

Dependence of Detonation Velocity of Explosives on Effective Atomic Number and Effective Electron Density of the Explosives

Tohe Tessema Teklemariam, Vijay Kumar Mittal*

Department of Physics, Jimma University, Jimma, Ethiopia

Email address:

teklema@yahoo.ca (T. T. Teklemariam), teklemariam.tessema@aau.edu.et (T. T. Teklemariam), Vijay_52_Mittal@yahoo.com (V. K. Mittal)

*Corresponding author

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Abstract: Detonation velocity is one of the most important characteristics of explosives. For solid hydro carbon-based explosives it is generally greater than 4000 m/s. Detonation velocity depends to some extent upon the particle size of the explosives, increased charge diameter and increased confinement of the explosive. There is no report indicating the dependence of detonation velocity on the effective atomic number and effective electron density of the explosive. In the present work, we have arbitrarily chosen eight explosives. Four of these have detonation velocity between 9400 and 10100 m/s, and the other four has detonation velocity between 4500 and 5300 m/s. Direct method was used to calculate effective atomic number and effective electron densities various explosives. On calculating effective atomic number and effective electron density, it was found that detonation velocity of explosives does depend upon these two parameters. For explosives with high detonation velocity, effective atomic number is high and effective electron density is low while for low detonation velocity explosives it is reverse. It was also found that the variation of effective atomic number and effective electron density as a function of gamma ray energy can be explained on the basis of three different gamma ray inter action mechanism of gamma rays with matter.

Keywords: Explosives, Detonation Velocity, Effective Atomic Number, Effective Electron Density

1. Introduction

An explosive is defined as a chemical compound which, when subjected to heat, impact, etc. undergoes very rapid, self-propagating, heat-producing decomposition. This decomposition produces gases that exert tremendous pressures as they expand at the high temperature of the reaction creating a fast moving wave front. Detonation Velocity (DV) or explosive velocity, also known velocity of detonation, is the velocity at which this shock wave front travels through the detonated explosive.

Solid explosives often have detonation velocities ranging between 4000 m/s to 10100 m/s [1].

Low explosives are compounds where the rate of decomposition proceeds through the material at less than the speed of sound i. e. shock wave front passes through the

material at sub sonic speed [1].

High explosives (HE) are explosive materials that detonate, meaning that the explosive shock front passes through the material at a supersonic speed [1].

Explosive velocity increases with smaller particle size of the explosive, increased charge diameter, and increased confinement (*i.e.* higher pressure).

In literature there is no report indicating that detonation velocity depends upon the effective Z (Z_{eff}) or effective electron density (N_{eff}) of the explosive. However, in literature there is one report where the effective Z and effective electron density of some commonly used explosives has been reported [2].

Therefore, in the present work we have decided to study the effect of effective atomic number Z_{eff} and effective electron density N_{eff} of the explosive on the DV. For this we

have chosen two types of explosives. The first category consists of explosives with high DV (> 9400 m/s) and the second is with relatively small DV (~ 4500 to 5300 m/s). For these two categories of explosives, we calculated the effective atomic number and effective electron densities.

Many researchers have made extensive effective atomic number and effective electron density studies on a variety of materials. For example, effective atomic number and effective electron densities were evaluated in composite materials like dosimetric materials [3, 4], alloys [5, 6], semiconductors [7, 8], glasses [9], biological samples [10], gamma ray detectors [11], liquid crystals [12], narcotic drugs

[13, 14] etc.

2. Methodology

The first category includes explosives where the DV is > 9400 m/s. These are ONC, DDF, HHTDD and HMX. In the second category are the explosives with common name as TAPP, MEKP, UN and HMTD with DV between 4500 m/s to 5300 m/s. These are shown in Table 1 and are taken from Wikipedia [15]. This table also shows the common name, chemical formula, density and detonation velocity of the chosen explosives.

Table 1. Common name, chemical formula of explosives chosen in the present work. Densities and detonation velocities are also displayed in the table.

Explosive	Chemical formula	Common name IUPAC name	Density (g/cm ³)	Detonation velocity (cm/s)
High detonation velocity				
ONC	C ₈ N ₈ O ₁₆	Octanitrocubane	1.979	10,100
DDF	C ₄ N ₈ O ₈	4,4'-Dinitro-3,3'-diazenufuroxan (E)-4-nitro-N-[(E)-(4-nitro-2-oxo-1,2,5-oxadiazol-2-ium-3-ylidene)amino]-2-oxido-1,2,5-oxadiazol-3-imine	2.02	10,000
HHTDD	C ₆ H ₄ N ₁₂ O ₁₄	Hexanitrohexaazatricyclododecanedione 2,6-Dioxo-1,3,4,5,7,8-hexanitrodecahydro-1H,5H-diimidazo[4,5-b:4',5'-e]pyrazine	2.16	9700
HMX	C ₄ H ₈ O ₈ N ₈	Her Majesty's Explosive 1,3,5,7-Tetranitro-1,3,5,7-tetraazoctane	1.91	9400
Low detonation velocity				
TAPP	C ₉ H ₁₈ O ₆	triacetone triperoxide 3,3,6,6,9,9-Hexamethyl-1,2,4,5,7,8-hexaoxacyclononane	1.18	5300
MEKP	C ₈ H ₁₈ O ₆	Methyl ethyl ketone peroxide 2,2'-Peroxydi(butane-2-peroxol)	1.17	5200
UN	CH ₅ N ₃ O ₄	Urea nitrate	1.69	4700
HMTD	C ₆ H ₁₂ O ₆ N ₂	Hexamethylene triperoxide diamine 3,4,8,9,12,13-Hexaoxa-1,6-diazabicyclo[4.4.4]tetradecane	1.57	4500

Calculation for effective atomic numbers and effective electron densities were done by direct method as discussed in detail in our earlier publications [11, 12]. Mass attenuation coefficients needed for these calculations were evaluated by WinXCom software [16].

Below, a brief discussion of the method used for evaluating effective Z and effective electron density is presented.

This method uses the concept of gamma attenuation when it passes through a material media [17]. Intensity (I) of the attenuated beam is related to its unattenuated beam intensity (I_0) by the Lambert–Beers law given in (1).

$$I = I_0 e^{-\mu x} \quad (1)$$

Where x is the thickness of the material in 'cm' and μ is its linear attenuation coefficient in cm^{-1} . The mass attenuation coefficient of the material (μ_m) was obtained from the value of its linear attenuation coefficient μ and density (ρ) of the material as given in (2) [17].

$$\mu_m = \frac{\mu}{\rho} \quad (2)$$

Since the materials under study (explosives) are composite materials, total μ_m of the explosive is given by the relation (3) [17]. Where w_i is the weight fraction of the i^{th} element.

$$\mu_m = \sum_i w_i \frac{\mu_i}{\rho_i} \quad (3)$$

To find the total weight fraction of each of the element in the explosives under study, an equation of weight fraction for

composite materials, (4) was used.

$$w_i = \frac{n_i A_i}{\sum_i n_i A_i} \quad (4)$$

Satisfying $\sum_i w_i = 1$

Where A_i and n_i are the atomic weight and the number formula units of the i^{th} element in the explosives, respectively.

The WinXCom software was used to obtain mass attenuation coefficient of the explosives under study [16].

The results obtained from calculations of mass attenuation coefficients were used to find for the total atomic cross-section σ_t using (5) [18].

$$\sigma_t = \frac{\mu_m M}{N_A} \quad (5)$$

Where M is the atomic mass of the material and N_A is Avogadro's number. For each of the explosive total electronic cross sections which depend on the total mass attenuation coefficient were obtained using (6). Total electronic cross-section σ_e for a particular explosive and its total atomic cross sections are related as shown in (6) [19].

$$\sigma_e = \frac{1}{N_A} \sum_i \frac{f_i A_i}{Z_i} \mu_m = \frac{\sigma_t}{Z_{eff}} \quad (6)$$

Where f_i is the fractional abundance of the element i with respect to the number of atoms such that $\sum_i f_i = 1$.

Finally, the ratio of total atomic cross-section σ_t and total electronic cross-section σ_e , as in (7), was used to find the effective atomic number of the crystals.

$$Z_{eff} = \frac{\sigma_t}{\sigma_e} \tag{7}$$

Number of electrons per unit mass (effective electron density) was determined using the relation given in (8) [19, 20].

$$N_{eff} = \frac{\mu_m}{\sigma_e} \tag{8}$$

In brief our calculations of the effective atomic number and effective electron densities are based on the following formulas presented in (7) and (8).

3. Results

Plot of mass attenuation coefficients for all the explosives as a function of energy are shown in Figure 1. All these curves are almost overlapping. So, it is not possible to draw any conclusion from these curves.

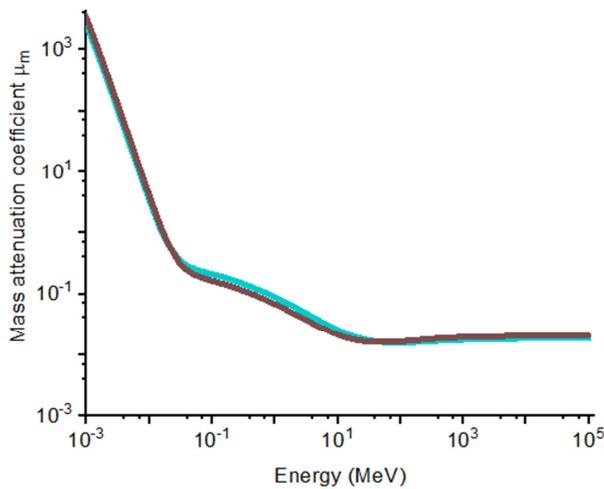


Figure 1. Mass attenuation coefficients for all the 8 explosives.

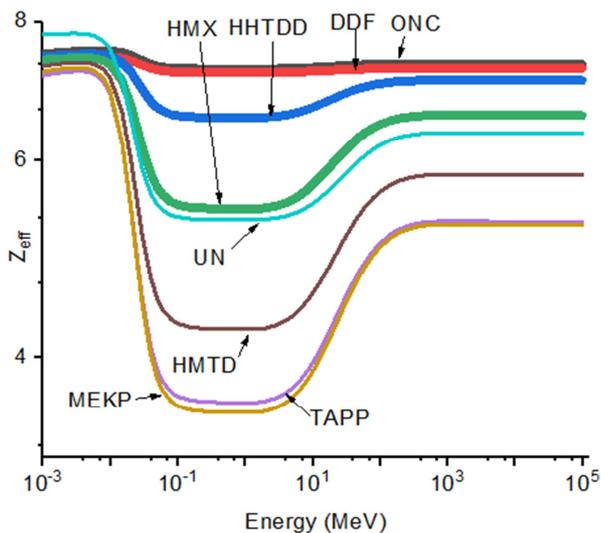


Figure 2. Z_{eff} vs. Energy of gamma rays. Thick curves are for high detonation velocity explosives, whereas thin curves are for low detonation velocity explosives.

In Figure 2, plot of Z_{eff} versus energy (MeV) for different

explosives are shown. Thicker lines correspond to the four explosives namely ONC, DDF, HHTDD and HMX. These are the explosives with $DV > 9400$ m/s. The other four thinner curves are for explosives UN, HMTD, TAPP and MEKP. For these explosives the DV is between 4500 to 5300 m/s. From the figure one can conclude that effective atomic number of high detonation velocity explosives is higher than those with low detonation velocity.

From Figure 2, it is evident that at low energy (< 0.01 MeV), Z_{eff} for all the explosives has a high value. In the energy range between 0.01 to 0.1 MeV, Z_{eff} decreases fast. Further in the energy range between 0.1 to about 10 MeV, Z_{eff} remains almost constant. Beyond this energy, it increases relatively slowly to attain a constant value.

In Figure 3 effective electron density as a function of gamma ray energy is shown for eight different explosives. As in Figure 2, thicker lines correspond to the four explosives namely ONC, DDF, HHTDD and HMX having high DV. The thinner curves are for explosives UN, HMTD, TAPP and MEKP having low DV. From the figure it is quite clear that for explosives with high DV, effective electron density is lower than those with low DV.

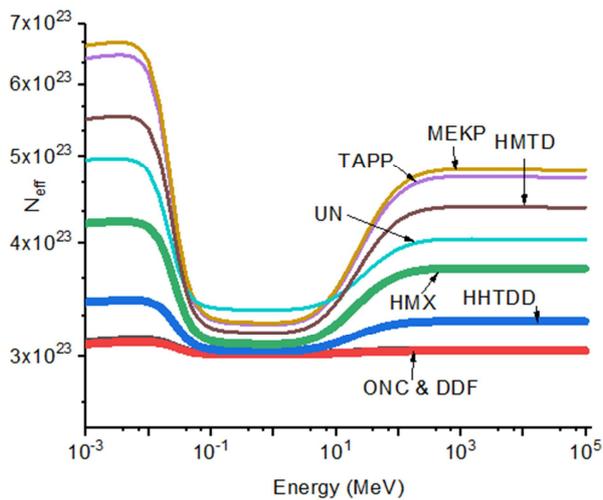


Figure 3. N_{eff} vs. Energy of gamma rays. Thick curves are for high detonation velocity explosives, whereas thin curves are for low detonation velocity explosive.

The behavior of Z_{eff} and N_{eff} as a function of γ -ray energy can be explained on the basis of partial importance of γ -ray interaction processes with matter. Gamma ray mainly interacts with matter via three different processes i. e. photo electric effect, Compton scattering and pair production.

In low energy region, photo electric effect dominates. In the intermediate region Compton scattering dominates and in the high energy region pair production is the main γ -ray interaction process.

In low energy region $0.01 < E < 0.5$ MeV, cross section for photo electric effect behaves as

$E^{-3.5}$. The values of Z_{eff} and N_{eff} also decrease almost in the same manner as photo electric cross section. Compton effect is negligibly small and probability of pair production is zero in this energy region.

In the intermediate energy region $0.5 < E < 5$ MeV, cross section for Compton scattering increases as E and cross section for photo electric effect decreases as $\frac{1}{E}$. Cross section for pair production increases as $\log_e(E)$. The net result is that total photon interaction cross section almost remains constant in the region. Therefore, the values of Z_{eff} and N_{eff} practically remain constant in the region.

Finally, in the high energy range $E > 5$ MeV cross sections for photo electric effect and Compton scattering are negligibly small while pair production cross section increases as $\log_e(E)$. This increase is very slow and also it almost saturates for $E > 100$ MeV. Z_{eff} and N_{eff} also show the similar behavior in this energy range.

4. Conclusions

In this experiment, we have arbitrarily chosen eight hydro carbon based organic explosives. Out of these, four have DV > 9400 m/s while the other four explosives have DV between 4500 and 5300 m/s. It has been found that for high DV explosives Z_{eff} is higher than those with low DV. Effective electron density N_{eff} , however is lower in high DV explosives compared to low DV explosives.

Therefore, looking at these eight explosives, we can conclude that DV of explosives depends upon the effective atomic number and effective electron density of the explosives.

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