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2, 4-Dinitroimidazole**

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A New Insensitive Explosive That Has Moderate Performance and is Low Cost: 2, 4-Dinitroimidazole

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Summary

2, 4-dinitroimidazole is a very shock insensitive material. The performance of the material is expected to be 60% greater than TNT. Costs appear to be low but are unresolved at this time. 2, 4-DNI may be a realistic alternative to TNT for mass-use bombs.

Introduction

LLNL is working together with the Army at ARDEC and the Los Alamos National Laboratory (LANL) in synthesizing and characterizing the energetic molecule 2, 4-DNI. For many mass-use applications 2, 4-DNI appears to be the best compromise of properties. TNT is less expensive, HMX has higher performance, PETN has hotter detonation products, and TATB is less sensitive than 2, 4-DNI. However, 2, 4-DNI appears to beat them all in terms of a property compromise for real world applications.

The cooperative activity is described in the following joint LLNLLANL-ARMY report. What is reported here are the results of recent shock loading studies, performance calculations, and sensitivity discussion.

Shock Loading

We have performed three shock loading experiments on a 2, 4-DNI-based formulation RX51AA. The formulation consists of 95.0wt% 2, 4-DNI and 5.0% Estane-5702. This material approximates the DOE/DoD HMX-based explosive LX-14 (95.5wt%HMX, 4.5%

Estane). RX51AA was pressed to a nominal density of 96.6% of theoretical maximum density (TMD). It should be noted that LX-14 has a higher nominal density of 97.3% TMD, and 0.5% less explosive by volume than RX51AA. These differences are expected to make RX51AA slightly more sensitive than a 2, 4-DNI-based material that was an exact match to LX-14.

The shock loading configuration is shown in Fig. 1. A smooth 100 mm bore powder gun was used to one-dimensionally shock the samples. Six *in situ* manganin pressure gauges were located at three different depths in the explosive. Pressure histories as a function of time are obtained at each location.

Figure 1. Experimental configuration and shock trajectory plot.

The experiment data are shown in Fig. 2. Figure 2a displays the pressure response of LX-14 at an input pressure of 22.7 kbar at: 0 mm, 6 mm, and 13 mm. As can be seen LX-14 has nearly transitioned to detonation after the shock has run 13 mm. At approximately the same shock pressure, the 2, 4-DNI-based material shows no reaction. In fact the shock velocity is actually decreasing. Table 1 lists the shock velocities between the different gauge stations for the three samples.

Nearly doubling the shock input pressure to 38.3 kbar is adequate to begin to initiate RX51AA. The reactions are slow and the shock front is only slightly accelerating. A typical high solids loaded plastic bonded explosive would show a prompt transition under these conditions. It should be noted that the oscillations in the first pressure

signal in Fig. 2c were due to the power supply of the gauge not being stabilized at the time of the shock arrival and is not a material response.

At 72 kbar the material has nearly transitioned to detonation 6 mm into the sample. The shock velocity between 6 mm and 13 mm is consistent with steady state detonation.

Figure 2. Pressure histories of: (a) LX-14 shocked at 22.7 kbar. (b) RX51AA shocked at 21.0 kbar. (c) RX51AA shocked at 38.3 kbar. (d) RX51AA shocked at 72 kbar.

Table 1. Shock velocity histories in RX51AA.

Shock Loading Pressure (kbar)	Region I (mm/ μ s)	Region II (mm/ μ s)	Behavior
2.10	2.96	2.79	decrease
3.83	3.51	3.58	same
7.0	4.59	8.00	transitioned

Performance of 2, 4-DNI

Table 2 lists the predicted performance of 2, 4-DNI compared to TNT. It can be seen that 2, 4-DNI is significantly better. As described in the following joint LLNL-LANL-ARDEC paper the detonation products appear to be very hot suggesting utility in non-ideal composite explosives.

Table 2. Explosive performance of 2, 4-DNI.

Detonation Parameters		Predicted Energy		
ρ (g/cc)	1.76	V/V _o	Relative to TNT	Relative to HMX
D (mm/ μ s)	7.961	2.2	+49	-27
u _p (mm/ μ s)	2.02	4.1	+56	-26
P _{CJ} (GPa)	27.8	6.5	+59	-26
V _{CJ} (cc/g)	0.424	10		-25
T _{CJ} (K)	3130	20		-25
E _{CJ} (cal/g)	485			

We have evaluated 2, 4-DNI for propellant applications. Although attractive as a high explosive it appears not to be of value as a propellant component. Table 3 summarizes the propulsion properties of pure 2, 4-DNI. It can be seen that the specific impulse (I_{sp}) is significantly below HMX and 1,3,3-trinitroazetidine (TNAZ). Tables 3 & 4 list the calculated performance of strategic and tactical propellants based on 2, 4-DNI. It is clear that there are no performance benefits with 2, 4-DNI for these propellant applications.

Table 3. I_{sp} of pure materials.

Material	HMX		TNAZ		2,4-DNI	
	Chmb	Exh	Chmb	Exh	Chmb	Exh
P (psia)	1000	14.7	1000	14.7	1000	14.7
Expansion ratio		8.36		9.15		7.86
I_{sp} @ <i>atms</i>		<u>265</u>		<u>273</u>		<u>237</u>
I_{sp} @ vacuum		286		296		254
T (K)	3276	1557	3522	1973	2992	1262
Mw	24.27	24.68	26.16	27.43	26.24	26.35
Mols gas/100 g	4.12	4.05	3.82	3.64	3.81	3.80
C* (ft/sec)	5389		5442		4871	

Table 4. Performance as a Class 1.1 aluminized propellant.

Material	HMX-based		TNAZ-based		2,4-DNI-based	
	Chmb	Exh	Chmb	Exh	Chmb	Exh
P (psia)	1000	14.7	1000	14.7	1000	14.7
Expansion ratio		10.13		10.10		10.31
I_{sp} @ <i>atms</i>		<u>273</u>		<u>274</u>		<u>259</u>
I_{sp} @ vacuum		298		299		283
T (K)	3706	2327	3853	2454	3475	2183
Mw	28.36	29.58	29.59	31.20	29.33	30.35
Mols gas/100 g	3.53	3.38	3.38	3.20	3.41	3.3
C* (ft/sec)	5381		5380		5104	

Table 5. Performance as a smokeless propellant (70/20/10 oxidizer/NG/NEPE).

Material	HMX-based				TNAZ-based				2,4-DNI-based			
	Chm	Exh	Exh	Exh	Chm	Exh	Exh	Exh	Chb	Exh	Exh	Exh
P (psia)	1000	14.7	5.8	2.3	1000	14.7	6.056	2.424	1000	14.7	5.66	2.50
Expansion ratio		8	16	32		8	16	32		8	16	32
I_{sp} @ <i>atms</i>		<u>255</u>	<u>271</u>	283		<u>263</u>	<u>279</u>	<u>293</u>		<u>233</u>	<u>248</u>	<u>258</u>
I_{sp} @ vacuum		274	286	295		284	295	305		250	261	270
T (K)	2945	1292	1073	903	3233	1514	1273	1068	2658	1098	931	881
Mw	22.73	22.84	22.84	22.87	24.12	24.43	24.43	24.43	23.78	23.83	24.07	24.7
Mols gas/100 g	4.40	4.38	4.38	4.37	4.15	4.09	4.09	4.09	4.2	4.2	4.15	4.05
C* (ft/sec)	5216				5356				4801			

Impact Sensitivity

Major differences in the impact sensitivity of 2, 4-DNI have been observed depending on the purity of the material. Unlike most materials the impact sensitivity increases with purity. Coburn, of LANL, has observed a correlation in sensitivity with the concentration of 4-nitroimidazole (4-NI).

We are examining this phenomenon in terms of crystal structure. The crystal structures for 2, 4-DNI and 4-NI are shown in Fig. 3. A crystal of 2, 4-DNI consists of ribbons of molecules. The hydrogen bonding network in 4-NI is similar, but it has totally planar packing resulting from extra H-bonds. 4-NI inclusions may stabilize the otherwise unstable 2, 4-DNI polymorphic structure as is shown in Fig. 3c.

Figure 3. (a) 2, 4-DNI non-planar crystal. (b) 4-NI planar crystal. (c) Postulated planar 2, 4-DNI + 4-NI planar crystal.

This phenomenon is being examined more closely. Although it is unlikely that the presence of 4-NI will effect the shock sensitivity of 2, 4-DNI, its inclusion may dramatically enhance the handling safety.

Conclusions and Future Directions

The shock loading studies on 2, 4-DNI have found the material to be less sensitive than any other conventional bonded explosives that we have made measurements on with the exception TATB-based materials. 2, 4-DNI significantly outperforms TNT. What remains to be done is an accurate determination of production costs. We are in the process of optimizing the synthesis of the material. We plan to scale 2, 4-DNI to a 5 kg quantity this year.

The 2, 4-DNI will be made available to other DoD/DOE laboratories. We are also evaluating the utility of 2, 4-DNI in the joint LLNL-Air Force Hard Structure Munitions High Explosive Program.