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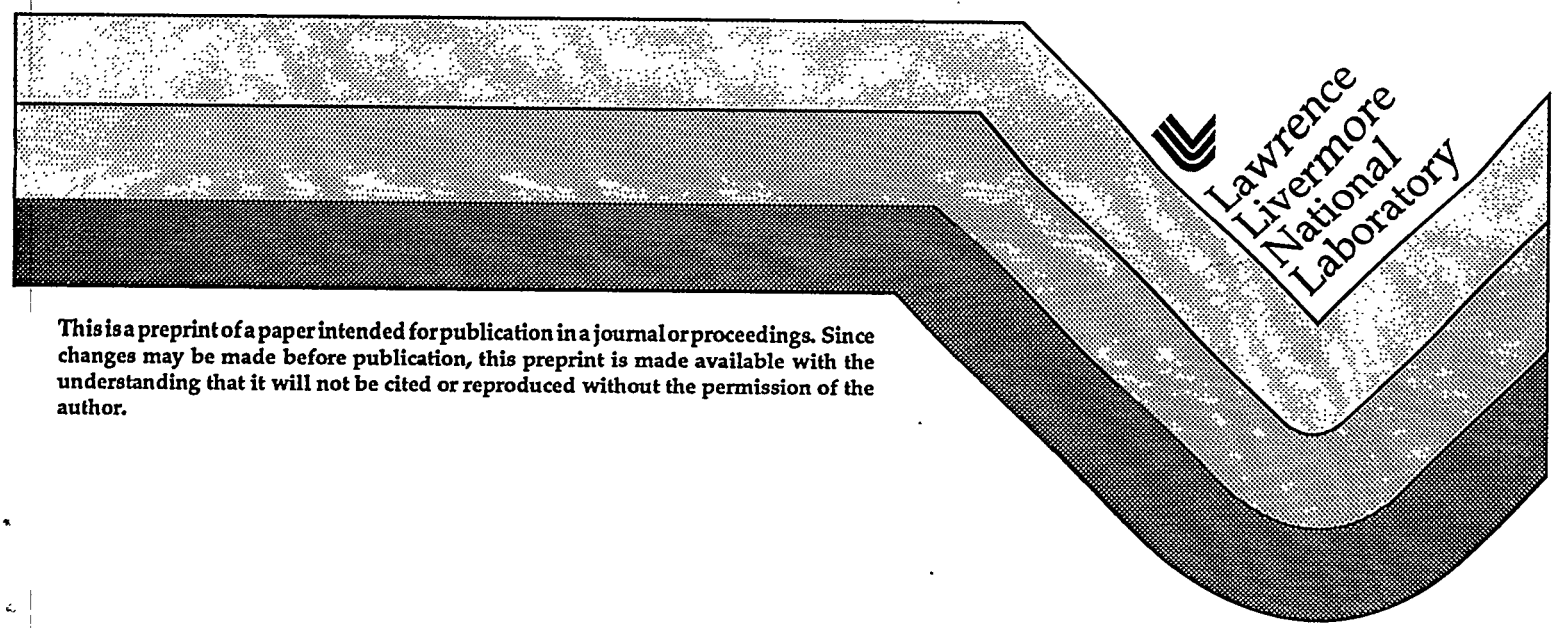

SHOCK INITIATION OF 2,4-DINITROIMIDAZOLE (2,4-DNI)

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The shock sensitivity of the pressed solid explosive 2,4-dinitroimidazole (2,4-DNI) was determined using the embedded manganin pressure gauge technique. At an initial shock pressure of 2 GPa, several microseconds were required before any exothermic reaction was observed. At 4 GPa, 2,4-DNI reacted more rapidly but did not transition to detonation at the 12 mm deep gauge position. At 6 GPa, detonation occurred in less than 6 mm of shock propagation. Thus, 2,4-DNI is more shock sensitive than TATB-based explosives but is considerably less shock sensitive than HMX-based explosives. An Ignition and Growth reactive flow model for 2,4-DNI based on these gauge records showed that 2,4-DNI exhibits shock initiation characteristics similar to TATB but reacts faster. The chemical structure of 2,4-DNI suggests that it may exhibit thermal decomposition reactions similar to nitroguanine and explosives with similar ring structures, such as ANTA and NTO.

INTRODUCTION

The five membered ring explosive 2,4-dinitroimidazole (2,4-DNI) was first synthesized by Lancini et al. (1) by nitrating 2-nitroimidazole. It was later obtained by the thermal rearrangement of 1,4-DNI (2). Currently 2,4-DNI is being made from 4-nitroimidazole, which is commercially available (3). This allows 2,4-DNI to be produced in large quantities in a cost effective manner. The goal of the synthesis project is to produce a relatively inexpensive explosive that has a higher energy density than TATB and TNT, yet is still insensitive. The small scale safety properties, thermal explosion behavior, and detonation velocity versus charge density of 2,4-DNI were reported by Jayasuriya et al. (3). In this paper, the shock sensitivity of 2,4-DNI was measured at three shock pressures using embedded manganin gauge techniques (4) and calculated using the Ignition and Growth reactive flow model (5) for shock initiation and detonation in the DYNA2D hydrodynamic code (6).

EXPERIMENTAL

The experimental geometry is shown in Fig. 1. A 12.7 mm thick, 60 mm diameter Lexan flyer plate impacted a target consisting of a 6 mm thick, 90 mm diameter Teflon buffer plate and a 25 mm thick, 50.8 mm diameter 2,4-DNI charge. The 2,4-DNI charge was held in place by a 3 mm thick Lexan ring. Six 0.3 mm thick Teflon-insulated manganin gauges were placed in pairs along the center line of the 2,4-DNI charge at distances of 0, 6, and 12 mm. Three experiments were fired in the 100 mm powder gun with Lexan flyer velocities of 0.979 mm/μs, 1.518 mm/μs and 2.273 mm/μs, producing initial shock pressures of approximately 2 GPa, 4 GPa and 6 GPa, respectively. The measured changes in resistance of the manganin gauge elements were converted to

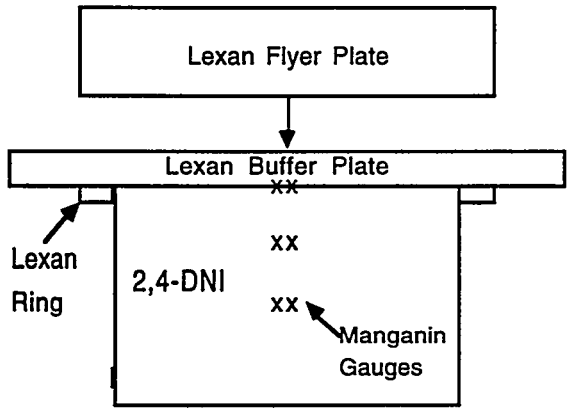

FIGURE 1. Experimental geometry for the shock initiation experiments on 2,4-DNI

pressure histories and compared to Ignition and Growth reactive flow calculations.

REACTIVE FLOW MODELING

The Ignition and Growth reactive flow model (5) has been incorporated into several hydrodynamic codes and used to solve many explosive and propellant safety and performance problems (7). The model uses two Jones-Wilkins-Lee (JWL) equations of state, one for the unreacted explosive and another one for the reaction products, in the temperature dependent form:

$$p = A\, e^{-R_1 V} + B\, e^{-R_2 V} + \omega C_v T \qquad (1)$$

where p is pressure in Megabars, V is relative volume, T is temperature, ω is the Gruneisen coefficient, C_v is the average heat capacity, and A, B, R_1 and R_2 are constants. The equations of state are fitted to the available shock Hugoniot data. The reaction rate law is:

$$dF/dt = I(1-F)^b(\rho/\rho_o - 1 - a)^x + G_1(1-F)^c F^d p^y \quad (0<F<Figmax \quad 0<F<FG1max)$$
$$+ G_2(1-F)^e F^g p^z \quad (F_{G2min}<F<1) \qquad (2)$$

where F is the fraction reacted, t is time, ρ is the current density, ρ_o is the initial density, p is pressure in Megabars, and I, G_1, G_2, a, b, c, d, e, g, x, y, and z are constants. As explained in previous papers (4), this three term reaction rate law models the three stages of reaction generally observed during shock initiation of heterogeneous solid explosives. The first term ignites some of the solid explosive as it is compressed by a shock or compression wave creating heated areas (hot spots) as the voids in the material collapse. Generally the amount of explosive ignited by a strong shock wave is approximately equal to the original void volume. The second term in Eq. (2) represents the relatively slow growth of reaction from the hot spots into the surrounding solid in a deflagration-type process. The third term in Eq. (2) describes the rapid transition to detonation observed when the growing hot spots begin to coalesce and transfer large amount of heat to the remaining unreacted particles, causing them to react very quickly and to create a high pressure pulse which overtakes the leading shock front and thus causes detonation. The equation of state parameters for 2,4-DNI, Lexan, and Teflon and the Ignition and Growth rate law parameters used in the reactive flow calculations are listed in Table 1. The measured pressure histories and those predicted by the Ignition and Growth model are compared in the next section.

COMPARISON OF RESULTS

Figure 2 compares the experimental pressure histories (solid lines) with those predicted by the Ignition and Growth model (dashed lines) for the lowest pressure 2,4-DNI experiment with a Lexan flyer velocity of 0.979 mm/μs, which imparts a 2 GPa shock pressure into the 2,4-DNI charge. The 0 mm gauges measured very little growth of reaction for the first 6 μs after impact, and then the pressure

TABLE 1. Equation of state and reaction rate parameters

1. Ignition and Growth Model Parameters for 2,4-DNI

Unreacted JWL	Product JWL	Reaction Rate Parameters	
ρ_o =1.67 g/cm^3			
A=2700 Mbar	A=6.113 Mbar	I=2.0e+8	G_2=25
B=-0.0519165 Mbar	B=0.1065 Mbar	a=0.0	e=0.667
R_1=13.0	R_1=4.40	b=0.667	g=0.667
R_2=1.30	R_2=1.20	x=15.0	z=2.0
ω=0.9	ω=0.32	G_1=9.5	F_{igmax}=0.3
C_v=3.0e-5 Mbar/K	C_v=1.0e-5 Mbar/K	y=1.0	F_{G1max}=1.0
T_o=298^{o}K	E_0=0.089 Mbar	c=0.667	F_{G2min}=0.3
Shear Modulus=0.035Mbar		d=0.333	
Yield Strength=0.002 Mbar			

2. Gruneisen Parameters for Inert Materials

$$p = \rho_o c^2 \mu[1+(1-\gamma_o/2)\mu - a/2\mu^2] \,/\, [1-(S_1-1)\mu - S_2\mu^2/(\mu+1) - S_3\mu^3/(\mu+1)^2]^2 + (\gamma_o + a\mu)E$$

where $\mu=\rho/\rho_o - 1$ and E is thermal energy

Inert	ρ_o(g/cm^3)	c(mm/ms)	S_1	S_2	S_3	γ_o	a
6061-T6 Al	2.703	5.24	1.4	0.0	0.0	1.97	0.48
Lexan	1.193	1.933	2.04	0.0	0.0	0.61	0.0
Teflon	2.15	1.68	1.123	3.98	-5.8	0.59	0.0

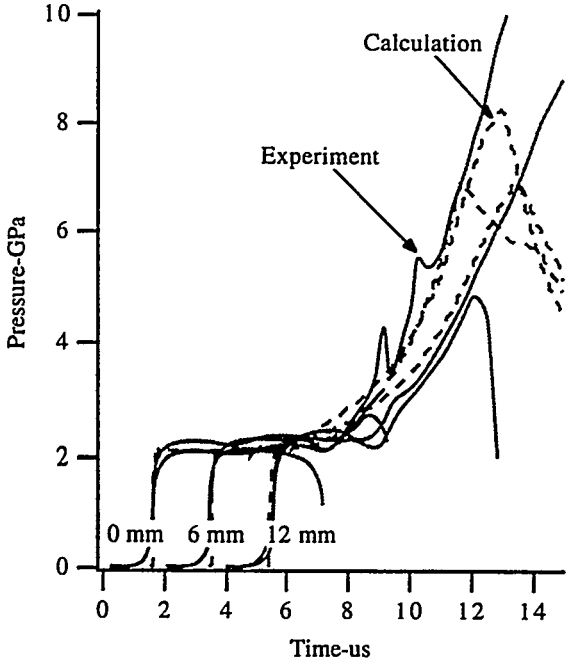

FIGURE 2. Pressure histories for 2,4-DNI impacted at 0.979 mm/μs by a Lexan flyer plate

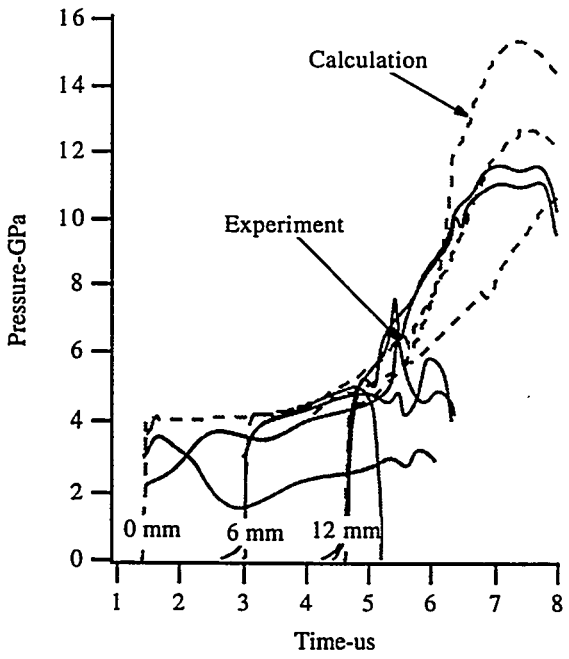

FIGURE 3. Pressure histories in 2,4-DNI impacted at 1.518 mm/μs by a Lexan flyer

rose slowly to 3 GPa over the next μs before the gauges failed. The 6 mm deep gauges recorded no pressure increase for the first 3 μs, followed by a continuous growth to over 10 GPa in the next 5 μs. The 12 mm deep gauges recorded similar pressure histories. The Ignition and Growth model pressure histories exhibit similar continuous energy releases up to about 8 to 9 GPa, corresponding to approximately 50% reaction. At this shock pressure, TATB-based explosives do not react (8), and HMX-based explosives exhibit a faster growth of reaction behind the shock front than does 2,4-DNI (9).

Figure 3 shows the experimental and calculated pressure histories for 2,4-DNI impacted by Lexan at 1.518 mm/μs, creating a 4 GPa shock. At this shock amplitude, TATB-based explosives do not react, while HMX-based explosives transition to detonation at run distances of less than 10 mm (10). The gauge records in Fig. 3 clearly show that 2,4-DNI is not close to detonating at the 12 mm gauge position. Although the 0 mm gauge records are not very good, the other 4 gauges clearly show some shock front amplitude increase at the 6 and 12 mm depths, followed by a pressure growth to 11 GPa over the next 3 μs at the 12 mm gauges. The Ignition and Growth model calculates these increases accurately by allowing about 3% reaction during shock compression (ignition) and a subsequent reaction rate with a p^1 dependence.

The experimental and calculated results for the highest Lexan flyer velocity experiment, 2.273 mm/μs, producing a 6 GPa shock are shown in Fig. 4. The 0 mm gauges record a rapid growth reaction to 12 GPa over 2 μs. The 6 and 12 mm gauges record high pressures characteristic of a detonation wave. The Ignition and Growth calculations agree closely with the gauge records and predict that detonation occurs just before the reactive shock reaches the 6 mm gauge. At a shock pressure of 6 GPa, HMX-based explosives detonate in about 4 mm, while TATB-based explosives do not decompose to any significant degree. Therefore, 2,4-DNI is much more reactive than TATB at 6 GPa, but but not as reactive as most explosive molecules.

SUMMARY

The shock sensitivity of 2,4-DNI has been determined using embedded manganin pressure gauges and the Ignition and Growth reactive flow model. Its shock initiation characteristics have been shown to be similar to TATB-based explosives in that a shock of sufficient strength to ignite a few percent of the charge then exhibits some amplitude growth as it propagates through the charge, followed by a growth of reaction that can be modeled with a linear pressure dependence. The transition to detonation then occurs in the usual fashion when the growing pulse pulse overtakes the leading shock front. Since it reacts

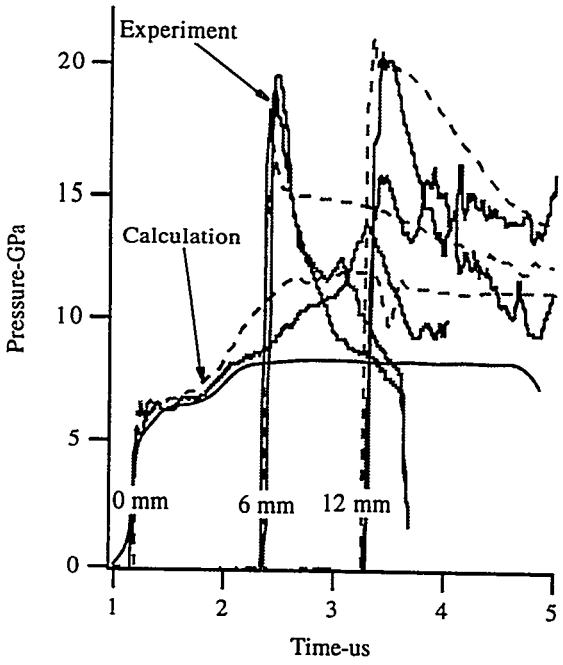

FIGURE 4. Pressure histories for 2,4-DNI impacted at 2.273 mm/μs by a Lexan flyer

relatively slowly at 2 and 4 GPa shock pressures, 2,4-DNI is definitely less shock sensitive than HMX. Since it reacts slowly at 2 and 4 GPa and detonates within 6 mm at 6 GPa, 2,4-DNI is more shock sensitive than TATB. However, since most hazard scenarios involve shock pressures well below 6 GPa, 2,4-DNI may be shock insensitive enough for many applications.

Williams et al. (11) have studied the thermal decomposition of several explosives with ring structures similar to that of 2,4-DNI, such as 3-nitro-1,2,4-triazol-5-one (NTO) and 3-amino-5-nitro-1,2,4-triazole (ANTA), and found that these compounds partially decompose forming a polymer-like residue called melon. Thus 2,4-DNI should decompose in a similar manner. Since at least one of these compounds, nitroguanidine, exhibits Group 2 explosive behavior (12), 2,4-DNI may also fall into this category.

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REFERENCES

1. Lancini, G. C., Maggi, N., and Sensi, P., *Farmaco (pavia), Ed. Sci.*, **18**, 390-395 (1963).

2. Sharnin, G. P., Fassakhov, R. Kh., and Orlov, P. P., USSR Patient 458553 (1975).

3. Jayasuriya, K., Damauarapu, R., Simpson, R. L., Coon, C. L., and Colburn, M. D., "2,4-Dinitroimidazole: A Practical Insensitive High Explosive," Lawrence Livermore National Laboratory Report UCRL-JC-ID-113364, March 1993.

4. Urtiew, P. A., Erickson, L. M., Hayes, B., and Parker, N. L., *Combustion, Explosion and Shock Waves* **22**, 597-614 (1986).

5. Tarver, C. M., Hallquist, J. O., and Erickson, L. M., in Eighth Symposium (International) on Detonation, Naval Surface Weapons Center NSWC 86-194, Albuquerque, NM, 1985, pp. 951 -961.

6. Whirley, R. G., Engelmann, B. E., and Hallquist, J. O., "DYNA2D User Manual," Lawrence Livermore National Laboratory Report UCRL-MA-110630, April 1992.

7. Tarver, C. M., Urtiew, P. A., Chidester, S. K., and Green, L. G., *Propellants, Explosives, Pyrotechnics* **18**, 117-127 (1993).

8. Tarver, C. M., *Propellants, Explosives, Pyrotechnics* **15**, 132-142 (1990).

9. Lee, E. L. and Tarver, C. M., *Phys. Fluids* **23**, 2362-2372 (1980).

10. Dobratz, B. M. and Crawford, P. C., "LLNL Explosives Handbook," Lawrence Livermore National Laboratory Report UCRL-52997, January 1985.

11. Williams, G. K., Palopolli S. F., and Brill, T. B., *Combustion and Flame* **98**, 197-204 (1994).

12. Price, D., Clairmont, A. R., and Erkman, J. O., *Combustion and Flame* **17**, 323-336 (1971).