Application of Nuclear Quadrupole Resonance to Detection of Explosives and Research Activities at CIAE

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The detection of explosives is a challenging topic. The nitrogen-14 nuclear quadrupole resonance technique exploits the transitions between the energy levels split by the quadrupole interaction to detect the presence of explosives. It is a very promising new technique owing to its unambiguous detection and identification of explosives with low false alarm, high sensitivity and fast detection. The explosive screening machines based on the nitrogen-14 nuclear quadrupole resonance have been used for aviation security at airports. This paper describes the principle and application of nitrogen-14 nuclear quadrupole resonance to detection of explosives and reviews the research activities in this domain at China Institute of Atomic Energy.

I. INTRODUCTION

Explosive detection is a challenging subject that attracts world-wide efforts. A number of detection techniques, e.g., trace detection, x-ray scanning, thermal neutron activation (TNA) and/or pulsed fast neutron analysis (PFNA) etc have been developed. Unfortunately, none of them have been proved to be fully satisfied. New techniques capable of exclusively detecting and identifying explosives are still essential, and the nitrogen-14 nuclear quadrupole resonance (^{14}N-NQR) technique has been proposed and the ^{14}N-NQR explosive screening machines and devices have been developed and used for aviation security at airports, for security checking at military areas and government buildings, post offices and customs, for landmine clearance and for personal scanning and car-bomb screening.

The ^{14}N nucleus is a non-spherically symmetric nucleus and has a quadrupole moment. The hyperfine quadrupole interaction of the quadrupole moment with the electric-field gradient causes the energy level splitting. The ^{14}N-NQR makes use of the transitions between the split energy levels, which determine the NQR frequencies. The energy level splitting depends on the crystalline and chemical structures of substances. As a result each substance is characterized by its NQR frequencies. There have been more than 30 NQR probe nuclei, one of which is ^{14}N. The NQR measurements have been performed for more than 10 thousand substances and no identical NQR frequencies have been observed.

The principle of NQR is the same as that of the well known nuclear magnetic resonance (NMR), and the only difference is that NQR makes use of an electric field gradient internally generated in substances rather then a strong magnetic field externally applied as in NMR. Almost all explosives contain ^{14}N and the ^{14}N-NQR has been proposed and used for explosive detection. Since the electric field gradient is determined by the crystalline structure, chemical bond and valence state of substances, the ^{14}N-NQR frequency is specific for each explosive and, therefore, is the fingerprint of explosives. The ^{14}N-NQR frequencies of different explosives are different and they are also different from those of other nitrogen-containing substances. Therefore, the ^{14}N-NQR technique can identify exclusively the existence and type of explosives and dispel other nitrogen-rich substance interference. The ^{14}N-NQR technique makes unambiguous identification of explosives possible and provides a capable way of unique detection and identification of explosives with low false alarm, high sensitivity, fast detection and easy operation.

This paper describes the principle of the ^{14}N-NQR technique and its application to explosive detection and presents a brief overview of research activities of investigating concealed explosive detection by the ^{14}N-NQR technique at China Institute of Atomic Energy (CIAE).

II. PRINCIPLE OF ^{14}N-NQR

Table I shows the elemental composition of explosives. It can be seen that explosives contain N (the abundance of ^{14}N is 99.634%) except $KClO_3$. The charge distribution of ^{14}N nucleus with a spin $I = 1$ is asymmetric as shown in Fig. 1. The charge distribution is expressed

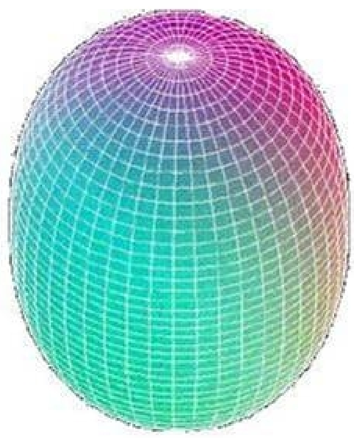

FIG. 1: Charge distribution of ^{14}N nucleus

TABLE I: Elemental composition of explosives (wt.%).

Explosives	Composition	C	H	N	O
Nitrocellulose	$C_6H_7N_3O_{11}$	24.24	2.37	14.14	59.23
Cyclonite (RDX)	$C_3H_6N_6O_6$	16.22	2.72	37.84	43.22
Pentaerythritol tetranitrate (PETN)	$C_5H_8N_4O_{12}$	19	2.55	17.72	60.73
TNT	$C_7H_5N_3O_6$	37.0	2.2	18.5	42.3
Tetryl	$C_7H_5N_5O_8$	29.28	1.76	24.39	44.58
Nitroglycerin (NG)	$C_3H_5N_3O_9$	15.87	2.22	18.5 6	3.41
Ammonium nitrate (AN)	$H_4N_2O_3$	0	5.04	35.01	59.97
Octogen (HMX)	$C_4H_8N_8O_8$	16.22	2.72	37.84	43.22
Black Powder	HNO_3 + Cl + S	–	9.3	35.2	10.3

by a quadrupole moment Q and the ^{14}N nucleus has a quadrupole moment of $Q \sim 0.015$ b. The NQR uses nuclei as a measuring probe, and the NQR performed with ^{14}N as a probe is called the ^{14}N-NQR. The quadrupole moment interacts with the local electric field produced by local electrons or more distant charges in crystals, see Fig. 2. This interaction leads to energy level splitting and preccessional motion of the probe nuclei, characterizing each particular environment of the atoms. The ^{14}N-NQR exploits the transitions between the split energy levels to detect the presence of explosives. Since the electric field is determined solely by chemical and crystalline structures, valence state etc, each transition occurs at a specific resonant frequency, which is called the NQR frequency. Each explosive is characterized by its own NQR frequencies that act as its fingerprint.

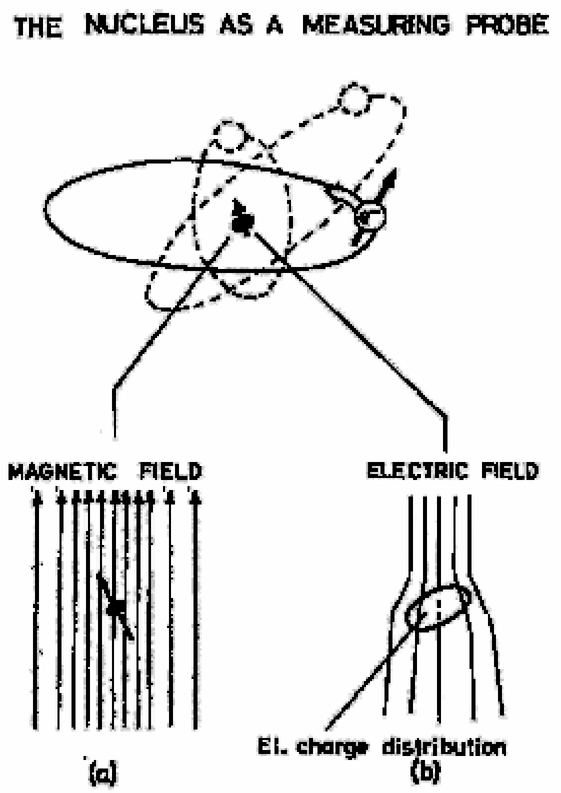

FIG. 2: Interaction of quadrupole moment with local electric field (bottom).

The ^{14}N nucleus has a nuclear spin $I = 1$ and the quadrupole interaction in a substance with a non-cubic structure splits the energy level into three energy levels with $m = +1, 0, -1$ as shown in Fig. 3. If a RF pulse with frequency ν_i is applied, the ^{14}N nuclei are excited to the higher energy level from the low energy level. After the RF pulse the ^{14}N nuclei are de-excited back to the low energy level by emitting a RF signal with a frequency ν_i. The ^{14}N-NQR detects this RF signal, the frequency of which is called the NQR frequency. There are three NQR frequencies for ^{14}N:

$$\nu_3 = \frac{e^2qQ}{4h}(3+\eta)\,, \quad \nu_2 = \frac{e^2qQ}{4h}(3-\eta) \tag{1}$$

and

$$\nu_1 = \nu_3 - \nu_2 \tag{2}$$

where Q is the quadrupole moment, $\frac{e^2qQ}{h}$ is the quadrupole coupling constant and η is the asymmetry parameter of the electric field gradient. With a known

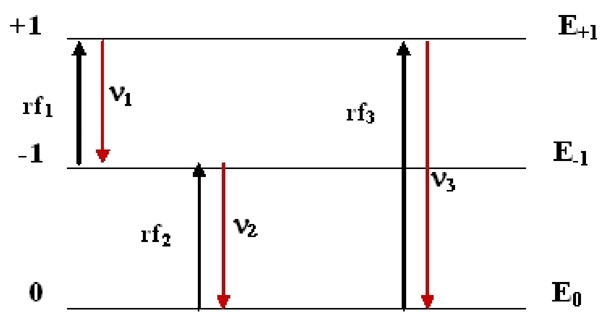

FIG. 3: Energy splitting and resonance frequencies for spin $I = 1$ nuclei.

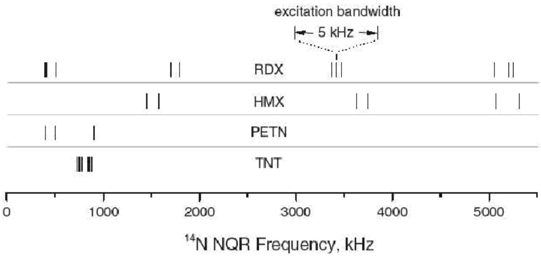

FIG. 4: ^{14}N-NQR frequencies of explosives.

Q, the quadrupole coupling constant or quadrupole interaction is determined by the electric field gradient (efg) only, which is firmly connected to crystalline structure, chemical bond, valence state, etc. The quadrupole coupling constant characterizes materials.

The efg is a tensor quantity:

$$V_{xy} = V_{xz} = V_{yz} = 0\,, \quad V_{zz} > V_{yy} > V_{xx} \tag{3}$$

(V_{zz} major component) and $\eta = (V_{xx} - V_{yy})/V_{zz}$ $(0 < \eta < 1)$ in the Cartesian coordinates along the efg principal axes. The V_{zz} and η define the strength and symmetry of efg.

The nuclear quadrupole resonance (NQR) frequency is given by

$$\nu_m = \frac{3eQV_{zz}}{4I(2I-1)h}(2m+1)\,. \tag{4}$$

Different substances have different eQV_{zz} and hence different quadrupole resonance frequencies. Therefore, the nuclear quadrupole resonance frequency is the fingerprint of each substance. All explosives can be identified uniquely by their own NQR frequencies. Figure 4 illustrates the ^{14}N-NQR frequencies for RDX, HMX, PETN and TNT. In addition it is worth to mention that the ^{14}N-NQR dispels completely the interference from other nitrogen-rich materials by the quadrupole resonance frequency. This is a significant advantage of this technique.

The NQR measurement is similar to the NMR measurement. In the NQR measurement the electric field gradient internally generated in substance is used rather then the strong magnetic field externally applied as in NMR. The NMR measurement can be conducted by varying either RF frequency or magnetic field to match the resonant condition, while the NQR measurement can be carried out by varying RF frequency only. Schematic drawing of the ^{14}N-NQR detection of explosives is shown in Fig. 5.

III. APPLICATION TO DETECTION OF EXPLOSIVES

The NQR process induces the nuclei of specific atoms to store RF energy for a short time and then rebroadcast a RF NQR signal to a detector. The precise NQR frequency gives rise to information on the presence of the atom and its bonding to the surrounding molecular structure. Thus the ^{14}N-NQR provides a reliable means for detecting explosives.

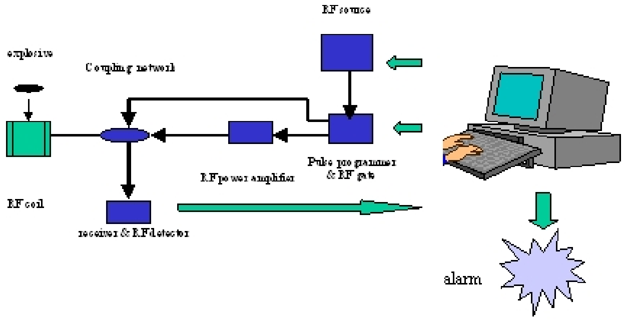

FIG. 5: Schematic drawing of ^{14}N-NQR detection of explosives.

The NQR spectroscopy was developed at the end of the 1940s. A pioneering experiment to determine the ^{14}N quadrupole interaction in $(CH_2)_6N_4$ etc was carried out in early 1950s. The ^{14}N-NQR was used to detect explosives at the end of 1970s. Since then the interest was aroused in using ^{14}N-NQR to detect explosives, landmines and drugs. The world's first machine of the ^{14}N-NQR explosive screening was used at Los Angeles International Airport for aviation security in 1995. Since then quite a number of ^{14}N-NQR explosive screening machines have been installed for screening checked-in and carry-on baggage at airports in the world.

The NQR technique is an important technique in materials science and solid state physics. It is used to detect the presence of material, to determine the quality, purity, temperature and pressure of material and to study the chemical composition, molecular structure and motion and electronic environment. Therefore, the NQR can be well employed to detect explosives. The detection of explosives by NQR has the following advantages: high selectiveness to particular explosive and ability to identify its type, high reliability with minimal false alarms, direct detection with short analysis time, non-contact method that allows for detecting explosives with low vapor density, non-destructive method without destroying electronically stored data and radio-technical method with no harmful types of radiation.

^{14}N-NQR has a spectrum of applications in explosive inspection. The detection of explosives such as RDX, PETN, HMX, tetryl and TNT for aviation security is its main application. The ^{14}N-NQR explosive screening machines have been installed at airports to inspect checked-in and carry-on baggage. Besides, applications can be made for security-checking at embassies, military areas and government and commercial buildings. The ^{14}N-NQR devices can be used also for mail and cargo screening at post offices and customs. Shoe scanner, corridor-type scanner and fare collection screening system can be used for personal scanning. Car-bomb screening system

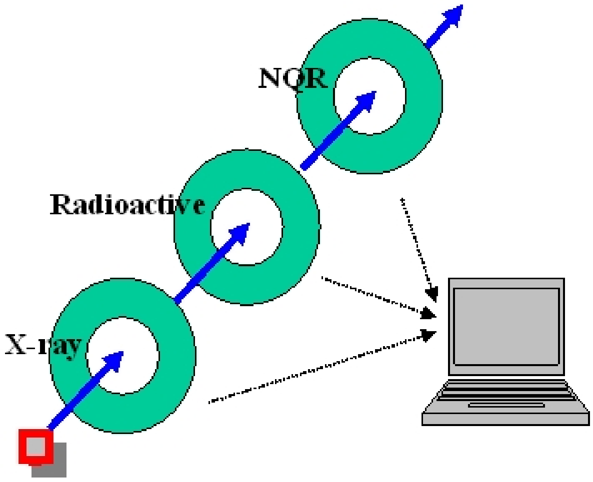

FIG. 6: Schematic drawing of combined baggage screening system.

has been developed to inspect explosives hidden in a car. Besides the explosive detection the NQR technique has a wide range of applications in narcotics detection, pharmaceutical quality control and assurance, material and mineral assay and landmine clearance.

Recently, R&D of the combined baggage screening system, i.e., ^{14}N-NQR detection in combination with x-ray scanning and radioactive material inspection, has been conducted for detecting metal weapon, radioactive material and explosive in sequence at one pass. The schematic drawing of the so-called combined baggage screening system is illustrated in Fig. 6.

IV. RESEARCH ACTIVITIES AT CIAE

The ^{14}N-NQR method was proposed to detect and identify concealed explosives in mid 1990s at CIAE. This

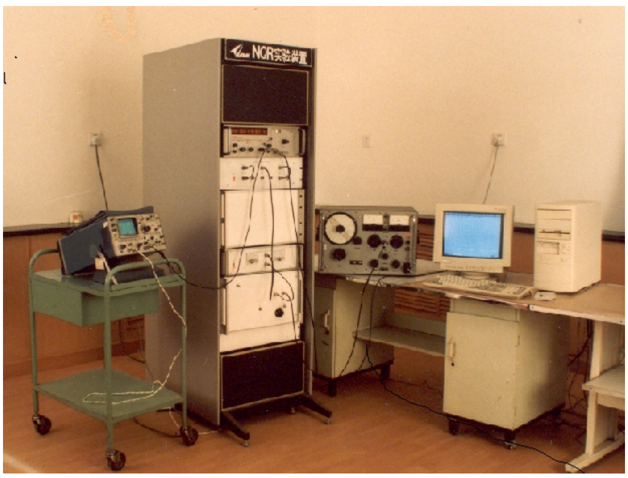

FIG. 7: View of early baby setting for RDX detection.

FIG. 8: Laboratory systems of RDX detection with probe volumes of 140 liters.

FIG. 9: Laboratory systems of RDX detection with probe volumes of 10 liters.

FIG. 10: Radioactive detection unit.

project of explosive detection by ^{14}N-NQR was supported at its early stage by China National Nuclear Group Corporation (CNNC) and by IAEA that provided three year research contracts. At present the research is also supported in part by IAEA under the TC CPR / 1 / 006 Project entitled "Investigation of Concealed Explosive Detection by ^{14}N-NQR".

In late 1990s a laboratory prototype ^{14}N-NQR system for RDX detection was developed. Figure 7 shows the early baby setting of the RDX detection system.

At present, we have developed two laboratory ^{14}N-NQR systems of RDX detection. The one with a probe volume of 140 liters is for carry-on baggage screening (Fig. 8) and the other with a probe volume of 10 liters is for mail screening (Fig. 9). We are now constructing a ^{14}N-NQR screening system with a probe volume of 160 liters. This system can detect RDX, HMX and PETN and be used for screening carry-on baggage at airports and railway and bus stations. A system with a 24 liter probe is being manufactured for detection of explosives in handbag, parcel, mail and small object.

According to the practical interest in China we are supported in part by IAEA under the TC CPR / 1 / 006 Project to investigate the ^{14}N-NQR system for detecting TNT and Black gun powder (KNO_3+C+S) in collaboration with King's College UK.

We have made substantial progress in developing a combined baggage screening system for radioactive materials and explosives in collaboration with QRSiences Australia. Figure 10 illustrates the detection unit of radioactive materials. A pair of the detection units has been installed in the explosive screening machine. This combined system inspects radioactive materials before the NQR detection of explosives.

V. SUMMARY

The ^{14}N-NQR detection of explosives makes use of the electric field gradient internally generated in substances to detect the presence of explosives and acts a fingerprint identification of explosives with low false alarm, high sensitivity, fast scanning and easy operation. The ^{14}N-NQR technique is a promising new means for and will play an important role in explosive detection.

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