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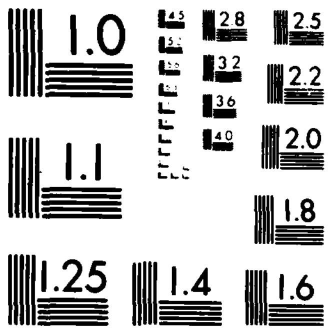
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MEMORANDUM REPORT BRL-MR-3425

# CRITICAL $P^2T$ VALUE COMPUTATION FOR EXPLOSIVES USING THE SHEAR BAND INITIATION MODEL

Evan Harris Walker

January 1985





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Recent computer calculations by Walker at BRL to model antifratricide shield functioning for artillery rounds has indicated a wide applicability of the critical $P^2T$ (or critical energy) values for predicting explosive initiation. While previous investigators have sought to give a theoretical explanation of the $P^2T$ criterion in explosive initiation, none has proposed a way to compute critical values of $P^2T$ from the mechanical and thermodynamic properties of explosives.

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20. Abstract (continued)

Frey at BRL has recently proposed a shear band mechanism as a source of hot spots in explosives subjected to rapid shearing. If the shear band mechanism is generally applicable, it must be possible to relate it to the critical values of $P^2T$ for different explosives. This would allow one to calculate this important sensitivity criterion from the mechanical and thermodynamic properties of explosives. Gibbons at BRL has observed shear banding in shocked explosives; however, the Frey model treats the shear velocity as an input parameter. Expressions have now been derived for the shear velocity across a band generated by shock loading, and for the density and dimensions of the shear bands. Using the thermodynamic properties of the explosive, this initial heating can be followed to full detonation. Similarly, by making the shock pressure a function of time to model stress relief waves in the shocked explosive, one can compute the conditions for failure to detonate. Thus, we obtain a complete model of shock initiated detonation based on more fundamental physical properties of explosives. This capability should make the control of sensitivity in explosives a more exact procedure.

TABLE OF CONTENTS

LIST OF ILLUSTRATIONS

## I. INTRODUCTION

The $P^2T$ criterion for the onset of detonation, first proposed by Walker and Wasley,[1] has become a central issue in the study of detonation mechanics. Although the criterion has been criticized, most recently by Moulard,[2] the criterion has been extensively employed and supported by experimental studies.[3-7] E. H. Walker[8] has recently employed the criterion successfully in a study comparing fratricide initiation in a variety of artillery shells with differing explosive fills. Thus, any satisfactory understanding of detonation onset will require an understanding of the $P^2T$ mechanism.

A number of studies[9-13] have sought to derive or calculate values for the $P^2T$ criterion, but none has provided a strictly physical theory free of *ad hoc* assumptions as to the origin and distribution of initiation sites, "hot spots", or the assumed initiating temperature distribution behind the shock front. Ramsey[14] argues such an assumption is not important to derive the relation $P^2T$=const., but evaluating this constant for different explosives must depend on the mechanism that gives rise to the initial heating and evolution of heat in the explosive. Howe, et al[15] have shown that shock initiation of detonation consists of two processes: an ignition process and a build up process. They present evidence that the build up to detonation is controlled by a heat transfer dominated grain burning process. The ignition process appears to arise from shock induced "hot spots."

The necessity of the hot spot concept of Bowden[16] and Eyring[17] arises from the fact that under shock initiation conditions the bulk temperature of the explosive is much too low to initiate decomposition. Various mechanisms have been proposed to account for the hot spots controlling the ignition process. Bowden and Yoffe[16] proposed adiabatic compression of gas as the principal mechanism, but also discussed plastic work in solid explosives as a mechanism. Mader[18] studied the mechanism of direct heating of the explosive by void closure; Seeley[19] has suggested jetting during void closure as the mechanism for hot spot formation; and Delpuech, et al[20] suggest shock induced free radical formation as playing the critical role in the initiation process.

## II. FREY'S SHEAR BAND MODEL

Recently Frey[21] has proposed a shear band theory for hot spot formation. Frey suggested these shear bands might arise during void closure or during shock induced displacement of the explosive near irregularities at the explosive-container wall interface, as shown in Figure 1. Starting with this hypothesis, Frey showed that shearing under pressure could lead to sufficiently rapid heating of the explosive to generate hot spots in the explosive adequate to give rise to initiation of the explosive. However, the shear velocities indicated by the shear band mechanisms shown in Figure 1 do not depend on the explosive material properties. As such, the $P^2T$ criterion as a property of the explosive would be difficult to understand.

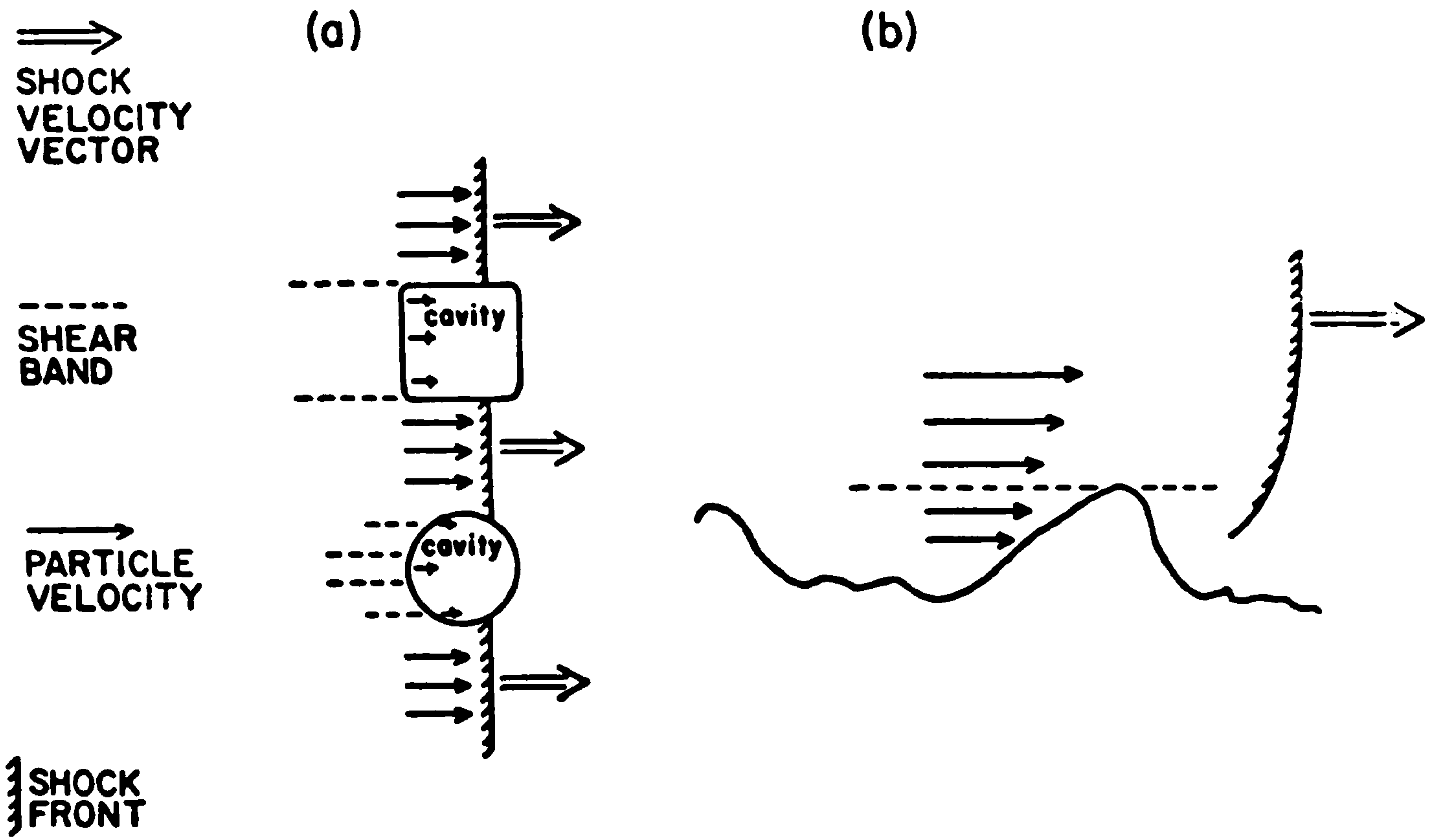


Figure 1. Schematic of the Sources of Shear Bands According to Frey's Model. (A) Shear bands produced in front of cubical and spherical cavities. (B) Velocity gradient producing shear bands near irregular interface.

Until recently, shear bands in shock loaded explosives had not been observed. Gibbons[22] has recently obtained scanning electron micrographs showing an extensive shear band structure in shock loaded comp B, Figure 2. The comp B also shows evidence of incipient reaction of the TNT matrix in the area of the shear bands. From the location of these shear bands, it is apparent that the shear bands do not result from either cavity collapse or container wall irregularities. The shear bands could also arise from the shear stress field in the explosive produced by deformation of the explosive container. However, that flow field depends primarily on the characteristics of the container and the container's response to impulsive loading, and only to a lesser degree on the properties of the comp B fill. Such an origin for shears leading to initiation of the explosive would not be likely to involve the $P^2T$ criterion. Another cause for the occurrence of the shear bands is required. A mechanism for shear band production that makes use of Frey's shear band theory and that provides a procedure for the computation of $P^2T$ criterion values for explosives is presented below. In a separate report,[23] we derive the $P^2T$ criterion based on the model presented here.

## III. SHEAR BAND PRODUCTION BY SHOCK LOADING IN HETEROGENEOUS EXPLOSIVES

Assume a shock passes through a material, such as comp B, consisting of grains of one material, RDX, embedded in a matrix of a second material, here TNT. The pressure p behind the shock is given in terms of the density $\rho$, sound velocity u, and particle velocity v by

$$p = \rho_0 uv \quad . \tag{1}$$

Although the pressure is the same in both the RDX grains and the TNT matrix, since the impedance, $\rho u$, differs in the two materials, the particle velocity will differ in the two constituents, as indicated in Figure 3. Table 1 shows the densities, sound velocities and particle velocities for RDX and TNT for a 2.5 GPa shock pressure. The resulting velocity difference is

$$v_s = v_1 - v_2 \quad . \tag{2}$$

From Table 1 this gives 70 m/s.

TABLE 1

Densities, Sound Velocities, and Particle Velocities for the Constituents of Comp B at 2.5 GPa*

| | $\rho_0$ (g/cm$^3$) | u(km/s) | v (km/s) |
|---|---|---|---|
| RDX | 1.80 | 3.53 | 0.395 |
| TNT | 1.61 | 3.34 | 0.465 |

*Computed from shock Hugoniot data in The LLNL Explosives Handbook, B. M. Dobratz. University of California, Livermore, CA 94550. See table 7.5.

A

B

Figure 2. Scanning Electron Micrograph of Shock Loaded Comp B. Magnitude of the shock was about 2.5 GPa. The grains are RDX particles which are embedded in the TNT matrix. The shear bands run principally between the RDX grains, although some shear bands run through the RDX grains. This area was discolored brown by incipient reaction of the TNT. (A) Magnification is 750X; (B) Enlargement of upper right of (A) at a magnification of 1500X.

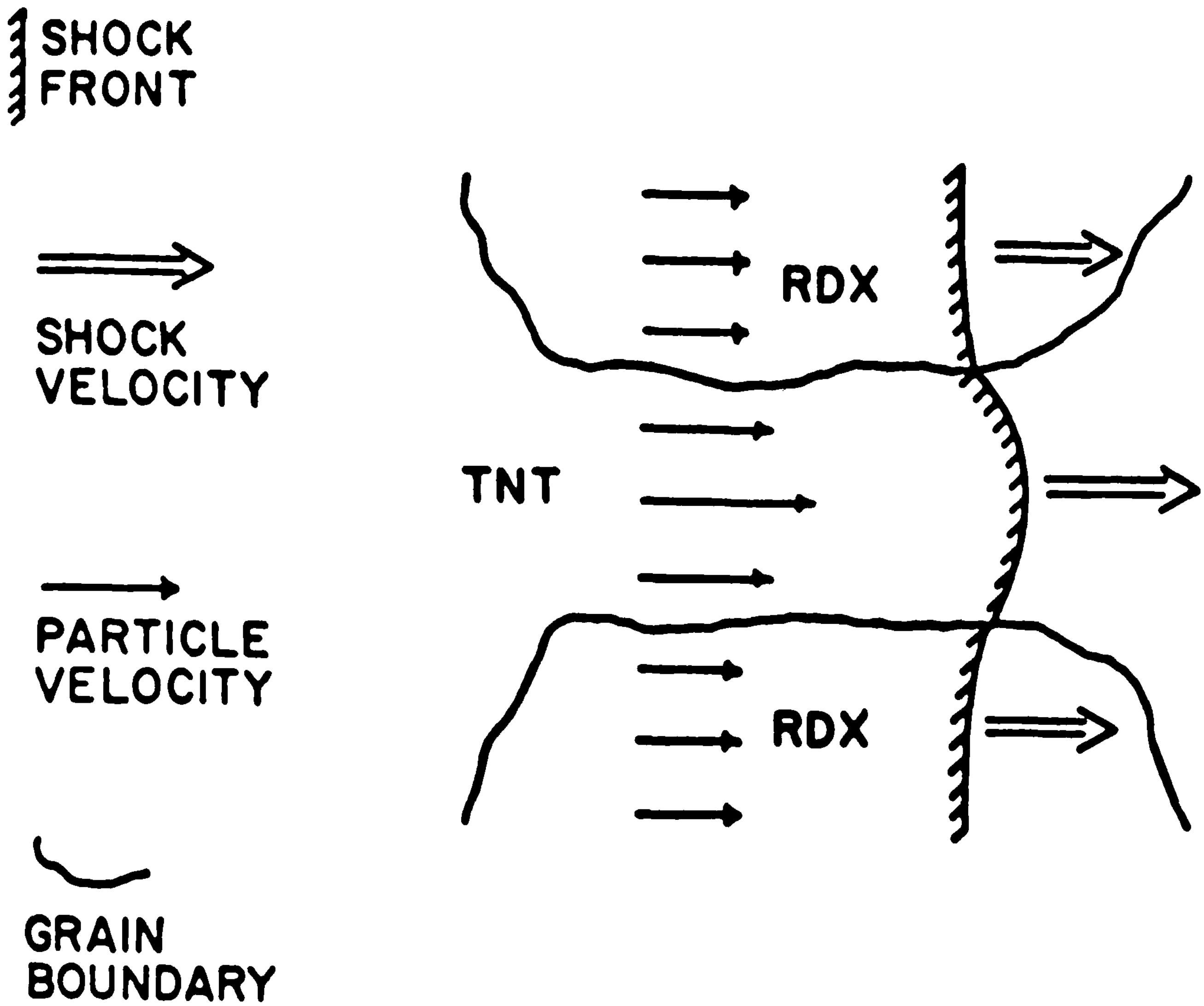


Figure 3. Schematic Representation of a Shock Passing Through a Heterogeneous Material. The shock velocities differ in the two materials as do the particle velocities. As a result, a velocity gradient will develop across these materials giving rise to shear.

It is to be noted that even in a single constituent explosive, a similar result will occur. The propagation velocity for a sound wave differs along various crystal orientations. In such materials, for individual grains, $u_{(100)}$ will differ significantly from $u_{(111)}$ or $u_{(010)}$ for example (where the subscripts refer to the principal axes along the crystal grains of the explosive.) Thus, we would obtain various shear velocities depending on crystal orientations. For a crystal having the (111) plane parallel to the (100) plane in a neighboring crystal we would have

$$v_s = v_{(100)} - v_{(111)} \quad (3)$$

Unfortunately, sound velocity data along different crystal axes for explosives is too sketchy for our present needs, so we will confine our interest to two constituent explosives.

We will also limit our treatment to the case in which the shear takes place in the matrix. In general, where the effective shear strength of the explosive approximates the shear strength of the matrix, we may treat the process of shear formation as taking place in the matrix. Where the shear strength approximates the shear strength of the grains, shear formation should be calculated for the grains. In other cases, we must make calculations for shearing that can occur in either the matrix or the grains. In such cases, the smaller of the calculated $P^2T$ values obtained is to be taken for the critical value characterizing the explosive. Thus, generalization of the present approach can be achieved in a straight forward way.

It should be noted that shear band formation described here constitutes the incipient mechanism for shear failure. Large scale mechanical failure of the explosive is associated with the arrival of relief waves from free surfaces (failure of the explosive's container walls, for example). The arrival of these relief waves lead to the growth of the incipient shears into larger shears that ultimately connect to form macroscopic cracks in the explosive.

## IV. SHEAR VELOCITY FOR TWO CONSTITUENT EXPLOSIVES

Writing $\rho_1, u_1$ for the density and sound velocity in the matrix and $\rho_2, u_2$ for the density and sound velocity for the included grains we write

$$v_s = p \frac{\rho_2 u_2 - \rho_1 u_1}{\rho_1 u_1 \rho_2 u_2} \quad (4)$$

where a negative result indicates shearing results from a slower matrix particle velocity. This velocity is the overall shear velocity between the two constituents of the explosive. It is not the shear band shear velocity however, as it does not take account of the number of shear bands (on average) in the matrix lying between two grains. As the shock passes between two grains, the displaced material will strain until relieved by the development of one or more shear bands.

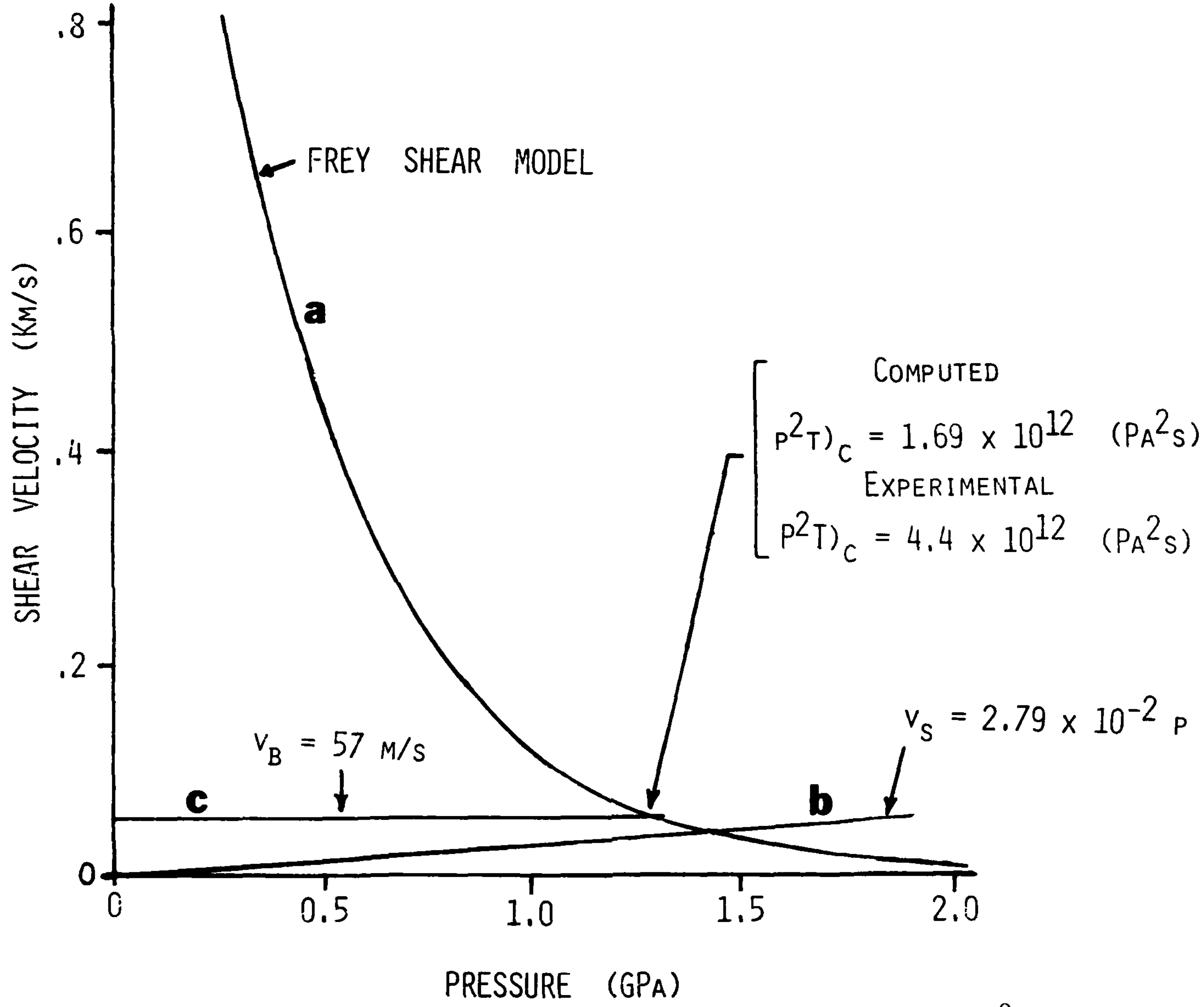


Figure 4. Shear Velocity Required to Achieve Thermal Explosion Criterion of $1000^{o}$K in 1 μs as a Function of Pressure (curve "a"), after Frey and a Plot of Equation (5) for the Shear Velocity Generated in Comp B Due to the Shock Pressure. The intercept point occurs at $v_s$ = 40.8 m/s, p = 1.42 GPa. Curve "c" is discussed in Section V. It incorporates the correction for the number of shear bands developed by the shear in matrix material as given by Equation 11 for $v_b$. The intercept occurs at $v_b$ = 57 m/s, p = 1.30 GPa.

In Frey's analysis, the shear velocity occurs as a parameter dependent on the circumstances of cavities and container irregularities. In the present case, we see that the velocity difference is dependent on the physical properties of the explosive. In the case of comp B, $v_s$ (km/s) is given, approximately, in terms of the pressure p (GPa) by

$$v_s = 2.79 \times 10^{-2} p \quad . \tag{5}$$

Frey[24] shows that there is a functional relation between shear velocity and the shock pressure, where time to reach a critical ignition temperature appears as a parameter, Figure 4. With Frey's computed results for the shear velocity versus shock pressure for TNT as shown in Figure 4, and the relation between shock pressure and shear velocity for the TNT matrix in comp B, as given in Equation 5, we can solve to obtain the shock pressure leading to a given ignition temperature in a specified time. From Figure 4, we obtain a solution of $v_s = 40.8$ m/s and $p = 1.42$ GPa. Assuming the ignition temperature of $1000^{\circ}$K as used by Frey, we calculate a $P^2T$ criterion of

$$P^2T)_{crit} = 2.02 \times 10^{12} \ (Pa^2 s) \ . \tag{6}$$

The result is to be compared with an experimental value of $4.41 \times 10^{12}$ $Pa^2s$. The difference in values obtained here arises from the fact that the shear velocity in Equation 5 is not the shear band shear velocity, but instead the overall shear velocity between the grains of RDX and matrix of TNT. Let us now turn to the question of the shear band density which will allow us to obtain the shear band shear velocity.

## V. SHEAR BAND DENSITY

To obtain the shear band shear velocity $v_b$, it is necessary to derive the density of the shear bands in the matrix material. Consider the material displacement as shown in Figure 5. After the shock passes through the explosive, a shear gradient will develop due to the resistance to shear at the matrix-grain interface. In a time t assumed to be very short (i.e., before shear banding develops) the material behind the shock will assume, approximately, a rhomboidal displacement as seen in Figure 5. Figure 5 shows one of these rhomboidal sections broken into several incipient shear bands of width d and strain $\delta d$ such that

$$\delta d = \frac{\text{total strain in time t}}{\text{number of shear bands}} = \frac{v_s t}{D/d} \quad . \tag{7}$$

The failure angle $\theta_{max}$ at which shear occurs is related to the strain $\delta d$ by

$$\frac{\delta d}{d} = \theta_{max} \quad . \tag{8}$$

Where $\theta_{max}$ is a property of the material. Of course, Figure 5 idealizes the regularity of the overall process.

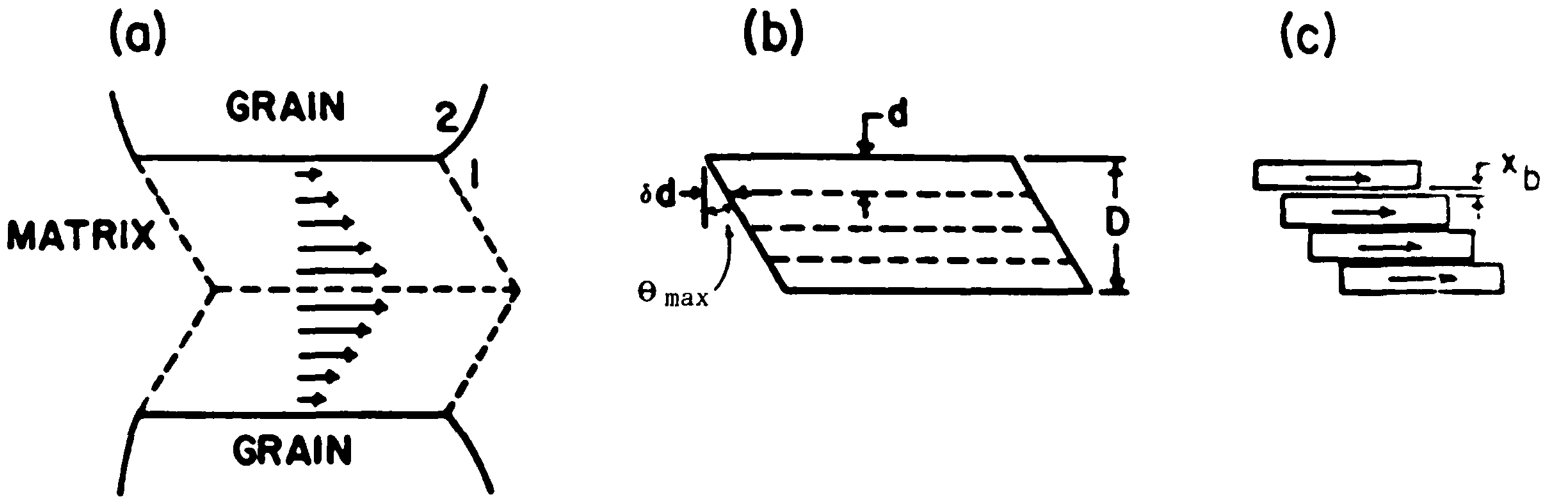


Figure 5. Schematic of Shear Band Formation. (a) Displacement of matrix material relative to grains due to passage of a shock, where it is assumed the difference in shock particle velocity develops into a velocity gradient as expected for viscous flow in a channel. The displacement indicated by the two rhomboidal regions indicates strains at an early time after passage of the shock. (b) Schematic of a rhomboidal region giving shear band and displacement dimensions just before formation of the bands due to development of slide planes. (c) Resulting displacement of material in the rhomboid of (b) as the critical angle $\Theta_{max}$ occurs.

The time at which this shearing occurs depends on the propagation of stress relief into the material as shear banding develops. Thus, in a time t such a relief wave can propagate only a distance $u_1t$. This means that the next nearest shear will be located at most a distance $u_1t$ away. Since the process is more nearly stochastic, the average value for the separation of the shear bands will be half $u_1t$. Since that distance is also d, we have

$$\tfrac{1}{2}u_1 t = d\,. \tag{9}$$

Therefore, from Equations 7, 8, and 9, we have

$$d = \frac{\theta_{max} D u_1}{2v_s}\,. \tag{10}$$

Now substituting from Equation 4 for $v_s$ we obtain

$$d = \frac{\theta_{max} D u_1 \rho_1 u_1 \rho_2 u_2}{2p\,(\rho_2 u_2 - \rho_1 u_1)}\,. \tag{11}$$

The number of shear bands in the gap between grains, n* is, approximately,

$$n^* = 2D/d = \frac{4p\,(\rho_2 u_2 - \rho_1 u_1)}{\theta_{max} u_1 \rho_1 u_1 \rho_2 u_2}\,. \tag{12}$$

$\theta_{max}$ is given in terms of the shear modulus G and shear strength $\sigma_{max}$ by $\sigma_{max}/G$. The shear modulus can also be expressed in terms of the Young's elastic modulus E and Poisson's ratio $\nu$ by $\tfrac{1}{2}E/(1+\nu)$. Thus,

$$\theta_{max} = 2\,(1+\nu)\,\sigma_{max}/E\,. \tag{13}$$

The value of the shear band shear velocity $v_b$ is given by dividing $v_s$ by n, where

$$n = n^*/2\,. \tag{14}$$

Since both $v_s$ and n are linear in p, $v_b$ is independent of p. We have from Equations (4) and (12)

$$v_b = \tfrac{1}{2}\,u_1 \theta_{max}\,. \tag{15}$$

For E = 5.4 GPa, $\nu$ = 0.3 and $\sigma_{max}$ = 0.07 GPa, we have from Equation (13)

$$\theta_{max} = 0.034 \tag{16}$$

for TNT. With $u_1$ of 3.34 km/s as given in Table 1, we obtain from Equation (15), $v_b$ = 57 m/s for the shear band shear velocity in the TNT matrix material.

From Figure 4, we see this yields an intercept at a shock pressure of 1.30 GPa. This value of the pressure acting for 1 μs yields for the computed $P^2T$ value

$$P^2T)_{crit} = 1.69 \times 10^{12}\ Pa^2s \quad . \tag{17}$$

This value is somewhat lower than the experimental value of $4.4 \times 10^{12}\ Pa^2s$. However, the criterion for initiation of the explosive used in Frey's calculation is similarly approximate. It should be pointed out that as treated here, this is only an initiation criterion, and not a detonation criterion, as time must be allowed for the incipient burn of the explosive at these hot spots to generate self sustaining pressures. In a separate report,[25] this problem is considered in some detail and shown to contribute only a small contribution to the $P^2T$ value we have here. Thus, using an expression for the shear band shear velocity under shock loading conditions, we can employ Frey's shear band theory to calculate $P^2T)_{crit}$ from the properties of explosive materials.

## VI. CONCLUSIONS

A theory relating shock loading to the development of shear bands in explosives has been presented. This theory together with Frey's shear band theory for the development of hot spots due to shear heating along these shear bands makes it possible to compute $P^2T)_{crit}$ values for explosives from the mechanical and thermodynamic properties of the explosive.

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24. See Ref. 21, Figure 7.

25. See Ref. 23, pg 12-13.

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