwise stretching of the plume. For oblique impacts, assuming a free-slip surface interaction, the debris cloud should expand symmetrically in the CM frame.

Therefore, we can write $u(z,t) = -u(-z,t)$. The CM velocity may be assumed to have the self-similar form

$$u(z,t) = \frac{z}{L(t)}\dot{L}(t)\ , \quad \text{for } |z| < L(t) \tag{5}$$

where $L(t)$ is the half-length of the debris plume and the over dot stands for a time derivative. Transforming to new similarity variables $\xi = z / L(t)$ and t, Eq. (3) has the general solution

$$\Sigma(\xi,t) = \frac{g(\xi)}{L(t)}, \quad \text{for } -1 \le \xi \le 1$$

$$= 0 \qquad \text{for } |\xi| > 1 \tag{6}$$

where $g(\xi)$ is an arbitrary "shape-preserving" plume profile. The variable ξ is also a Lagrangian variable since the amount of mass contained within a cell bounded by any two planes ξ_1 and ξ_1 remains fixed even though the plume expands. Also the highest velocity the fragments can have is $\upsilon_{\max} = \upsilon_{cm} + \dot{L}$, and the least is $\upsilon_{\max} = \upsilon_{cm} - \dot{L}$. For a point-like impact ("explosion") we could take $L(t) = \Delta\upsilon \cdot t$ where $t = 0$ is the moment of impact. In that case, the velocities of the fragments lie within the range $\upsilon \in (\upsilon_{cm} - \Delta\upsilon, \upsilon_{cm} + \Delta\upsilon)$, and the total length of the plume at time t will be $L_{plume} = 2L(t) = 2\Delta\upsilon \cdot t$. From experimental measurements, a typical value for the dispersion coefficient is $\Delta\upsilon / \upsilon_{cm} \sim 1/3$. We could also choose a family of profiles having the "Super-Gaussian" structure:

$$g(\xi) = C\exp\left(-\lambda\xi^{2k}\right) \quad \text{for } -1 \le \xi \le 1 \tag{7}$$

The parameter λ can be adjusted to conform to actual SPI plume half widths currently being studied at ORNL. The k parameter controls the "flatness" of the profile: to avoid a discontinuity in the derivative of the profile at the center-of mass location, $\xi = 0$, we must use values of k greater than unity. Transforming back to the laboratory frame the velocity and density become

$$\upsilon(s,t) = \upsilon_0 + \frac{\dot{L}(t)}{L(t)}\left(s - \upsilon_{cm}t\right) \quad |\, s - \upsilon_{cm}t \,| \le L(t)\,, \tag{8a}$$

$$\Sigma(s,t) = \frac{C}{L(t)} \exp\left[-\lambda \left(\frac{s - \upsilon_{cm}t}{L(t)}\right)^{2k}\right] \qquad |\, s - \upsilon_{cm}t \,| \le L(t)\,, \tag{8b}$$

The left (back) and right (front) moving boundaries of the plume are respectively, $s_- = \upsilon_{cm}t - L(t)$ and $s_+ = \upsilon_{cm}t + L(t)$. With M_0 the mass of the pre-impact pellet, the mass constraint

$$\int_{s_-}^{s_+} \Sigma(s,t)\,ds = \int_{-1}^{1} g(\xi)\,d\xi = M_0\,, \tag{8c}$$

determines the normalization constant:

$$C = \frac{M_0 k \lambda^{(2k)^{-1}}}{\Gamma\left(1/2k\right) - \Gamma\left(1/2k,\, \lambda\right)}\,, \tag{8d}$$

where $\Gamma(z)$ and $\Gamma(y,z)$ represents the ordinary and incomplete gamma functions, respectively. It can be verified that these formula satisfy the continuity equation (2) in the laboratory frame. The mass flux Φ_M (kg/s) passing through any *fixed surface* s is therefore, $\Phi_M = \Sigma(s,t)\upsilon(s,t)$ (kg/s). As a consistency check, the following general relation can be verified by making some straightforward mathematical transformations,

$$\int_{t_F}^{t_B} \Sigma(s,t)\upsilon(s,t)\,dt = M_0\,, \tag{9}$$

where t_F and t_B are respectively the times that the front surface and back surface of the plume cross the fixed surface, as implicitly given by

$$s = \upsilon_{cm} t_F + L(t_F)$$
$$s = \upsilon_{cm} t_B + L(t_B). \tag{10}$$

The time for the plume to enter the plasma is $\Delta t = t_B - t_F$. In the case of a point-like impact, $L = \Delta\upsilon \cdot t$, this time is given by

$$\Delta t = \frac{2s_1}{\upsilon_0}\left[\frac{\Delta\upsilon / \upsilon_{cm}}{1-(\Delta\upsilon / \upsilon_{cm})^2}\right], \tag{11}$$

and the *full length* of the plume at the moment the back surface crosses the plasma surface s_1 will be

$$2L_1 = \frac{2s_1(\Delta\upsilon / \upsilon_{cm})}{1-(\Delta\upsilon / \upsilon_{cm})}. \tag{12}$$

For example, taking $\upsilon_{cm} \sim 300\,\text{m/s}$, dispersion coefficient $\Delta\upsilon / \upsilon_{cm} \sim 1/3$, and $s_1 = 40\,\text{cm}$, we get $\Delta t = 1\,\text{ms}$, and $2L_1 = 40$ cm. As previously emphasized [1], the SPI delivery time is "delta-function" like, unlike gas injection, which takes more than 10 ms.

Now the fate of the shattered pellet material once inside the plasma depends on how the debris mass is distributed among the different fragment sizes. The fragment discreteness enters the problem, because the bigger fragments travel farther in the plasma than smaller fragments. The fragment size distribution function is $\bar{f}(r,s,t)$, where $\bar{f}(r,s,t)drds$ is the number of fragments with a radius between r and $r+dr$ located between s and $s+ds$, at time t. The size distribution is assumed to be independent of the space coordinate, so separation of variables can be used to write $\bar{f}(r,s,t) = h(s,t)f(r)$. Details of the source model including the size distribution will be reported in future work.

What is the center of mass velocity υ_{cm}? If the pellet were gliding along a perfectly smooth walled tube with a gradual bend angle then we could say that $\upsilon_{cm} = \upsilon_0$ where υ_0 is the original velocity of the intact pellet before encountering the tube surface. However pellets do not seem to glide; instead, they appear to impact the bent section of the breaker tube suddenly at some oblique angle which is close to the angle of the bend. For such sudden impacts there is no transfer of momentum from the normal component to the tangential component via the normal forces acting on the pellet by the tube wall that allows for the *continuous* change in the pellet's direction. For sudden impacts, and again for free-slip conditions, we must invoke conservation of momentum tangent to the impacting surface, giving

$$\upsilon_{\text{cm}} = \upsilon_0 \cos\theta \ , \tag{13}$$

where υ_0 is the pellet velocity, and θ is the angle between the pellet's line of flight and the surface (neglecting curvature of tube wall). Thus, if we want a high debris cloud velocity then we should try to achieve shallow impact angles, $\theta << 1$. Energy conservation can be written as

$$\frac{1}{2} M_0 \upsilon_0^2 = \frac{1}{2} M_0 \upsilon_{\text{cm}}^2 + E_x \ , \tag{14}$$

where excess energy E_x is the remaining energy available for pellet disintegration and dispersion of the fragment debris in the CM system. (The equation here assumes wall is thick so that no energy will be transferred to it during the impact.) From these two conservation equations, we have

$$E_x = \frac{M_0}{2} \upsilon_0^2 \sin^2\theta \ , \tag{15}$$

the excess energy can be further partitioned as

$$E_x = E_f + E_k \ , \tag{16}$$

where E_f is the energy expended in shattering the pellet into many fragments, and E_k is the collective kinetic energy of the expanding fragments. Now E_k itself can be divided into the kinetic energy of the fragment ensemble in the CM frame associated with longitudinal expansion, $\int (\rho u^2 / 2) dV$, which can be calculated based on the above model, and the radial kinetic energy associated with plume divergence, which is just the remainder.

Ib. Cleavage fracture of cryogenic pellets and nominal fragment size

The process of impact fragmentation creates new surfaces. This takes work energy. The specific energy expended in creating new free surfaces is γ (J/meter squared). We have worked out what its value is for pure deuterium ice in APPENDIX A. For now, let us suppose that each fragment is spherical in shape. If we generate N fragments with mean radius $\bar{r}$, then the total energy expended in fracturing will be $E_f = 4\pi r^2 N\gamma$, or upon eliminating N this is

$$E_f = \frac{3M_0\gamma}{\rho_0\bar{r}}, \tag{17}$$

where, ρ_0 is the mass density of the solid. Warm fragments, especially the small ones with large surface to volume ratios, can generate vaporous material, although the process will be arrested as vaporization of any isolated body is accompanied by its cooling. This is a problem left for future work. We will show that only a small potion of the excess energy goes into fracturing, i.e., $E_f << E_k$. The energy based fragmentation theory [1,2] provides the following relation

$$a = 3\left(\frac{\rho_0\dot{\varepsilon}^2}{5\gamma}\right)^{1/3}, \tag{22}$$

where $\dot{\varepsilon}$ is the time rate of change of the deformation strain, and a is the fragment surface area to volumetric ratio: for spherical fragments this would be $a = 3/r$. Consequently, the mean fragment size is

$$\bar{r} = 3\left(\frac{5\gamma}{\rho_0\dot{\varepsilon}^2}\right)^{1/3}, \tag{23}$$

Using the results in Part II, it can be shown that the type of deformation strain on the large pellet caused by impact is one of *shear stress* that leads to *cleavage fracture*, rather than one of *simple tensile forces* that cause to spallation from the rear surface of the pellet as is the case in high velocity metallic projectiles that have orders of magnitude higher material strengths. We see no visible evidence for rear surface spallation from images taken by Combs et al of dual-layer neon/deuterium pellets impacting inclined steel plates [See Ref 1 in Part II]. An estimate of the shearing strain rate is given by

$$\dot{\varepsilon} = \dot{\tau}_{shear} = \frac{1}{2}\left(\frac{\partial \upsilon_z}{\partial r} + \frac{\partial \upsilon_r}{\partial z}\right) \sim \frac{\upsilon_n \sin\theta}{D_p}, \tag{24}$$

where $\upsilon_n = \upsilon_0 \sin\theta$ is the normal impact velocity component, D_p is the diameter of the large pellet, z is the direction normal to target surface, r is tangent to surface, and: (1) cylindrical pellet axis is assumed parallel to flight direction (no pitch, no yaw) and (2) negligible sliding friction (free-slip surface conditions). Putting (24) into (23) gives the final estimate of the mean fragment diameter

$$d_{frag} = 6\left(\frac{5\gamma D_p^2}{\rho_0 \upsilon_0^2 \sin^4\theta}\right)^{1/3}, \tag{25}$$

Let us put some numbers into this formula. For pure deuterium SPI we calculated in Appendix A the free surface energy density to be $\gamma = 0.00406\ \mathrm{J/m^2}$. Taking, $D_p \sim 0.0144\ \mathrm{m}$, $\upsilon_0 \sim 500\ \mathrm{m/s}$, $\theta \sim 22.5\,\mathrm{deg}$, $\rho_0 = 200\ \mathrm{kg/m^3}$, gives $d_{frag} = 0.946\ \mathrm{mm}$. This result is in good accord with the mean fragment diameter of 0.916 mm based on size histogram data from the 2009 ORNL experiments. Size data was obtained by impacting the debris cloud on a downstream brass witness foil and measuring the size of crater impacts scattered over the surface of the foil. However, the witness foil method is not capable of detecting fragments below certain size: certainly fine-scale fragment granules cannot be accounted for in this type of diagnostic. It is therefore possible that the experiments could overestimate the mean fragment size because the experiments are only sampling the large fragments in the tail of the size distribution function. The strain rate is $\dot{\varepsilon} \sim$ 5000/s. In the fracture of shale oil at this strain rate the nominal fragment size would be a few mm [1]. This is because the strength of material, related to the surface energy γ is so much higher than it is for the cryogens, although the mass density of shale oil is larger by a factor of ten. More recent experiments carried out in May 2016 used a pellet composed of a homogeneous mixture of neon and deuterium (60% neon, 40% deuterium molar concentrations), shattered by injecting it into an S-bend curved tube. In this experiment the parameter are: $D_p \sim 0.01$ m, $\upsilon_0 \sim 440$ m/s, $\theta \sim 12.5$ deg, $\rho_0 = 834$ kg/m^3 (see first equation in Part II), giving $d_{frag} = 1.25$ mm. This result is very encouraging because the S-bend witness plate diagnostic showed that a significant amount of the debris cloud was composed of chunky fragments with diameters of this order. A more detailed analysis of the data is forthcoming. Finally, in February 2016 a breaker tube with a 65 degree bend was used to shatter a neon-deuterium composite pellet traveling at velocity $V_0 = 500$ m/s. The pellet parameters are given in the next section. Using the formula (25) we found that the nominal fragment was very small, $d_{frag} = 0.301$ mm. Images of the spray of debris material coming out of the tube indicated that most of the material was in the form of fine scale mist or fog; it was well collimated and visible so it could not have been a pure vapor. The brass witness foil did not show any visible impact craters, indicating that the solid fragments produced had to have been much smaller and/or have much reduced speed compared fragments produced in the other two experiments, consistent with the theory result.

Now the ratio E_f / E_x can be written as

$$\frac{E_f}{E_x} = \frac{6\gamma / \bar{r}}{\rho_0 \upsilon_0^2 \sin^2 \theta}, \tag{26}$$

For the 2009 experiment this ratio is $E_f / E_x = 2.1 \times 10^{-5}$. Since $E_f << E_x$, then $E_x \cong E_k$. The fundamental implication here is that SPI impacts are of such strength that the excess energy is orders of magnitude above the threshold energy for fragmentation onset E_x^{thres} in which no kinetic energy is generated, $E_k \to 0$ and $E_x^{thres} = E_f$. A simple everyday analogy would be in the dropping of a fragile object, for example a glass sphere. Dropped from a certain height a glass sphere just barely shatters with its fragments lying close to the impact location because there is no residual kinetic energy available to scatter its fragments. In other words there is a threshold onset velocity that is just sufficient to cause catastrophic failure and shattering. If the sphere is dropped from a much greater distance, the fragments may scatter out to great distances simply because there is more impact energy available for the collective kinetic energy of the fragments. For metallic projectiles this threshold velocity is about 2 km/s [3]. For the cryogens it must be orders of magnitude smaller because the strength of material, related to γ, is so much lower. As shown in the Part II the impact pressures generated are extremely large ~ 146 MPa (see Eq. 29) compared to the shear strength of solid deuterium ~ 0.1 MPa for typical pellet temperatures. To reduce the stress and strain rates we can think of alternate, more benign options for shattering a large pellet into larger fragments while simultaneously maintaining a large forward-directed CM debris cloud velocity. These options can be taken up in future investigations.

Appendix A to Part I: Calculation of the surface energy and cohesive energy of solid deuterium

To motivate the study of the fracture we start with our model for the theoretical cohesive strength for the solid deuterium. We relate this critical parameter to the empirically known elastic constants of continuum mechanics, which are fairly well known for solid deuterium and to a lesser extent neon and argon. We want predict the conditions leading to pellet fracture under tensile stress. This exercise serves to lay the foundation for the proposed theoretical approach and bridge the gap between the continuum mechanics and the atomic physics approach to fracture mechanics. Atomistic simulations yield "*ab initio*" information about crack tip formation and deformation at length scales unattainable by experimental measurement and unpredictable by continuum elasticity theory and, hence, gives additional insights into the complex mechanisms of materials failure.

The intermolecular/atomic bonds formed in the condensed phase of deuterium, neon, and argon are much simpler than in metallic bonding, which requires quantum mechanical density functional theory for its description, since valence electrons are free to roam about. In the cryogens the intermolecular forces are dominated by the weak Van der Waals forces. The potential energy in the solid state can be written as a sum of effective interaction potentials

$$U_i \approx 1/2 \sum_{i<j} \phi(d_{ij}) \quad , \tag{A1}$$

where $\phi(d)$ is the two-body interaction potential energy of an isolated pair separated by distance d_{ij}. The dominant piece is the (12-6) Lennard-Jones (LJ) potential, which is certainly valid for inert gas solids. For pure ortho-deuterium, which prevails at temperatures above 4.2 K, the LJ potential is approximately valid since the D_2 molecules are in the ground rotational state (rotational quantum number $J=0$) and interact essentially via spherically symmetric van der Waals forces [V. V. Goldman, J. Low Temperature Physics **24** 297 (1976)]. Many body forces such as the three-body Axilrod-Teller-Muto (ATM) force also play a role to some extent and should be included. Following [I. F. Silvera and V. V. Goldman (J. Chem Phys. 69 4209 (1978)], we incorporate the three-body ATM interaction in two-body form as a $1/d_{ij}^9$ potential so as to capture the basic three-body distance scaling. Simplifying further to include only nearest neighbor interactions, we propose this expression

$$U(x) = U_0\left(\frac{1-q}{x^{12}} - \frac{2+q}{x^6} + \frac{2q}{x^9}\right), \qquad x = d/d_0 \quad , \tag{A2}$$

where d is the distance between nearest neighbor molecules comprising the crystal lattice (lattice spacing), and d_0 is the zero-pressure equilibrium spacing where the potential energy is minimized, $U = -U_0$. Ortho-D_2 crystallizes in a hexagonal close packing (HCP) structure. Ne and Ar solidify in the face-centered cubic (FCC) arrangement). In the HCP lattice, 12 D_2 molecules surround a central molecule so that d is the same for any two neighboring molecules. Therefore, U represents the *deviation in energy per molecule* as *all molecules* are simultaneously displaced from their equilibrium position in the lattice. The work per molecule required to separate all the molecules to an infinite distance apart $d \to \infty$, $U \to 0$ is the binding energy per molecule U_0. For solid D_2, $U_0 = 0.0114$ eV, and the molecular volume density is $n_0 = 3\times 10^{28}$ m^{-3}, so $d_0 = 2^{1/6} n_0^{-1/3} = 0.361$ nm, the latter is in agreement with [M. Nielsen and H.B. Moller, Physical Review B **3**, 4383 (1970)]. and [S.N. Ishmaev et al., Sov. Phys. JETP **62**, 721 (1985)]. In our representation, the constant $q(>0)$ describes the strength of the repulsive $1/x^9$ ATM force, determined by matching empirical data for the bulk modulus K (at zero pressure) with the theoretically calculated value using Eq. (A2).

During impact, large shear stresses develop in the pellet. Only shear stress or tensile stress tension causes fracture, not pure compression. We ask now what is the theoretical tensile stress that causes fracture in solid D_2. Fracture is caused by a crack growing catastrophically: if the cracks are unstable they propagate link up and cause the material can break apart or fracture into smaller pieces. The process of crack growth reduces the potential energy associated with the surrounding stress fields. The pressure is given by $P = -\partial F/\partial V$ at constant temperature (which is essentially zero in this case), where F is the free energy of the solid, and V is the volume. The unit cell of the HCP crystal lattice is a convex polyhedron named *triangular orthobicupola*, formed by connecting the centers of the 12 molecules surrounding the central core molecule. The fractional number of molecules per unit cell is therefore $N_{cell} = 10/3$, and the cell volume is $V_{cell} = 5\sqrt{2}r^3/3$. The free energy per unit cell is clearly $F_{cell} = U \cdot N_{cell}$. So if I assume that the unit cell remains geometrically similar under contraction/dilation the pressure in the solid is actually

$$P(x) = -\frac{N_{cell}\partial U/\partial r}{\partial V_{cell}/\partial r} = \frac{2^{3/2}U_0}{d_0^3}G(x) \quad , \tag{A3}$$

where

$$G(x) = \frac{2(1-q)}{x^{15}} - \frac{2+q}{x^9} + \frac{3q}{x^{12}} \quad . \tag{A4}$$

The bulk modulus $K = -VdP/dV$ evaluated at zero pressure is $-(1/3)dP/dx$ evaluated at $x = 1$, so

$$\begin{aligned} K &= \frac{U_0 8\sqrt{2}}{d_0^3}(1-q/4) \\ &= 440.7(1-q/4) \quad \text{MPa} \end{aligned} \tag{A5}$$

Two references quote values for the bulk modulus of solid deuterium: 318 MPa from [I. F. Silvera and V. V. Goldman (J. Chem Phys. 69 4209 (1978)] and 335 MPa from [D. A. Young, Phase Diagrams of the elements, Univ. California Press, Berkeley, 1991, p. 268-285]. We therefore choose $q = 1$ in Eq. (B5), which gives a calculated value K = 331 MPa. Both P and U are plotted in Fig. (1) as a function of normalized lattice spacing x. (Not shown in this report) *The solid is under tensile stress (* $P < 0$*) for* $x > 1$*, and compressive stress* $P > 0$ *for* $x < 1$. The maximum tensile stress $\sigma_{coh} = -P_{coh}(>0)$, denoted by point A, represents the *theoretical cohesive strength* of the material. This is

$$\sigma_{coh} = 2^{3/2}\left(\frac{3}{4}\right)^4 \frac{U_0}{d_0^3} = 34.87 \quad \text{MPa} \quad , \tag{A6}$$

If the tensile stress exceeds the value, “runaway” debonding occurs resulting in material fracture. Knowing the planar density of the HCP lattice, we can calculate the surface free energy:

$$\gamma = \frac{1}{2\cdot 3^{1/2}} \frac{U_0}{d_0^2} = 0.00406 \text{ J/m}^2 \quad , \tag{A7}$$

This is an important quantity used in the text, because energy is required to form new surfaces created in the fracture process, and this energy has to come from the elastic strain energy associated with the stress pulse at impact. It is not surprising that γ turns out to be somewhat larger than the empirical value of the surface tension for liquid deuterium near the triple point, $\gamma_{liq} = 0.0038 \text{ J/m}^2$ [5]. Since Young's modulus E is related to Poisson's ratio ν and the bulk modulus K by $E = 3K(1-2\nu)$, we can now express σ_{coh} in terms of γ and E, respectively

$$\sigma_{coh} = 2^{5/2} 3^{1/2} \left(\frac{3}{4}\right)^4 \frac{\gamma}{d_0} \quad , \tag{A8a}$$

$$\sigma_{coh} = \frac{9E}{256(1-2\nu)} \quad , \tag{A8b}$$

Measured values of ν for solid D_2 range from $\nu = 0.3$ to 0.31 [5]. The threshold stress required to shatter the pellet is actually considerably lower than the theoretical value σ_{coh}. Real materials contain initial defects in the form of small cracks or voids. Since the stress field is locally concentrated near such flaws what matters then is the tensile stress at the crack tip. We shall explore crack growth and link up in a future investigation.

References to Part I

[1] L.R. Baylor et al, *Fusion Science and Technology* **68**, 211 (2015)

[2] D.E. Grady, *J. Appl Phys*, **53** 322 (1982)

[3] D.E. Grady, *J. Mech Phys Sol*. **36** 353 (1988)

[4] I.H.G. Livingstone, et al *Int. J. of Impact Eng*. **26** 453 (2001)

[5] P.C. Souers, *Hydrogen Properties for Fusion Energy*, University of California Press, Berkeley, 1986

Part II Deformation of mitre tube by pellet impact and impact pressures

IIa. The ORNL experimental data

In February 2016, a breaker tube with a 65 degree bend was used to shatter a neon-deuterium composite pellet traveling at velocity $V_0 = 500$ m/s. The composition of the solid pellet was a homogeneous mixture of 0.414 moles of D_2 (0.828 moles of D) and 0.551 moles of Ne. The total mass of the pellet is therefore $M_{pell} = 12.7885$ g, with mass fraction of Ne given by $X_{Ne} = M_{Ne} / M_{pell} = 0.8696$. Using respective values for the mass density of pure solid Ne and D_2, $\rho_{Ne} = 1.444$ and $\rho_{D_2} = 0.2$ g/cm^3, the mass density of the mixture is given by

$$\rho_{pell} = \left[\frac{X_{Ne}}{\rho_{Ne}} + \frac{1 - X_{Ne}}{\rho_{D_2}} \right] = 0.7973 \text{ g/cm}^3 .$$

The pellet shape was a right cylinder measuring 25 mm in diameter, and based on the above data its length should be $L_{pell} =$ 32.676 mm. The breaker tube was actually a thin-walled mitre bend tube consisting of 304 stainless steel with a wall thickness measuring $h = 3.175$ mm. The pellet struck the inside of the tube at oblique angle $\vartheta = 65$ degrees, so its normal impact velocity was $V_{n0} = V_0 \sin\vartheta = 453.15$ m/s. The kinetic energy of the pellet is $E_k = 1.5986$ J, so its component normal to the surface is $E_{kn} = 1.313$ J. The impact caused permanent "dishing" of the wall with a maximum deflection depth of 3.8 mm below the original surface.

IIb. Linear-Elastic deformations using bending moment concepts

To begin with, we ask why was there a permanent plastic deformation in the mitre tube instead of an elastic one in which the tube wall returns to its original un-deformed position after impact. To do that we first solve for the deformation contour under static loading conditions in the elastic regime using a moment-curvature approach applicable to thin beams and plates. The outer diameter of the mitre tube is $D_t = 50.8$ mm so that the circumference of the tube is $C = \pi D_t = 159.6$ mm. Since the diameter of the pellet $D_{pell} = 25$ mm is much less than the circumference of the mitre tube we shall neglect the curvature of the wall. Thus we may imagine that the pellet strikes a perfectly flat circular plate of radius $r = D_{pell} / 2$ clamped at its edge. The deformation contour of a thin circular plate with a uniform pressure applied to its surface is a difficult problem. A simpler but analogous problem to solve is the thin beam clamped at both ends with a distributed load over its surface. Let the length, width and thickness of the beam be $L, D,$ and h, respectively. Affix the coordinate system along the axis of the beam such that the x coordinate runs along the length of the beam $-L/2 < x < L/2$ and $x = 0$ locates the mid-length cross section of the beam. The "neutral" sheet of the beam is the surface $y = 0$, so the y coordinate is upward from the neutral sheet: $y = h/2$ is at the top surface of the beam and $y = -h/2$ is at the bottom surface. The load causes the beam to sag. Precisely it is the neutral sheet that is sagging. The displacement of neutral sheet at cross section x is defined as $w(x)$ and it is a *negative* quantity for downward loads. The goal is to find the $w(x)$ profile and the maximum displacement w_0 which occurs at the mid-length section, $x = 0$. The sagging of the beam leads to a "bending strain". Lets look at the mid-length cross section where we see that the beam shape has a positive curvature. The beam is bent such that in the upper portion of the beam $y > 0$ the material elements in the cross section experience compression (negative strain), while in the lower section of the beam the material elements are stretched (positive strain). In the limit of small deflections, the bending strain in any cross section is given by $\varepsilon_{xx} = -y\kappa$, where the curvature in this limit is obviously

$$\kappa = \frac{d^2 w}{dx^2} . \tag{1}$$

In a linear-elastic material, the bending stress within any cross section x will be

$$\sigma_{xx} = -Ey\frac{d^2w}{dx^2}, \qquad \sigma_{ij} = 0 \; (i, j \neq x), \tag{2}$$

where E is the modulus of elasticity (Young's modulus). Thus we see that if the neutral sheet has positive curvature then to the left side of the section there will be a differential force $dF = \sigma dydz$ pushing outward (compressive stress and strain) for $y > 0$ and pulling inward (tensile stress and strain) for $y < 0$. Such anti-symmetric internal forces generate an internal torque (induced couple) about the neutral axis $y = 0, x = x$. Integrating the differential torque $dT = y\sigma dydz$ over the whole cross section gives the total induced couple. Static equilibrium is expressed by the moment-curvature equation [1,2],

$$EI\frac{d^2w}{dx^2} = M(x), \tag{3}$$

which states that that the internal couple balance the external torque $M(x)$ applied to the left side of the section, where $I = Dh^3/12$ is the area moment of inertia about the neutral axis for such a beam. At the mid-plane cross section the external torque is positive $M(0) = M_0 > 0$, i.e., it tends to make a rotation about the neutral line in the clockwise direction. This equation is solved in the region $0 < x < L/2$. The external torque to the left of the section at $x = x$ is just M_0 minus the *counterclockwise* torque due to the distributed load between $x = 0$ and $x = x$. Hence, for a uniform load with force per unit length $\overline{p}$ (applied uniform pressure $p = \overline{p}/D$), Eq. (3) becomes

$$EI\frac{d^2w}{dx^2} = M_0 - \frac{\overline{p}x^2}{2}. \tag{4}$$

Integrating Eq. (4) two times gives two more unknown constants in addition to the unknown M_0. These three unknowns are determined by applying three boundary conditions: at a clamped end the vanishing of displacement and slope, $w(L/2) = w'(L/2) = 0$, and by symmetry $w'(0) = 0$. The final solution is given by

$$w(\xi) = w_0 \left(1 - \xi^2\right)^2 . \tag{5}$$

where

$$w_0 = -\frac{pL^4}{32Eh^3}, \quad \xi = x/(L/2) . \tag{6}$$

The shape of the profile is identical same as that of the circular plate if $\xi = r/a$ where a the radius of the plate, and the maximum deflection w_0 is close to that given by Eq. (6) is if L is replaced by $2a$.

Next, we calculate the critical deflection w_{0c} corresponding to the elastic limit, and show that this critical deflection is much less than the experimentally measured deflection $w_{0\exp} = 3.8$ mm indicating that the impact resulted in plastic deformation. The elastic limit occurs when the maximum stress $\sigma_{xx,\max}$ is equal to the yield stress σ_Y . Now the maximum stress occurs at $\xi = 1$ and $y = h/2$, whence

$$w_{0c} = -\frac{1}{16}\frac{\sigma_Y}{E}\frac{L^2}{h} . \tag{7}$$

For 304 SS we use the following values:

$$\begin{aligned} E &= 203 \text{ GPa} \\ \sigma_Y &= 310 \text{ MPa} \end{aligned} . \tag{8}$$

Putting $L = D_{pell}$ and $h = 3.175$ mm, we obtain $w_{0c} = 0.0188$ mm, which is much less than $w_{0\exp} = 3.8$, indicating that the deformation is deeply plastic. Before constructing a non-linear plastic deformation model we want to demonstrate that the mechanical work done to deform the beam (plate) is equal to the stored strain energy. Then the principle of virtual work can be used to infer the impact pressure. We will use this principle in the plastic deformation case to back out the impact pressure based on the measured deflection.

First we calculate the bending strain energy. This is

$$U_{strain} = \int \left(\int \sigma_{xx} \, d\varepsilon_{xx} \right) D dy dx \, . \tag{9}$$

After doing the inner integral we obtain

$$U_{strain} = \frac{DE}{2} \iint y^2 \left(\frac{d^2 w}{dx^2} \right)^2 dy dx \, . \tag{10}$$

Substituting in Eq. (5) we obtain

$$U_{strain} = \frac{128}{15} \frac{EDh^3 w_0^2}{L^3} \, . \tag{11}$$

The mechanical work done in creating the deformation is given by

$$U_{mech} = \int p \cdot \delta V_D \, . \tag{12}$$

where V_D is the volume displaced by the deflection

$$V_D = \int_{-L/2}^{L/2} Dw(x)dx \ = \frac{8}{15} DLw_0 \ . \tag{13}$$

Inserting the differential volume $\delta V_D = (8/15)DLdw_0$ into Eq. (12), and eliminating p by means of Eq (6), proves that

$$U_{mech} = U_{strain} \ . \tag{14}$$

Therefore we can say in general that if we can calculate the strain energy we can calculate the impact pressure by principle of virtual work:

$$\frac{\partial U_{strain}}{\partial V_D} = p \ . \tag{15}$$

We will now use this principle to calculate the expected impulsive pressure in the realistic case where strain energy is purely plastic.

IIc. Permanent Plastic deformations using virtual work principle

When the stress is above the yield stress the material will experience permanent or plastic deformation. The aim of this section is to derive a formula to that allows us to infer the pellet impact pressure from a measurement of the maximum wall deflection for such plastic deformations. In the linear elastic regime, the stress-strain relation for compression and tension is linear and symmetrical, $\sigma = E\varepsilon$. Near the yield point and beyond the linear relation breaks down. For ductile metals the stress-strain curve exhibits a rounded elastic-plastic transition with no sharply defined yield point. The relationship is often given by the Ramber-Osgood equation [3]:

$$\varepsilon = \frac{\sigma}{E} + \left(\frac{\sigma}{K}\right)^{1/n} , \tag{16}$$

in which the total strain (under tension only) is the sum of the elastic reversible component and the plastic irreversible one, with K being the strain-hardening coefficient and n the strain-hardening exponent characterizing the degree of non-linearity of the stress-strain curve. In the high strain plastic deformations of mitre tubes observed in the SPI experiments [Baylor, 2016 private communication] it is possible to neglect the elastic strain in comparison with the plastic one. In this case the material is called "plastic/rigid" [N. Cristescu, "Dynamic Plasticity", (1967) North Holland publishing co. Amsterdam] allowing the use of the approximate relation:

$$\sigma = K\varepsilon^n , \tag{17}$$

For 304 SS, $n = 0.43$, $K = 1400$ MPa, and $E = 203$ GPa. I compared this simple formula against an experimental stress-strain curve and found that for a strain of 0.1 the simple formula gives a tensile stress value of 520 MPa, while the experimental curve gives 445 MPa. So the formula is only 17% larger. The ultimate tensile strength of the steel is 620 MPa which occurs for a maxmum strain of 0.53. The deformations encountered in the ORNL experiments have associated strains less than maximum, for otherwise the pellet would have perforated the wall of the mitre tube.

We use a cylinder coordinate system (r,θ,z) where r,θ are in the plane of the plate. We cannot at this level of investigation compute the displacement profile. Instead we will assume that it has the same shape as that of the elastic beam in the previous section. The circular plate and the beam have the same deflection profile if we replace half-length of beam with radius of plate a. Hence,

$$w(\xi) = w_0\left(1-\xi^2\right)^2 \quad \xi = r/a , \tag{18}$$

except that the maximum plastic displacement w_0 is not yet known. The radius of the deformation region is assumed equal to the radius of the pellet $a = D_{pell}/2$. The plastic strain energy per unit volume is given by

$$u_{plastic} = \int (\sigma_{rr}\, d\varepsilon_{rr} + \sigma_{\theta\theta} d\varepsilon_{\theta\theta})\,. \tag{19}$$

Employing Eq.(17) gives

$$u_{plastic} = \frac{K\varepsilon_{rr}^{n+1}}{n+1} + \frac{K\varepsilon_{\theta\theta}^{n+1}}{n+1}\,. \tag{20}$$

The strains measure displacements *between* particles in a medium and it is a tensor quanity $\vec{\varepsilon} = \partial(\vec{x} - \vec{X}) / \partial\vec{X}$. For axisymmetric deformation, plate particles are stretched out along the radial coordinate so the displacement $\vec{x} - \vec{X}$ is oriented in the radial direction $|\vec{x} - \vec{X}| = u_r$, with $u_\theta = 0$. Hence, in this coordinate system

$$\varepsilon_{rr} = \frac{\partial u_r}{\partial r}, \qquad \varepsilon_{\theta\theta} = \frac{u_r}{r}\,,\ \varepsilon_{zz} = 0,\ \varepsilon_{r\theta} = 0,\ \varepsilon_{\theta z} = 0,\ \ \varepsilon_{rz} = 0 \tag{21}$$

Now $du_r = ds - dr$, with

$$(ds)^2 = (dr)^2 + (dw)^2\,. \tag{22}$$

Whence,

$$\varepsilon_{rr} = \sqrt{1 + \left(\frac{dw}{dr}\right)^2} - 1\,. \tag{23}$$

Now in the ORNL experiment the wall deformation depth w was significantly smaller than the radius of the deformation a. Thus, we are justified in expanding the radical, yielding

$$\varepsilon_{rr} \approx \frac{1}{2}\left(\frac{dw}{dr}\right)^2 . \tag{24}$$

Neglecting $\varepsilon_{\theta\theta}$ compared to ε_{rr}, Eq. (20) is approximately

$$u_{plastic} \approx \frac{K}{n+1}\left\{\frac{8w_0^2}{a^2}\xi^2(1-\xi^2)^2\right\}^{(n+1)} . \tag{25}$$

The total strain energy of plastic deformation (Joules) is now

$$\begin{aligned} U_{plastic} &= \int_0^1 u_{plastic} 2\pi h a^2 \xi d\xi \\ &= \frac{2\pi 8^{\nu}}{3}\frac{\Gamma(\nu)\Gamma(2\nu)}{(1+3\nu)\Gamma(3\nu)} a^{(2-2\nu)} h K w_0^{2\nu} \end{aligned} . \tag{26}$$

where $\nu = n+1$, and $\Gamma(z)$ is the gamma function. Inserting the experimental value of the maximum deflection $w_0 = 3.8$ mm we obtain

$$U_{plastic} = 32 \text{ J}. \tag{27}$$

Note that $U_{plastic} << E_{kn} = 1313$ J. Is not surprising that only a fraction of the normal kinetic energy was spent in deforming the mitre tube wall. If the pellet were to strike the wall and stick to the wall without rebounding, i.e., if the pellet were imbedded and remained intact (no breakup), then all of its normal kinetic energy would be converted to deformation strain energy: $U_{plastic} \approx E_{kn}$. But that is not the case here. Instead the pellet broke apart and its debris material spread out laterally along the surface of the wall at high velocity very much like what was seen in the sequence of images taken by a high-speed camera observing the impact of a high-velocity cryogenic pellet against a thick steel plate [1]. These images show that the pellet at the point of impact forms a thin circular saucer-like structure, its material expanding primarily in the radial direction parallel to the surface of the plate. The radial velocity of this debris material is at least as high as the pellet's normal velocity. Therefore a large amount of the initial kinetic energy of the pellet was transferred to kinetic energy associated with the saucer-like expansion of its broken debris material. Since the kinetic energy of the debris material following impact cannot be disregarded, it is not inconsistent that the theory says that only a small fraction of the initial kinetic energy was used to deform the wall. The more pertinent questions are (i) "what does the theory say about the relation between the measured wall deflection and the impact pressure", and (ii) "does the inferred impact pressure agree with what we would expect from a separate model of impact pressure?" We have two impact models to consider. One will be the correct one. Using Eq. (15) and (26) and the differential displacement volume for a deformed circular plate $\delta V_D = (\pi/3)a^2 \delta w_0$ our plastic deformation model predicts a pellet impact pressure of

$$p = 4\nu 8^{\nu} K \frac{\Gamma(\nu)\Gamma(2\nu)}{(1+3\nu)\Gamma(3\nu)} \left(\frac{h}{a}\right)\left(\frac{w_0}{a}\right)^{2\nu-1} . \tag{28}$$

Plugging in the numbers from the experiment:

$\nu = 1.43,\ a = 12.5\ \text{mm},\ h = 3.175\ \text{mm}$

$K = 1400\ \text{MPa},\ w_0 = 3.8\ \text{mm}$

yields

$$p = 147\,\text{MPa}. \tag{29}$$

Is this a reasonable result? To find out we shall calculate the expected impact pressure from the linear impulse-momentum law

$$M_{pell}V_{n0} - M_{pell}V_{nf} = \int_0^{t_0} F\,dt\ . \tag{30}$$

where again V_{n0} is the initial normal velocity of the pellet and V_{f0} is the final normal velocity of the pellet or its debris material, F is the impact force on the wall, and t_0 is the duration of the contact. Clearly short contact periods require the existence of large forces in order to satisfy Eq. (30). The pellet mass can be written as $M_{pell} = \rho_{pell} A_{pell} L_{pell}$ where $A_{pell} = \pi a^2$. For perfectly plane contact, $F = pA_{pell}$, Eq. (30) can be written as

$$\rho_{pell} L_{pell} (V_{n0} - V_{nf}) = \int_0^{t_0} p\, dt \, . \tag{31}$$

In the first impact model, model A, the pellet behaves as a perfectly elastic body during its contact with the surface. At the moment the pellet makes contact with the surface a stress (pressure) wave with sound velocity c is sent towards the back of the pellet with velocity in the lab frame given by $c - V_{n0}$, while the back surface moves downward at velocity V_{n0}. Therefore, the sound wave meets the back surface at time $t_+ = L_{pell} / c$, whereupon it reflects forming a release wave. Now the release wave travels into the stationary compressed pellet material at velocity $c - V_{n0}$. Since the pellet material is compressed its length is contracted to $L'_{pell} = L_{pell}(1 - V_{n0} / c)$ the time for the reflected wave to reach the target surface is also t_+. Hence, the duration of the contact is $t_0 = 2t_+$. When the release wave meets the target surface the pellet becomes detached and rebounds with the same velocity $V_{nf} = -V_{n0}$. We know that doesn't happen but still if it did it would produce an impulsive pressure on the plate given by

$$p = \rho_{pell} V_{n0} c \, . \tag{32}$$

This is the so-called "water hammer" pressure valid for wave propagation in elastic media. From Section IIa we found $\rho_{pell} = 797 \text{ kg/m}^3$, $V_{n0} = \upsilon_0 \sin\theta = 500 \cdot \sin(65^\text{o}) = 453 \text{ m/s}$. and $c \sim 1000$ m/s, giving $p = 360$ MPa. Actually the impact pressure are larger because the compression of the volume is so large that the linear elastic model breaks down. We have done a rigorous model for pure deuterium and neon pellets using empirical bulk modulus data and arrive at respective impact pressures of 235 and 1685. It is more difficult to do a rigorous model for the actual composite pellet but if we average our non linear results we arrive at a mean pressure of 960 MPa. In any case these impact pressures are much higher than the prediction of Eq. (29). But as we said, we could have guessed that this elastic impact model was not physical from the start because the pellet does not rebound. Instead there is material failure, and break up material at contact flows sideways forming the saucer-like debris flow. Thus, in reality the rebound velocity is zero, $V_{nf} = 0$. Thus in model B, Eq (31) gives

$$\rho_{pell} L_{pell} V_{n0} = \int_0^{t_0} p\, dt \ . \tag{33}$$

The duration of the impact in model B is now simply $t_0 = L / V_{n0}$. There is no elastic stress wave in model B because material failure prevents such large elastic pressure from developing behind the 1-D elastic wave. The duration of contact also agrees with the sequence of image in Ref [1] showing saucer-line debris structure after pellet impact on a thick rigid plate. Plugging this into Eq (33) we get

$$p = \rho_{pell} V_{n0}^2 = 163 \text{ MPa.} \tag{34}$$

this result is in close agreement with our prediction in Eq. (29). This indicates that impact model B is the correct physical picture. What actually happens is that an elastic wave starts to propagate upon impact but never makes to the opposite side of the pellet. In a rotated coordinate system of 45 degrees, the compressed material behind the wave has a maximum shear stress of magnitude given by

$$\tau = \frac{p}{2} \text{ MPa.} \tag{35}$$

The shear stress is exceeding larger than the shear strength of the cryogens $\tau >> \tau_S$, which is on the order of a few tenths of a MPa. Therefore what happens is that the pellet material flows as though it were a shearless fluid giving the expected impact pressure of Eq, (34). The material in not under tension as would be the case during the propagation of the release wave but rather the interior of the pellet undergoes a shear strain rate given by Eq. (24) of Part I.

References for Part II

[1] S.K. Combs et al, *Fusion Science and Technology* **60**, 473 (2011)

[2] W. Goldsmith, “Impact: The Theory and Physical Behavior of Colliding Solids”, Edward Arnold, London, UK, 1960.

[3] J. M. Gere, S. P. Timoshenko, “Mechanics of Materials”: Forth edition, Nelson Engineering, (1996), *ISBN 0534934293*

[4] https://en.wikipedia.org/wiki/Ramberg-Osgood

Part III Models for the size distribution of fragments

The particle size distribution is critical because only solid fragments larger than > 0.1 mm will penetrate deeply. Both velocity and size distributions need to be determined in order to complete the neutral source model discussed in Part I.

Model 1 Statistical Fragmentation Model

Mott and Linfoot [1] made an attempt to understand the breakup of exploding munitions, specifically pipe bombs and shells. Their model described the random fragmentation of a two-dimensional plate, an extension of a one-dimensional model for the multiple fragmentation of a line (rod) subject to tension forces. The 1-D model found that the fractures lengths, masses in this case, were distributed randomly along an infinite line according to a Poisson process. It is appropriate to idealize the mass distribution of exploding shell fragments in a 2-D surface geometry because for a thin shell the fragment mass m is proportional to its area Σ. In the case of a plate with infinite surface areas, the probability density distribution of fragment masses, i.e. the number of fragments between m and $m+dm$ was predicted to be

$$f(m) = \alpha K_0(\beta m^{1/2}) , \qquad (1)$$

where α and β are normalization constants. Since fragment size scales like $r \sim \Sigma^{1/2} \sim m^{1/2}$, the appropriate size distribution is found by means of the relation $f(r)dr = f(m)dm$ obtaining

$$f(r) = \alpha r K_0(\beta r) . \qquad (2)$$

Model 2 Energy-Based Fragmentation Model

The fracture energy is the potential energy arising from the creation of new surfaces. The potential energy of a fragment is the surface energy $U_s = \sigma A$ where $A =$ surface area of fragment, and $\sigma =$ surface energy density (analogous to the surface energy associated with the surface tension of a liquid). Using Boltzmann statistics, the probable amount of fragment mass of specific energy ε within a differential range $d\varepsilon$ is $m(\varepsilon)d\varepsilon$, where $m(\varepsilon) = Ae^{-\beta\varepsilon}$. For a fragment with characteristic size $\sim r$, surface area $\sim r^2$, and mass $\sim \rho_0 r^3$, the specific energy will be $\varepsilon \sim \sigma / r\rho_0$. Hence, $m(\varepsilon) = Ae^{-\beta/r}$ where β stands for a different constant. However, $m(\varepsilon)d\varepsilon = m(r)dr$, so $m(r) = Ar^{-2}e^{-\beta/r}$. Because $m(r) \propto r^3 f(r)$, the size distribution becomes

$$f(r) = Ar^{-5}e^{-\beta/r} . \tag{3}$$

Model 3 Maximal Entropy Fragmentation Model

Using the principle of the entropy maximization [2], an alternate fragmentation distribution relation can be formulated. It is assumed that the mass M of the unbroken body is distributed into J mass bins in ascending order of mass such that the *jth* mass bin corresponds to the fragment mass $m_j \equiv j\Delta m$ and Δm is the mass interval for all the bins. Let n_j be the number of fragments with mass between m_j and m_{j+1}, then the total number of fragments is $N = \sum_j n_j$ $N = \sum_j n_j$, and from mass conservation $M = \sum_i n_i m_i$ because all fragments occupying the *jth* mass bin interval are *indistinguishable*, the number of distinct fragment arrangements, "microstates", available to this system is

$$W = \frac{N!}{n_1!n_2!n_3! \ldots n_j!} . \tag{4}$$

The information entropy associated with this system is $S = \ln W$. Taking the infinitesimal limits, $\Delta m << M$, $\mathrm{n_j} \to \mathrm{f(m)dm}$, the entropy may be expressed as

$$\begin{aligned} S &= \ln N! - \int \ln[f(m)!)]dm \\ &\approx \ln N! + \int f(1 - \ln f)dm. \end{aligned} \tag{5}$$

The entropy is maximized, $\delta S = 0$, by taking the variation in f subject to the constraints $\delta N = \delta M = 0$. This procedure yields a Boltzmann–like mass distribution function

$f(m) = \alpha e^{-\beta m}$, where α and β are different normalization constants. The mass distribution derived is identical to the 1-D distribution based on Poisson statistics. The size distribution immediately follows from this:

$$f(r) = \alpha r^2 e^{-\beta r^3} \ . \tag{6}$$

The three different models will soon be compared with the experimental data for solid deuterium pellets in order to discover which model fits the data best. When available, data for neon pellets would allow us to come up with scaling laws for the *mean fragment size* because in the science of fracture mechanics, mean fragment size has a dependence on material properties, mainly lattice energy, which is larger for solid neon.

REFERENCES to Part III

[1] Mott, N. F., & Linfoot, E. H. (1943, February). A theory of fragmentation. United Kingdom Ministry of Supply, AC3348.

[2] Grady, D. E., & Kipp, M. E. (1985). Geometric statistics and dynamic fragmentation. *Journal of Applied Physics, 58*, 1210.

Part IV Summary and future directions

This work developed theoretical models for the nominal size of the debris cloud and the impact pressures of the pellet impacting the wall. The size and pressure predicted indicates that pellet breakup is cause by cleavage fracture (shear stress) rather than tensile forces which would have caused spallation on the rear surface. The impact pressures closely agree with predictions of a separate theoretical model dealing with plastic deformation of a thin flat circular plate struck by a cryogenic pellet. Future work should continue to look deeper into the physics of pellet fracture. Crack formation and link up is one physics problem that need more attention. Most of the literature deals with hard projectiles impacting equivalently hard targets, or projectiles striking thick solid targets in which the ram pressure of the projectile is on the order of the yield strength of its material, in which case the projectile suffers a permanent "rigid-plastic" deformations. The situation in SPI is opposite: the projectiles are soft compared to the targets and the ram pressures of the projectiles are orders of magnitude larger than its yield strength. The analytical work should be supplemented by finite element numerical analysis. ANSYS modeling simulation software, version 16, is available at General Atomics at present. This may be used to model the frozen pellet and the steel impact structure with a dynamic analysis. The material models will be non-linear for the steel structure and also for the pellet if such data is available. The analysis will be made in tiny time increments whereby the pellet is moving incrementally with the initial velocity until impact begins. The stress and strains in the pellet material will be calculated and failure in the pellet updated. ANSYS programming language APDL allows the user to write code to create the geometries and manipulate the model as the impact progresses. Different impact angles, including pitch and yaw pellet orientation effects could be studied for a variety of situations and it may be possible to explore new and better ways to shatter the pellet so that most of the debris material in in the form of chunky material.