Static charge development and impact sensitivity of high explosives

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Abstract

One of the causes of accidental explosion of explosives is due to static electricity. The present study deals with the development of static electric charge resulting from compression of single crystals of pentaerythritol tetranitrate (PETN), trinitrotoluene (TNT), *N*-2,4,6-tetranitro-*N*-methyl aniline (tetryl) and cyclotrimethylene trinitroamine (RDX). The charge developed on PETN and TNT is "true piezoelectric", whereas on tetryl and RDX, it is tensorial piezoelectric in nature. Measurement of the piezoelectric coefficient, dielectric constant and compressibility of these explosive crystals reveals the anisotropic character of these crystals. The static field developed under the laboratory experimental conditions, when extrapolated to the condition of detonation, bears an inverse relation with the figure of insensitivity of the respective high explosives.

1. Introduction

The development of piezoelectric charge on crystals of high explosives is a phenomenon of fundamental importance [1–6]. The molecular structure and the spatial orientation of the molecule in the three-dimensional periodic array of crystals determine the extent of polarization of the molecule under an applied stress. Some accidental explosions have been ascribed to static electricity [7–10]. Therefore, a study of the development of charge and the field produced thereby under an applied stress was considered important. Such studies made on PETN, RDX, TNT and tetryl are reported here.

2. Experimental methods

2.1 Growth of crystal

Large single crystals of PETN, RDX, TNT and tetryl were grown from their saturated solutions in acetone. Initially each explosive was purified by

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repeated crystallization from acetone solution. A saturated solution of each individual purified explosive was made at room temperature. Some seed crystals were obtained after a few days of storage in a clean environment. Large single crystals of approximately 3–5 cm in length were grown in 2–3 months using these seed crystals [11]. Good, blemishless portions of the crystals were chosen, cut and polished to get crystals of the desired shape and habit.

2.2 Measurement of charge

A special cell for measurement of charge developed on a crystal face under varying loads was designed and fabricated [11]. The crystal was held between two electrodes, one of which was grounded. The charge developed on the face was measured using a Kistler dual mode charge amplifier, Model 503-D 145 and recorded on a strip chart recorder. The quantity of charge generated under varying loads from 100 g to 2 kg was plotted graphically as charge vs. load. The piezoelectric coefficient d, viz. charge per unit force (picocoulombs/g) was obtained from the slope of the linear plot.

$$d = \text{Charge (pC)}/\text{Load (g)}$$

2.3 Measurement of dielectric constant

The dielectric constants of the crystals were calculated along each direction by measurement of the capacitance of the crystals. A Wayne–Kerr capacitance bridge and a specially designed point electrode assembly [11] were used for this purpose. The voltage generated in a given direction is calculated as:

$$V(\text{volts}) = \frac{Q(\text{coulombs})}{C(\text{farads})} = \frac{d \times \text{load}}{0.088\,54\,\varepsilon\,A/t}$$

where A is the area in cm^2, t is the thickness in cm and ε is the dielectric constant of the crystal.

2.4 Measurement of mechanical property

Compressibility of the crystals was measured with the Instron testing machine, Model No. TICM.

3. Results

Table 1 presents the average values of piezoelectric coefficients, dielectric constants and Young's modulus of single crystals of PETN along the directions perpendicular to (110) and (001) for over 25 crystals in each direction. It is observed that opposite charges are generated on opposite faces confirming the crystal's true piezoelectric nature. Secondly, the direction perpendicular to (110) is more compressible and develops more charge. Table 1 also presents the values for single crystals of TNT, RDX and tetryl. TNT is a "true piezoelectric"

TABLE 1

Piezoelectric coefficient, dielectric constant and Young's modulus for single crystals of PETN, RDX, Tetryl and TNT

Explosive	Directions perpendicular to	Piezoelectric coefficient ($\times$ 10 pC/g)	Dielectric constant	Young's modulus ($\times 10^{-6}$ g/cm^2)
PETN	(110)	(3.20 ± 0.40)	(3.50 ± 0.12)	(1.24 ± 0.30)
	(001)	(1.50 ± 0.30)	(4.57 ± 0.17)	(3.80 ± 0.80)
	(001)	(0.75–0.01)	(4.29 ± 0.04)	(1.25 ± 0.15)
RDX	(120)	(0.50–0.01)	(4.70 ± 0.02)	(4.80 ± 0.50)
	(110)	(0.50–0.05)	(4.25 ± 0.11)	(2.65 ± 0.30)
Tetryl	(011)	(0.30–0.05)	(4.88 ± 0.16)	(2.65 ± 0.50)
	(010)	(0.25 ± 0.05)	(3.19 ± 0.07)	(1.20 ± 0.40)
TNT	(001)	(0.07 ± 0.02)	(3.89 ± 0.23)	(3.20 ± 0.30)

TABLE 2

Maximum static electric field across the explosive crystals

Properties of the crystals	PETN	RDX	Tetryl	TNT
	Directions perpendicular to			
	(110)	(001)	(100)	(010)
Piezoelectric constant, ($\times 10^3$ pC/g)	3.20	0.75	0.50	0.25
Capacitance across 1 cm^3 crystal (pF)	0.31	0.38	0.38	0.28
Static field under 1 kg load (volt/cm)	10.33	1.97	1.33	0.89
Static field at threshold pressure ($\times 10^{-5}$ volt/cm)	94.0	29.9	27.9	22.3

in nature and the direction perpendicular to (010) develops more charge and is more compressible. The Young's modulus of TNT along the direction perpendicular to (010) has been found to vary from 1.20×10^6 to 0.40×10^6 g/cm^2. Single crystals of RDX and tetryl behave in a unique way, which is reflected in the varying values of piezoelectric coefficients. The piezoelectric coefficients for RDX were found to vary from 0.75×10^{-3} to 0.01×10^{-3} pC/g and 0.50×10^{-3} to 0.01×10^{-3} pC/g for the directions perpendicular to (001) and (120) respectively. Similarly for tetryl, the static charge development was found to vary over a wide range. Both RDX and tetryl develop like charges on opposite faces. Further, it has been found that the directions perpendicular to (001) and (100) respectively develop more charge and are more compressible.
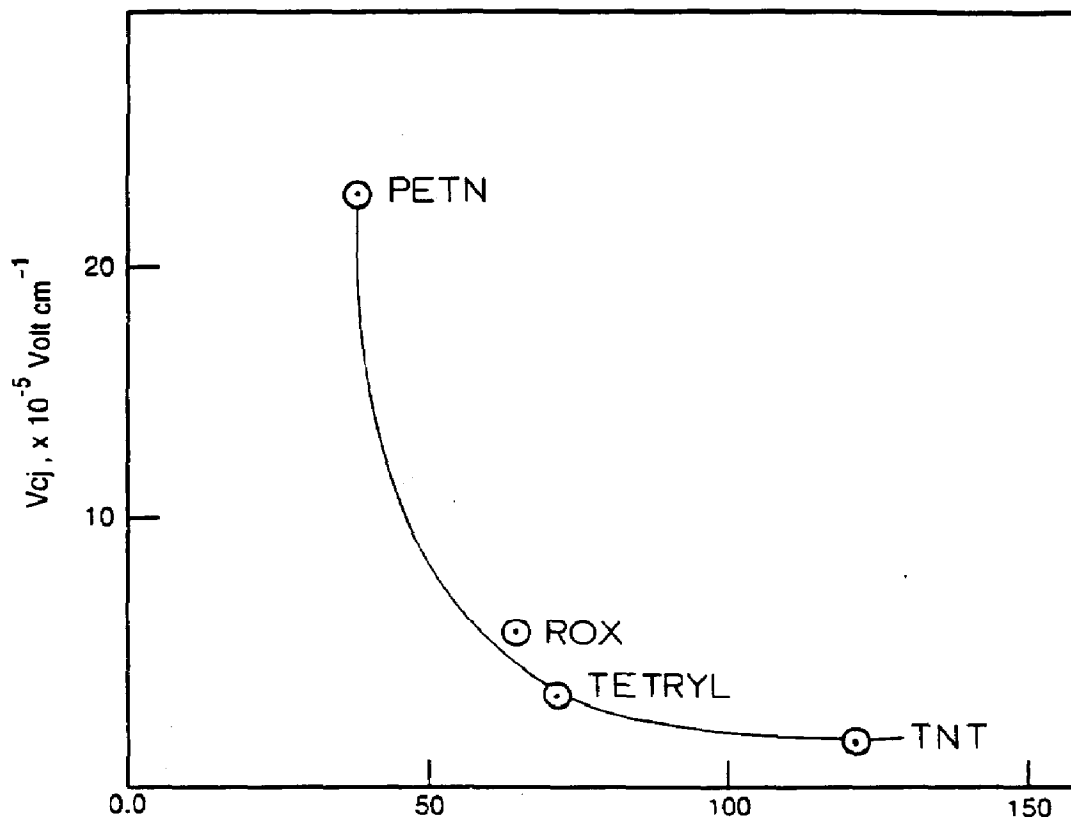
Fig. 1. Computed voltage at detonation pressure (V_{cj}) of high explosives vs. figure of insensitivity.

Table 2 presents the computed values of maximum static field developed under 1 kg load and at reported values of threshold pressure for the initiation of detonation. The experimental observation when extrapolated to the condition of detonation results in a very high field of the order of 10^5 volt/cm. The average values over 25 crystals at CJ (Chapman–Jouguet) pressures are 21.0×10^5, 5.31×10^5, 3.01×10^5 and 1.75×10^5 volt/cm for PETN, RDX, tetryl and TNT crystals respectively. Figure 1 shows the graphical relationship between the field generated at detonation pressure and the figure of insensitivity of the explosives.

4. Discussion

The results presented in Table 1 refer to the physical phenomenon, viz. piezoelectric charge development, dielectric constant and Young's modulus of the crystals along different directions. The charge development on PETN and TNT is "true piezoelectric" in nature which can be explained on the basis of crystal symmetry. PETN belongs to the tetragonal [12] class with symmetry $\overline{4}2\,m$ which falls under the piezoelectric category [13]. TNT crystallizes in

either orthorhombic or monoclinic structures. The orthorhombic class has point group *mm2*, which falls into the pyroelectric class. A pyroelectric crystal necessarily possesses piezoelectric properties, so TNT shows true piezoelectric charge. RDX is orthorhombic [14] with space group *mm*, and tetryl is monoclinic [15] with space group 2/*m*; these do not fall under the "true piezoelectric" category. The charge developed on RDX and tetryl may be attributed to the deformation of quadrupoles which is observed in tensorial piezoelectric materials [16]. The variation in magnitude of the piezoelectric constant, on RDX and tetryl is possibly due to variation in structural imperfections in the crystals. The variation in Young's modulus of TNT along the direction perpendicular to (010) is attributed to the twinning nature of the crystals [13]. The anisotropic characteristics of the crystals are obvious from the data presented in Table 1. This characteristic of nonequivalent properties based on the direction of measurement results from crystallization in a system of low symmetry. Each molecule under investigation is of a complex structure, and the group orientation in space is even more complex. The nitro groups are linked to the parent molecules in different ways. PETN has four $O-NO_2$ groups; TNT has three $C-NO_2$ groups of an aromatic ring; RDX has three $N-NO_2$ groups in an alicyclic ring; and tetryl, the most complex of all has three $C-NO_2$ groups of an aromatic ring and an $N-NO_2$ group. However, physically, these explosives have certain common characteristics. They all form soft crystals of low crystal symmetry. The crystals have low dielectric constants in the range of 3 to 5, and high compressibility in relation to ionic crystals. They have high resistivity, which enables them to develop electrostatic charge. Under compressive force they all develop electrostatic charges which may be either true or tensorial piezoelectric in origin.

It has been observed from Table 1 for single crystals of PETN, RDX, tetryl and TNT that the directions perpendicular to (110), (001), (100) and (010) develop high magnitudes of piezoelectric charge respectively. Koch [17] and Garg et al. [18] observed higher values of velocity of detonation (VOD) along the same direction for PETN, RDX and TNT crystals. Dick [19] has observed that PETN crystals shocked in directions parallel to (110), (001), (101) and (100) give different run distances to detonation, which showed a dependence of shock initiation sensitivity on the crystal orientation. This indicates that charge development along different directions of an explosive crystal may be used as an index to ascertain its sensitivity along the direction. The reported values [20] of sensitivity to mechanical impact (F of I) for PETN, RDX, tetryl and TNT are 38, 64, 72 and 120 respectively (with sensitivity inversion with the value of F of I). It has been noted that the maximum static electric field developed across the crystals under 1 kg force decreases as the F of I increases (Table 2). Further, an interesting correlation of this static field with impact sensitivity was observed by extrapolating this result to the condition of detonation. At detonation pressure the crystal is supposed to undergo mechanical fracture because mechanical fracture occurs [21] even at 10^2 psi but the charge development, being an electrical phenomena, will require less time compared

to the fracture which is a mechanical process [22, 23]. So the field generated across the crystal in the initiating threshold pressure [24] should thus be an index of the sensitivity of the crystal. Thus the static field at threshold pressure shows an increase with the sensitivity of the crystal (Table 2).

The pressure which relates to the detonation pressure of explosives is the Chapman–Jouguet (CJ) pressure. Coleburn [25] reported the CJ pressure for PETN, RDX, tetryl in pressed form and TNT in cast form as 240, 284, 226 and 187 kbar, respectively. Figure 1 shows the graphical relation between the field generated at CJ pressure with the figure of insensitivity.

The extrapolated electrical field developed on these crystals at detonation pressure is of the order of 10^5 to 10^6 volt/cm, compared to 10^7 volt/cm reported by Maycock and Grahenstein [4] for the highly sensitive s-HMX crystal. It is worth noting that dielectric breakdown voltage of some explosive compositions [26] and explosives [27] are of the order of 10^5 volt/cm. Hence, the field generated on the explosive crystal at detonation is sufficiently high to cause dielectric breakdown in them. As a result, a large amount of heat is liberated and the condensed material is vaporized to an ionized condition. This dielectric breakdown in the predetonation stage is supported by the observation of Clay et al. [28], that the ionization is a major factor for initiation of detonation.

Acknowledgement

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