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EDITORIAL

Magnetic Resonance Detection of Explosives and Illicit Materials

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This special issue of *Applied Magnetic Resonance* is devoted to magnetic resonance detection of explosives and illicit materials. This special issue presents papers on a very specific and important area of nuclear quadrupole and magnetic resonance (NQR and NMR) applications for detection of various solid-state and liquid explosive materials, illicit substances and medicine counterfeiting.

The detection of explosives is an issue of extremely importance for modern civilization. There are remains of explosives after the wars and local conflicts as well as the explosives which are used by terrorists around the world. In the aviation and public security, there is a problem of non-invasive detection of the explosives in the baggage, suits, cars, and others. In spite of the availability of various detectors, there are a number of problems to be resolved, such as increasing the sensitivity, shortening the detection time, decreasing the scanner cost, etc. In addition, an enormous number of various explosive materials are known that imposes a requirement for an effective technique to detect a vast range of possible threats. A bomb or a mine has plastic or metal enclose (usually hermetically sealing the content) and may also contain extra materials in addition to the explosive itself that makes a number of detection techniques not possible to use. Available detection techniques can be divided on the two large group of bulk and trace explosive detection methods. Although some trace detection techniques have proven their high effectiveness (such as dogs, ion mobility/mass/Raman/terahertz spectrometry, etc.), their application is unlikely to resolve an issue of the reliable explosive

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detection in many practical situations. It is obvious that the most effective device should combine a few methods to increase reliability of the explosive detection. For that reason all bulk detection methods, especially X-ray/neutron/gamma detection techniques as well as NMR/NQR detection, are extensively studied nowadays.

It should be stressed that minimum false alarms will be given by the techniques which are directed to detect not the metal or plastic enclose or fuses but the explosive itself. In other words, they should provide the chemical-specific identification of explosive. Such selectivity is provided by spectroscopic techniques which are well known for researchers working in both basic and applied science. Fortunately, only a few explosive types are commonly used in spite of the fact that there are hundreds of mine types and a lot of explosives materials.

Among various spectroscopic techniques, NQR and low-field NMR are considered as very promising bulk explosives detection methods, based on the chemical identification of content.

Most of the explosive and narcotic substances contain nitrogen in their structure. Nitrogen nucleus has a quadrupole moment, i.e., it has non-spherical shape and it is characterized by nuclear spin $I = 1$. Non-spherical (quadrupolar) nuclei interact with the electric field gradient from the neighbor charges forming non-degenerate energy levels for various nuclei axis (i.e., nuclear spin) orientations. The application of a radiofrequency field excites transitions between these energy levels. The transition frequencies depend on the electric field gradient of a crystal specified by the local symmetry and magnitude (i.e., configuration of neighboring ions which is unique for every chemical compound). Thus, the NQR frequency spectrum serves as a "passport" of a chemical compound. As a local characteristic of the specific crystal structure, the NQR frequency is not sensitive to variations in the explosive composition. Therefore making a mixture of explosives with other materials (such as the plasticizers) does not change the NQR spectrum. Furthermore, the NQR signal amplitude is proportional only to the amount of explosive present, and does not depend on the spacial distribution of explosive in the detected volume. Thus, NQR can detect explosives in diluted or sheet configurations which usually are not visible in X-ray imaging devices. Therefore combining NQR with X-ray scanners can provide much more reliable detection of explosive threats in the checkpoints of airports and other security-important places.

However, low sensitivity of NQR technique as well as low-field NMR is a topical problem. The very low signal-to-noise ratio (SNR) is affected by spurious signals from resonant acoustic ringing and by radiofrequency interference (RFI) which exists every time in the case of a non-laboratory (field) environment. Magnetic oscillation which are detected in NQR or low-field NMR are much weaker (usually several orders of magnitude) than the parasitic effect produced by external sources. Therefore the special methods to mitigate the influence of external sources of radiofrequency interference have to be applied. The NQR signal of small amount of detected substances could be as weak as the thermal noise in the detector circuit. The problem of a low SNR of ^{14}N NQR detection is especially important for some low-frequency explosives, such as trinitrotoluene (TNT) and ammonium nitrate (AN). For that, researchers are working for novel ultra-sensitive sensors for NQR detection, such as atomic magnetometer, SQUID-based or GMR-HTS hybrid probes, etc.

On the other hand, NQR technique cannot be applied in the case of liquid substances. Fortunately, they can be successfully detected by NMR technique. Taking into account the restriction on application of high magnetic fields to scan the luggage and people, only low-field NMR (with frequencies which are close to or even below those of NQR on ^{14}N nuclei) can be applied. In this case, however, we have to discriminate between various liquids by the relaxation and diffusion parameters of ^{1}H signal which is not easy task either.

Therefore, for development of NQR/NMR detection technique, one has to increase the sensitivity of ^{14}N NQR, to develop approaches immune to RFI and acoustic ringing and to develop new approaches for detection of liquid substances by low-field NMR.

There are two main topics in this issue: the application of NMR for the detection of liquid explosives and the development NQR methods for the detection of the explosives.

The first successful application of the NMR method for the detection of liquid explosives was demonstrated by Burnett [1] and later by Kumar et al. [2]. In this issue, Pablo Prado and his co-workers (USA) present a compact version of the NMR explosives detector for liquids in bottles. The proposed system configuration does not require a large magnet generating uniform magnetic fields, rather it inspects the liquid using a compact probe positioned on the wall of the bottle. Other solution for detection of liquid explosives was presented in this issue by Hideo Sato-Akaba and Hideo Itozaki (Osaka University, Japan). It should be noted that NMR in Earth's magnetic field was proposed by Packard and Varian as early as 1954 [3]. For years, Earth's NMR was used mainly in geophysical magnetometry as well as in the educational demonstrations of NMR. Recent progress in experimental techniques allows a wider range of applications of Earth's magnetic field NMR [4]. The work of Dr. H. Sato-Akaba and Prof. H. Itozaki presents an application of this technique for the liquid identification in 500 ml PET bottles. Earth's field NMR apparatus has been developed and optimized to measure the spin–lattice relaxation times of various liquids. They showed that the lower detection limit of pure water was as small as 1 ml. In this special edition we also included an interesting paper of Matsyendranath Shukla and Kavita Dorai, presenting a novel multiple-quantum correlation NMR scheme to separate components of a mixture according to their diffusion coefficients. Although this paper does not discuss applications for detection of explosives and illicit materials, it shows a potential of NMR technique for the determination of parameters of individual molecules in liquid mixtures that is important for a broad range of possible applications.

NQR explosives detection was firstly proposed by Robert Pound in Harvard University in 1951. Later this technique was developed in USA, Russia, UK, Australia, and other countries [5]. The NQR works presented in this issue concern various aspects of NQR explosives detection. Taras Rudakov from Lynx Engineering Limited (Australia) presents the research paper on the detection of an ammonium nitrate based explosives. Karen Sauer and Michael Malone from George Mason University (USA) studied the frequency-offset effects in CPMG sequence for nuclear spin of 1 in the presence dipole–dipole interaction both theoretically and experimentally. Jamie Barras and his co-workers from the group of

Prof. John A.S. Smith from King's college (London, UK) demonstrated the development of the portable medicines authentication device based on NQR. Jaroslav Turecek (Police Academy of the Czech Republic) with co-authors (Australia and Czech Republic) reported about the development of an inexplosive RDX simulant suited to a wide range of measurement methods, including NQR. Tara Prasad Das et al. (USA) presented a theoretical study of the nuclear quadrupole interaction parameters for the ^{14}N nuclei in the RDX and β-HMX explosives, and the cocaine and heroin drugs. The calculations are based on the first principles calculation using the one-electron Hartree–Fock approach. Georgy Mozzhukhin et al. (Russia & Turkey) present experimental study on three-frequency multipulse NQR for explosives detection which are based on theoretical studies of Prof. Dmitry Ya. Osokin [6]. The paper of Thérèse Schunk et al. (France) deals with the effects of the particle size, density and HMX content on the NQR line parameters (intensity and linewidth) of RDX at 3.41 MHz. It has been shown that no simple correlation exists between the line parameters and particle size, while a significant effect of the HMX content on the line parameters is observed. Janez Seliger and Veselko Žagar present a very detailed review on ^{1}H-^{14}N nuclear quadrupole double resonance (NQDR) techniques which can be used to measure the ^{14}N NQR frequencies and spin-lattice relaxation rates under various experimental conditions.

It is very important for all researchers working in this field to have financial support to conduct these non-routine (developmental) and quite extensive studies. Everyone who has worked in the applied science and technology knows how many troubles should be resolved before an idea (proof of principle) come to practical realization. Therefore an adequate financing is very important to have adequate technical possibilities for conducting the applied research work.

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