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THE INITIATION OF EXPLOSIVE CHARGES BY RAPID SHEAR (2)

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10 ROBERT E. FREY DR.
BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MD 21005

I. Introduction.

Friction and/or shear have been suggested by many people as possible sources of ignition in solid explosives. Although these two mechanisms are usually considered to be distinct, on a microscopic scale they are essentially the same. On a macroscopic scale, friction involves sliding interfaces and is described in terms of the coefficient of friction and the stress normal to the interface. The rate of heat generation at the surface is the product of the sliding velocity times the coefficient of friction times the normal stress. On a microscopic level, friction is caused by surface irregularities (asperities) which deform as the surfaces slide. The frictional heating is caused by viscoplastic work on the asperities. In this paper, I will consider the conditions required for ignition as the result of shear deformation and viscoplastic heating.

A cursory examination of this question leads one to the conclusion that the deformation must be localized in some way if ignition is to occur. The plastic work per unit mass resulting from the deformation of a material is given by the following relation [1]:

$$w_p = \frac{1}{\rho} \sum_i \int_0^{e_i^f} S_i de_i \quad (1)$$

where S_i is the principal deviatoric stress, e_i is the principal

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deviatoric strain, e_i^f is the final value of the deviatoric strain and ρ is the density. Consider the homogeneous deformation of a cylinder of explosive so that the length decreases and the radius increases. Assume that the Tresca yield condition holds. Then $e_r = e_\theta = -\frac{1}{2} e_z$, $S_r = S_\theta = -\frac{1}{2} S_z$, and $S_r - S_\theta = Y$, where Y is the yield strength of the explosive, and the usual notation of cylindrical coordinates has been used. The change in temperature of the explosive is given by

$$\Delta T = - \int \frac{Y}{\rho C} de_z = - \int \frac{Y}{\rho C} \frac{dz}{z} = \frac{Y}{\rho C} \ln \frac{z_o}{z_f}$$

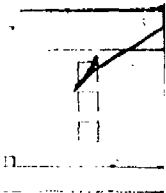
where C is the heat capacity, z_o is the initial length, and z_f is the final length. For composition B, Y is about 0.07 GPa and C is about 1.25 joules/ $^{\circ}$ C. To obtain a 100° C change in temperature requires z_o/z_f obtain a value of approximately 28. Clearly homogeneous deformation can result in initiation only in extreme circumstances.

There are several circumstances which may lead to very high shears in localized regions. Some of them are the following:

1. Sliding friction. As explained above, on a microscopic scale sliding friction involves shear deformation, and very high strains may occur in narrow layers. In particular, friction between a rotating shell and the explosive fill has been suggested as a cause of premature ignition in artillery shells [2]. It has also been suggested as a mechanism for the propagation of reaction during nondetontative explosions in confined explosive charges [3].

2. The collapse of spherical cavities. During ductile cavity collapse, a thin layer of material at the boundary of the cavity sees very high strains. This situation has been considered by Carroll and Holt [4]. Their analysis indicates that, in the absence of melting, extremely high temperatures can be obtained in small volumes around a collapsed cavity. This has been suggested as an ignition mechanism during shock wave initiation of explosives.

3. Adiabatic shear bands. Adiabatic shear bands in metals have been discussed by Recht [5]. A shear band is likely to form in a deforming material when thermal softening exceeds work hardening. In this case, deformation in any plane causes the material in that plane to weaken and tends to concentrate further deformation in the same plane. In metals, thin bands of material can be heated to the



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melting point. Winter and Field [6] have applied Recht's analysis to explosives and concluded that explosives should be highly susceptible to shear banding. Afanasev [7] and co-workers have observed them in nonexplosive organics.

4. Extrusion of explosive into cracks. If a crack develops in the metal confinement around an explosive while the explosive is under pressure, ignition could result when the explosive extrudes into the crack. This has been suggested as a possible ignition mechanism when confined explosives are impacted by projectiles at velocities too low to cause shock wave initiation [3].

In all of these circumstances, melting tends to limit the temperature which can be achieved. Once the melting point has been reached, any further heating must be strictly by viscous processes. The melting point increases with pressure, and melting is a more important consideration at low pressure than at high pressure. From data in the International Critical Tables, the rate of increase of melting point with pressure for many organic materials is 20 to 30° per kilobar. For instance, for TNT the melting point increases about 25°/kilobar at atmospheric pressure. The rate of increase decreases as pressure increases. To obtain a crude estimate of the effect of melting on hot spot ignition, I assumed that the melting point of several explosives increased at about 20°/kilobar and computed the time to explosion at the melting point as a function of pressure. Kinetic constants were taken from Rogers [8]. The results are shown in Figure 1. For reactions which occur in 1 microsecond or less, which is typical of the shock initiation regime, melting is important in preventing initiation at pressures below 1.0 GPa in PETN, RDX, or HMX and for pressures below 3.0 GPa in TNT. For reactions which occur in a millisecond time frame, which might be typical of artillery setback conditions, melting is significant for pressures below 0.4 GPa in RDX and 1.5 GPa in TNT. In this paper I will investigate the conditions under which viscoplastic heating can lead to ignition when melting is considered.

II. Ductile Cavity Collapse.

Carroll and Holt treated spherical cavity collapse in an elastic-plastic fashion [4] and in an elastic-viscoplastic fashion [9]. Application of their equations shows that, in the absence of melting, extremely high temperatures are produced in a thin layer around the collapsing cavity. Figure 2 shows the temperature as a function of applied pressure for a Comp-B charge where the initial porosity (actual volume/fully compacted volume) is 1.03. Extremely high temperatures are predicted in a very thin layer around the collapsing cavity. At a

pressure of 2.0 GPa, the surface of the cavity reaches a temperature of about 600°C. However, only a very thin layer is significantly heated. Figure 2 also shows the temperature of the isotherms enclosing the hottest 0.01% and the hottest 1% of the material. These isotherms are much cooler.

The analysis of Carroll and Holt does not include thermal softening, melting, or heat conduction. Since the heated region is close to the surface of the cavity, where the pressure is low, one can suspect that the inclusion of these factors might alter the results significantly. We have modified Carroll and Holt's formulation slightly to include these effects and also added a viscosity which varies with temperature and pressure. For simplicity, we use a rigid-plastic model (i.e., we assume that the elastic strains are negligible). The principal assumptions of the Carroll and Holt model are the following:

1. The flow in the vicinity of the cavity is spherically symmetric.
2. The material is incompressible.
3. The following constitutive relation applies:

$$\dot{e}_{ij} = \frac{1}{2G} S_{ij} + \frac{1}{2\mu} (1 - Y/\sqrt{3I}) S_{ij},$$

where $\dot{e}_{ij}$ is a component of the deviator strain rate tensor, S_{ij} is a component of the deviator stress tensor, G is the shear modulus, μ is the viscosity, Y is the yield strength, and I is the second invariant of the deviator stress. For the spherically symmetric, rigid-plastic case considered here, this reduces to

$$S_r = 2\mu\dot{e}_r + \frac{2}{3}Y$$

$$S_\theta = 2\mu\dot{e}_\theta - \frac{1}{3}Y,$$

where S_r , S_θ , $\dot{e}_r$, $\dot{e}_\theta$ refer to the principle deviator stresses and principle deviator strain rates, and the usual notation for spherical coordinates has been used.

Carroll and Holt considered a hollow sphere with outer radius b , inner radius a , and porosity α , defined as the ratio of the

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actual volume to the fully compacted volume, where $\alpha = b^3/(b^3 - a^3)$.
The equation of motion for this system is

$$\frac{\partial \sigma_r}{\partial r} + \frac{2}{r} (\sigma_r - \sigma_\theta) = \rho \ddot{r},$$

where σ_r and σ_θ are the principle stresses, r is the radius, and dots imply differentiation with respect to time. Following Carroll and Holt, we note that

$$\sigma_r - \sigma_\theta = S_r - S_\theta = \mu \dot{e}_r + Y,$$

and apply the boundary conditions,

$$\sigma_r = 0 \text{ at } r = a$$

$$\sigma_r = -P \text{ at } r = b,$$

where P is the applied pressure.

We also note that

$$\dot{e}_r = + \frac{2}{3} \frac{\dot{B}}{r} \frac{1}{3},$$

where $B(t) = a_0^3 - a^3 = b_0^3 - b^3 = a_0^3 (\alpha_0 - \alpha)/(\alpha_0 - 1)$

and a_0 , b_0 , and α_0 are the initial values of a , b , and α . The equation of motion can then be integrated with respect to the radius and the result expressed as the following differential equation for α :

$$P \int_a^b \frac{2Y}{r} dr - \int_a^b \frac{4\mu}{3} \frac{\dot{B}}{r^3} dr = F(\ddot{\alpha}, \dot{\alpha}, \alpha)$$

$$F(\ddot{\alpha}, \dot{\alpha}, \alpha) = \frac{\rho a_0^2}{3(\alpha_0 - 1)^{2/3}} \left[\frac{\dot{\alpha}^2}{6} \left[\frac{-4}{(\alpha - 1)^{2/3}} - \alpha \frac{-4}{3} \right] - \ddot{\alpha} \left[\frac{-1}{(\alpha - 1)^{1/3}} - \alpha \frac{-1}{3} \right] \right]. \quad (2)$$

The rate of plastic work at any point in the flow may be computed from equation (1), giving the following result:

$$\dot{W}_p(r) = \frac{2}{3} Y \frac{\dot{B}}{r^3}, \quad (3)$$

where $\dot{W}_p$ is the rate of plastic work per unit volume. We have integrated equation (2) numerically. Simultaneously, we integrate the heat equation for the material around the cavity,

$$\frac{\partial T}{\partial t} = \frac{K}{\rho C} \left[\frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right] + \frac{\dot{W}_p}{\rho C} \quad (4)$$

where T is temperature, t is time, K is heat conductivity, ρ is density, and C is heat capacity. This equation was also integrated using finite differences and a computational mesh which concentrated most of the points in the region close to the surface of the cavity. At each time step, equation (2) was integrated to obtain α , $\dot{\alpha}$, $\ddot{\alpha}$, a , and b . Then $\dot{W}_p$ could be determined and equation (4) integrated to determine $T(r)$ at the next time step.

Good data on the temperature dependence of the yield strength and on the temperature and pressure dependence of the viscosity of common explosives are not available. We assumed that the melting point increased with pressure at the rate of $200^\circ/\text{GPa}$ and that the yield strength was zero above the melting point and decreased to zero in a linear fashion over a range of 30°C below the melting point. We assumed that the viscosity varied in the following way with temperature and pressure:

$$\mu = \mu_0 \exp\left(\frac{P}{P_0}\right) \exp\left(\frac{E}{T} - \frac{E}{T_0}\right), \quad (5)$$

where μ_0 is the viscosity at temperature T_0 , E is an experimentally determined activation energy for viscous flow, and P_0 is an experimentally determined constant. Pressure and temperature relations of this type are discussed by Frenkel [10] and have some theoretical support. The pressure dependence shown in equation (5) agrees well with data from the International Critical Tables. Some data is available for TNT, and we will use this material in all of the calculations reported here. We determined an approximate value for E , $3,880^\circ\text{K}$, on the basis of two data points [11]. We estimated P_0 to be 0.165 GPa , a value which is typical of organic liquids and fits the experimental data reported in the International Critical Tables for nitrobenzene. Other required parameters are shown in Table I.

TABLE I - MATERIAL PROPERTIES USED IN CALCULATIONS

Parameter	Value
Y	0.07 GPa
v_0	$1.39 \times 10^{-2} \text{ Kg/(msec) at } 85^\circ\text{C}^{35}$
C	$1.29 \times 10^5 \text{ joule/(Kg}^\circ\text{C)}^{35}$
K	$0.262 \text{ joule/(m}^\circ\text{C sec)}^{35}$
ρ	$1.64 \times 10^3 \text{ Kg/m}^3^{35}$
E	$3,880^\circ\text{K}$
P_0	0.165 GPa

Figure 3 shows the results of the calculation for a case where the pressure increased from zero to 2.0 GPa over a period of 20 nanoseconds (this simulates a shock wave in a porous medium). The peak temperature never exceeds the normal (one atmosphere) melting point. In this situation, the deformation is concentrated in the region close to cavity where the pressure and melting point are low. Viscosity is not sufficient to elevate the temperature significantly above the melting point. Therefore, ignition by this mechanism is unlikely in TNT. Although we have not performed calculations on other explosives, we can infer that they would not be heated much above the normal melting point either. Since RDX has a rather long thermal explosion time at the melting point, it is probably not susceptible to ignition by this mechanism in a millisecond time scale.

III. Friction and/or adiabatic shear bands.

We have already commented on the similarity of friction and adiabatic shear bands at the microscopic level. In each case, large deformations are concentrated in a narrow region. In a shear band, the concentration occurs because thermal softening exceeds work hardening, as explained above. At a sliding interface, the concentration occurs because the interface region is weaker than the rest of the material. We have calculated the time evolution of temperature in a shear band or at a sliding interface when melting occurs. Our intention was to perform the simplest possible calculation while retaining the essential features of the real world.

In the model, we impose a velocity gradient across an arbitrary thickness of explosive. The magnitude of this thickness does not influence the results of the calculation. We arbitrarily induce a shear band by specifying the initial temperature in a thin layer to be high enough so that thermal softening occurs. The time evolution of the system is followed by making use of the following assumptions:

1. The shear stress is constant in all planes parallel to the shear band at any instant; i.e.,

$$\mu(x) \frac{dv}{dx} + \sigma(x) = f(t) \quad (6)$$

where μ is viscosity, x is distance perpendicular to the shear band (perpendicular to the direction of flow), v is velocity, σ is shear strength, and f is the shear stress applied at the shear band. f is independent of x but may vary with time. This assumption is a quasi-steady state assumption. It requires that the flow at any instant must have the form it would have at steady state given the temperature distribution which exists at that time, but it permits the flow to change as the temperature distribution changes.

2. The total shear velocity (the integral of dv/dx with respect to x) is independent of time. This condition and the previous one determine f via the following equation:

$$\int \frac{dv}{dx} dx = \int \frac{f - \sigma(x)}{\mu(x)} dx = v_t, \quad (7)$$

where v_t is the total shear velocity. At any time if $\sigma(x)$ and $\mu(x)$ are known, this equation can be used to determine f , and equation (6) can be used to compute dv/dx as a function of x . As the shear band develops, the velocity gradient will become concentrated in a narrow region and dv/dx will be zero over most of the space. In this situation, the integrals in equation (7) must be evaluated only over the region where dv/dx is positive. This is accomplished by choosing the limits on the second integral, which is evaluated numerically, so that the shear stress f is minimized.

3. The solid is rigid-perfectly plastic with a shear strength which decreases to zero at the melting point. As in the previous discussion, the shear strength is assumed to decrease linearly to zero in a 30°C range of temperature below the melting point.

4. The viscosity varies with temperature and pressure in the manner described by equation (5).

5. The rate of viscoplastic work per unit volume is given by the following expression:

$$\dot{W} = \frac{1}{2} \mu \frac{dv}{dx}^2 + \sigma \frac{dv}{dx}$$

6. The heat generated per unit mass by chemical decomposition can be computed on the basis of simple Arrhenius kinetics, as follows:

$$\dot{Q} = QA \exp(-E_a/T)$$

where Q is the heat of reaction per unit mass, A is the frequency factor, and E_a is the activation energy.

7. One dimensional heat equation applies; i.e.,

$$\frac{\partial T}{\partial t} = \frac{K}{\rho C} \frac{\partial^2 T}{\partial x^2} + \frac{\dot{Q}}{C} + \frac{\dot{W}_p}{\rho C} \quad (8)$$

Equation (7) was integrated numerically using finite differences. At each time-step, $\sigma(x)$ and $\mu(x)$ were determined from the known temperature distribution and dv/dx was determined from equations (6) and (7). Melting is handled in one of two ways. In one procedure, all of the material is considered to be a single phase, but the shear strength goes to zero when the temperature exceeds the melting point. This procedure neglects the heat of fusion. In the other procedure, two phases and a phase boundary are included in the calculation. The velocity of the phase boundary (the rate of growth of the melt layer) is determined from an energy balance at the boundary:

$$V_b \rho Q_f = K_e \frac{\partial T_e}{\partial x} - K_s \frac{\partial T_s}{\partial x}$$

where V_b is the velocity of the boundary, Q_f is the heat of fusion, and subscripts e and s refer to the liquid and solid phases. When this procedure is used, a dynamic mesh is used in both phases to avoid the necessity of rezoning as the boundary moves. This is accomplished by introducing a variable, y , defined as follows:

$$y = \frac{x_{bo}}{x_b} x$$

where x_{bo} is the initial position of the boundary and x_b is the position of the boundary at any time. x and its derivatives are expressed in terms of Y and substituted into equation (8). The resulting equation

is solved by finite differences. When expressed in terms of y , the computational grid automatically expands or contracts to adjust to the moving boundary. No significant differences were noted in the results of the two types of calculation. Surprisingly, the second procedure gave slightly higher temperatures, but this may be due to numerical error. All of the results reported here were accomplished with the second procedure.

Calculations were performed using material properties for TNT as listed in Table I. In addition, the following values for Q , A , and E were taken from Rogers [8]:

$$Q = 300 \text{ Cal/}({}^{\circ}\text{C g})$$

$$A = 2.51 \times 10^{11} \text{ sec}^{-1}$$

$$E_a = 34.4 \text{ KCal/mole}$$

Since the model is only an approximation of reality and since many parameters are not known precisely, the results should be considered in a qualitative rather than a quantitative sense. Figure 4 shows how the computed temperature at the center of the shear band varies with time for a case where the shear velocity was 0.2 km/sec and the pressure was 1.03 GPa. The temperature asymptotically approaches a maximum value. The time required for significant heating to occur is very short. The initial width of the heated region, which triggers shear band formation, affects the time history at the shear band but does not affect the maximum temperature. Figure 5 shows the time history for several calculations with the same pressure and shear velocity but different initial widths. There is an optimum initial width which gives the most rapid heating rate. With smaller initial widths, the temperature in the shear band may decrease for a while before it begins to increase. For larger initial widths, the temperature increases more slowly. In the absence of reaction, the maximum attainable temperature is a strong function of pressure. Figure 6 shows how the maximum temperature varies with shear velocity and pressure. At low pressures, melting limits the attainable temperature even for very high shear velocities. High pressure increases both the melting point and the viscosity and permits much higher temperatures to be attained at lower shear velocities.

On the basis of these calculations, it appears very unlikely that friction could be responsible for a premature ignition in a TNT shell during gun launch. The maximum pressure during gun launch is less than 0.2 GPa, and the sliding velocity between the rotating shell and the explosive is less than 30 m/sec. Under these conditions, the

temperature would not rise significantly above the melting point (of course, the presence of high melting point grit would change the picture drastically). We have not done any calculations on RDX because we do not have data for its viscosity. However, we can make a rough estimate of what would happen in RDX by using the TNT parameters but adjusting the melting point and T_0 (from equation (5) for the viscosity) upwards to account for the difference in melting point between TNT and RDX. If we do this, we obtain the same curves which we obtained for TNT but with all of the temperatures higher by 124°C (the difference in melting point between RDX and TNT). On this basis, it appears that RDX should also be insensitive to friction under setback conditions. These conclusions should be checked by experiment, and a program to do so is currently in progress at WRL. At present, the experiments support the theoretical conclusion.

Under shock initiation conditions, shear bands would be expected to form in the vicinity of collapsing cavities. Figure 7 shows in a schematic fashion how this might happen. In this situation, both the pressure and the shear velocity could be much higher than in the setback situation. An estimate of the maximum shear velocity can be obtained by taking the difference between the free surface velocity and the particle velocity behind the shock. This difference is approximately equal to the particle velocity. A 1.03 GPa shock in TNT has a particle velocity of about 0.2 km/sec. Figure 8 shows how the computed shear band temperature varies with time in this case. Thermal explosion occurs after about 50 nanoseconds. However, if the shear stops before thermal explosion occurs, the temperature in the shear band decreases rapidly due to the steep thermal gradients, and reaction does not occur. This is also shown in Figure 8. An estimate of the maximum slip distance at a shear band of this type is the dimension of the cavity in the direction of shock motion. The duration of the shear is this distance divided by the shear velocity. Consequently, we can estimate, very approximately, the critical cavity size required for initiation by this mechanism at any shock pressure. Table II shows these estimates for cavities in TNT.

TABLE II - CRITICAL CAVITY SIZES FOR SHOCK IGNITION IN TNT,
COMPUTED ON THE BASIS OF SHEAR BAND IGNITION

Shock Pressure (K bar)	Particle Velocity (Km/sec)	Time to Explosion (Microsecond)	Critical Cavity Size
4.9	0.1	4700	4.7cm
7.5	0.15	1.75	0.26mm
10.3	0.20	0.05	0.1mm

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Liddiard's data [12] showed a critical pressure of about 0.7 GPa for the ignition of TNT by long duration shocks. Since the maximum cavity size in a TNT charge of reasonable quality would be about 0.1 to 0.3 mm, the computed numbers are in reasonable agreement with experiment.

IV. Summary and Conclusions.

The role of shear in the initiation of reaction in high explosive has been examined theoretically. The calculations show that, for initiation by shear to occur under realistic conditions, some localization of the deformation must occur. When localized shear occurs, pressure is a critical parameter which controls the occurrence of ignition. High pressure during shear deformation enhances the chances for ignition by raising both the melting point (thereby increasing the heating due to viscoplastic work) and the viscosity of the melt (hence, increasing viscous heating). This pressure effect is extremely important in causing an explosive to be sensitized to shear deformation, and should be kept in mind when one assesses explosive hazards. For a low melting explosive, such as TNT, pressures in excess of 0.5 GPa are required for ignition at any shear velocity likely to occur. For higher melting explosives, lower pressures can lead to initiation.

The calculations show that typical pressures encountered during gun launch are unlikely to cause ignition of either TNT or RDX by this mechanism. However, when ignitions occur as a result of other causes, the resulting higher pressures make this mechanism a serious potential source of secondary ignitions which lead to violent explosions. This mechanism is also considered to be an important pathway by which interround propagation occurs, when munitions within a storage array are subjected to multiple fragment impacts and severe crushing. (See reference 3.)

Ductile cavity collapse does not lead to conditions which cause ignition. During ductile cavity collapse, the strain is concentrated in regions where the pressure and viscosity are low, and the temperature which may be obtained is limited by the melting point. Brittle cavity collapse, such as might be expected under shock loading conditions, can lead to the formation of shear bands and high temperatures can be attained. This is also expected to occur when the explosive is extruded into cracks in the confining steel case while the munition is under pressure. This latter sequence of events is viewed as a very probable source of ignition when the casing fails under launch or when subjected to crushing.

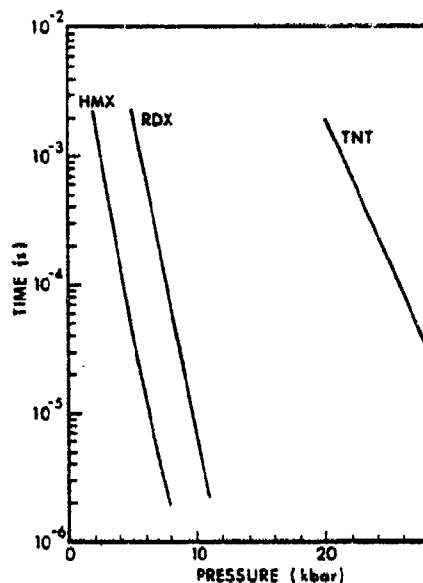


Figure 1 - Thermal Explosion Time at the Melting Point vs Pressure.

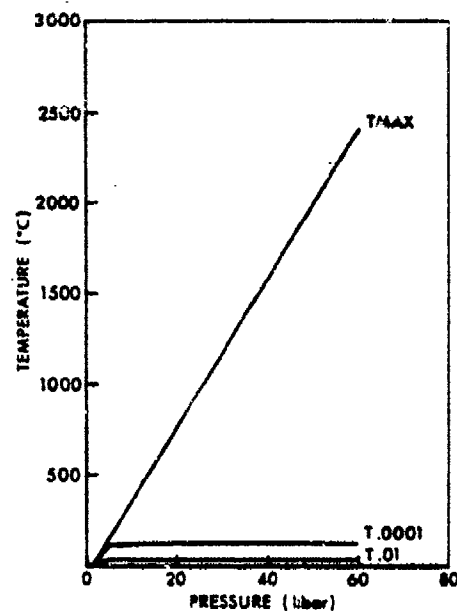


Figure 2 - Temperature vs Pressure After Cavity Collapse (Carroll & Holt's Model).

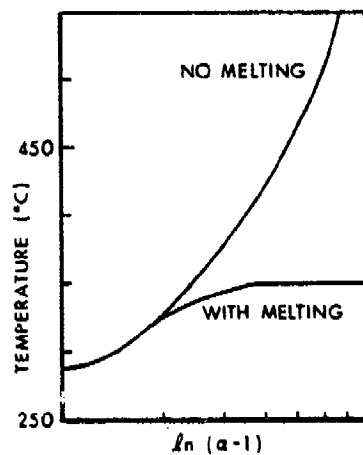


Figure 3 - Temperature vs Porosity During Cavity Collapse When Melting and Heat Conduction Occur.

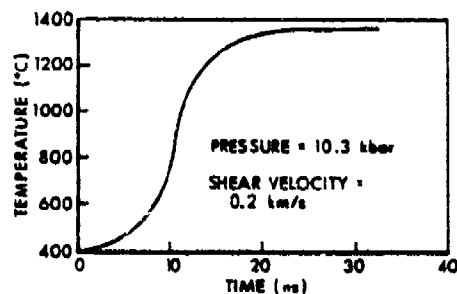


Figure 4 - Temperature vs Time in a Developing Shear Band.

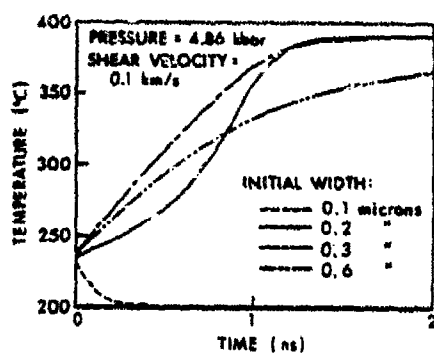


Figure 5 - The Time History of a Shear Band as a Function of the Width of the Initial Heated Region.

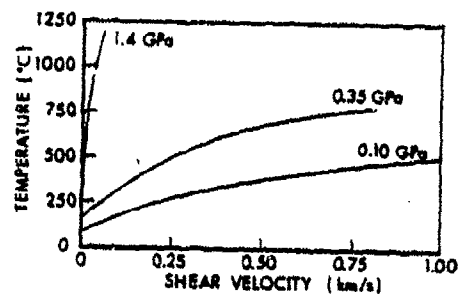


Figure 6 - The Effect of Shear Velocity and Pressure on Peak Temperatures in a Shear Band.

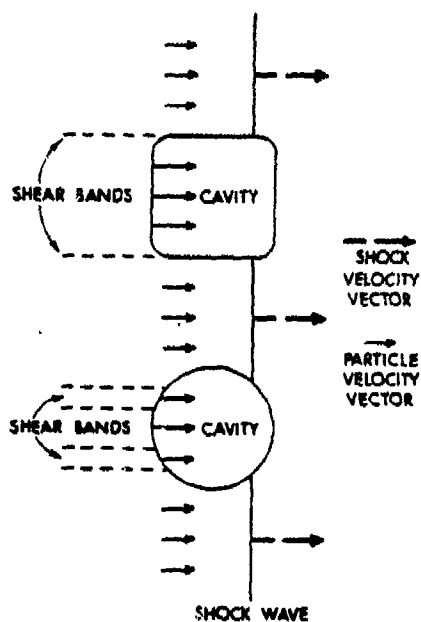


Figure 7 - Schematic Drawing Indicating How Shear Bands Could Be Formed in a Shocked Explosive.

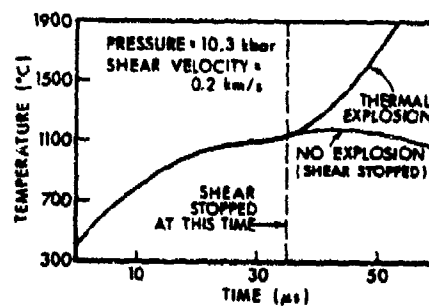


Figure 8 - Temperature vs Time in a Shear Band.

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