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 TUTORIAL

Nuclear Quadrupole Resonance for Substance Detection

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ABSTRACT This review paper provides a comprehensive overview of recent advances in nuclear quadrupole resonance (NQR) spectroscopy for substance detection, highlighting its principles, methodologies, and applications. The paper elucidates the fundamental physics underlying NQR spectroscopy, emphasizing the interaction between nuclear quadrupole moments and electric field gradients. It explores the various experimental techniques and instrumentation developments that have enabled the sensitive detection and precise characterization of substances containing quadrupolar nuclei. A significant portion of the survey is dedicated to discussing the diverse applications of NQR spectroscopy, including the detection of explosives, drug pharmaceuticals, and material authentication. Furthermore, the survey examines the challenges and limitations associated with NQR spectroscopy, including issues related to signal-to-noise ratio (SNR), temperature dependency, and substance restrictions. Strategies to overcome these challenges are discussed, offering insights into the future directions of NQR spectroscopy research that includes artificial intelligence (AI), internet of things (IoT) integration, incorporating a cloud database for NQR parameter storage, and multi-modal analysis.

INDEX TERMS Electric quadrupole moment, substance detection, security screening, instrumentation.

I. INTRODUCTION

Nuclear Quadrupole Resonance (NQR) is a distinctive and versatile detection technique that has garnered significant attention across diverse scientific and applied disciplines. Offering insights into the characteristics of materials at the atomic level, NQR has proven valuable for the analysis of compounds containing quadrupolar nuclei [1]. Operating on the principles of nuclear physics and spectroscopy, this technique exploits the fundamental interaction between nuclear quadrupole moments and the surrounding electric field gradients, revealing unique resonance frequencies that serve as crucial signatures for identification and analysis [2], [3].

In an era marked by rapid technological advancements, the field of security and law enforcement faces an ever-evolving challenge: the need for state-of-the-art techniques to detect and identify substances of interest. With an increasing

global demand for enhanced security measures, traditional methods have proven insufficient in keeping pace with the complexity of contemporary threats such as the ones listed in Table 1. Researchers and scientists have thus turned their attention to NQR spectroscopy as a promising solution. NQR spectroscopy's unique ability to detect specific compounds through their inherent nuclear properties has garnered significant interest in recent years, filling a crucial void in the arsenal of law enforcement and security agencies who seek more accurate, non-invasive, and up-to-date tools to combat evolving threats.

NQR has significant potential to transform the process of substance detection and identification. Its significance stems from its exceptional ability to provide a molecular "fingerprint" of various materials, enabling precise identification even in complex and challenging scenarios. Unlike most spectroscopic methods, NQR relies on interactions between atomic nuclei and nearby electric field gradients, which produces resonant frequencies that are specific to

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TABLE 1. Major types of substance detection methods used by law enforcement agencies.

Level of Detection	Methodology	Efficiency	Properties
Visual Inspection	Observational	Low	Limited to visible substances or paraphernalia
Presumptive Testing	Chemical color test	Moderate	Field tests using reagents like Marquis or Dile-Koppanyi reagent kits.
K-9 Units	Canine scent detection	Moderate to High	Trained dogs detect a wide range of substances
X-Ray Scanning	Imaging technology	Moderate to High	Used at security checkpoints to detect contraband
Mass Spectrometry	Laboratory analysis	High	Accurate but typically used in a controlled laboratory setting
Gas Chromatography	Laboratory analysis	High	Precise identification of substances in a controlled environment
Liquid Chromatography	Laboratory analysis	High	Often used for analyzing substances in liquid form in laboratories

each compound and crystal structure [4], [5]. This intrinsic specificity allows NQR to discriminate between closely related compounds that may confound other techniques. Moreover, NQR's non-invasive nature and its capacity to work across a range of substances offer distinct practical advantages [6]. This characteristic is particularly vital in security applications, where it plays a pivotal role in the detection of concealed explosives, narcotics, and pharmaceuticals.

Despite the promising potential of NQR spectroscopy in the realm of substance detection, researchers grapple with several formidable challenges that must be surmounted to make it a leading technique in this domain. One of the most significant hurdles lies in the temperature dependency of NQR signals [7]. NQR spectroscopy is highly sensitive to variations in temperature, which can adversely affect the reliability and accuracy of the results. Additionally, signal-to-noise ratio (SNR) is a persistent challenge [8]. Obtaining clear and discernible NQR signals from the background noise, especially in complex real-world scenarios, remains a formidable task. Furthermore, NQR spectroscopy is limited to the detection of solid substances, excluding the vast realm of liquids and gases [9]. Addressing these challenges is paramount for NQR spectroscopy to reach its full potential and establish itself as a forefront technology for substance detection in the ever-evolving landscape of security and law enforcement.

Even with its current drawbacks, the significance of NQR is underscored by its role in enhancing safety and security across various sectors. By providing rapid and accurate substance identification, NQR has proven to be important in preventing potential threats and ensuring product authenticity in industries such as consumables (food items) [10], [11], explosives (RDX, TNT, and others) [12], [13], [14], [15], and pharmaceuticals (drugs and nutritional supplements) [16], [17]. This survey paper aims to comprehensively explore the principles of NQR, challenges that impact the technique, and current substance detection applications that utilize NQR. The paper also does a deep dive into future research directions for NQR and ongoing research along these lines.

II. NUCLEAR QUADRUPOLE RESONANCE: THEORY AND PRINCIPLES

A. HISTORY OF NQR

The theoretical foundations of NQR can be traced back to the early 20th century with the development of quantum mechanics and nuclear physics [18]. During this time, physicists Edward M. Purcell and Robert V. Pound independently

discovered Nuclear Magnetic Resonance (NMR), a technique that revolutionized spectroscopy and allowed for the study of nuclear properties. In the early 1950s, Felix Bloch and William W. Hansen at Stanford University introduced the concept of NQR by recognizing that atomic nuclei with a non-zero electric quadrupole moment could experience resonance when exposed to an external RF field. In the 1960s, NQR started gaining attention as a potential analytical tool for various applications, including material analysis and chemical detection. Early applications of NQR included studying the properties of nuclear quadrupole nuclei in solids, which provided valuable insights into molecular environments of these materials. Over time, NQR gained prominence in explosive detection due to its specificity to explosives containing quadrupolar nuclei such as ^{14}N or ^{35}Cl . In the 1980s, significant efforts were made to utilize NQR for security purposes, especially in airport screening to detect concealed explosives. Advancements in electronics, designs, and pulse sequences have improved the sensitivity and applicability of NQR. Today, NQR continues to evolve and find applications in various disciplines, solidifying its status as a valuable and versatile detection technique.

B. PHYSICAL PRINCIPLES OF NQR SPECTROSCOPY

NQR is grounded in fundamental principles that merge nuclear physics with spectroscopy. It relies on atomic nuclei possessing electric quadrupole moments, which arise from the non-spherical distribution of electric charge within atomic nuclei with spin quantum number $I > 1/2$ [19]. In particular, nuclei with odd numbers of protons and/or neutrons have ellipsoidal, rather than spherical, nuclear charge distributions. When such a nucleus is placed in an electric field gradient (EFG), the interaction between its non-spherical charge distribution and the field gradient leads to quantized energy levels [20]. These hyperfine levels correspond to different orientations of the nucleus with respect to the principal axis system of the EFG tensor. As the nucleus transitions between these energy levels, it absorbs or emits energy in the form of electromagnetic radiation. Thus, quadrupolar nuclei exhibit quantized energy transitions in an EFG, leading to resonance frequencies that are unique to each nucleus and its local environment.

The process of NQR spectroscopy relies on this resonance phenomenon [21]. It utilizes either continuous wave (CW) or pulsed radio frequency (RF) excitation to induce transitions between the hyperfine energy levels, with the corresponding resonant frequencies serving as a chemical fingerprint [22].

The characteristic electromagnetic signals (or NQR resonance signals) generated during these transitions are observed during an NQR experiment. These fingerprints encode information on molecular structures, symmetry, and neighboring atomic interactions. Unlike NMR, which relies on an external magnetic field, NQR exploits the built-in EFG between the positively-charged nucleus and negatively-charged electrons to generate these distinctive resonant transitions [23].

The NQR technique is non-invasive, non-destructive, and applicable to most solids, including single crystals and powders. Moreover, the sensitivity of EFGs to the local environment surrounding the nuclei endows NQR spectra with exceptional specificity and the ability to differentiate substances with similar chemical compositions. In particular, factors such as nearby atoms, molecular symmetry, and electronic interactions influence the EFG experienced by the nucleus. Consequently, substances with different chemical environments (including molecular and/or crystal structures) exhibit unique resonance frequencies.

The intrinsic specificity of NQR resonance frequencies to nuclear and chemical properties is pivotal, allowing NQR to operate as a form of molecular “signature”. The high sensitivity of NQR resonance frequencies and line widths to local structure further augments its capacity for substance-specific identification [24]. The EFG experienced by a nucleus is influenced by factors like neighboring atoms, molecular symmetry, and electron distributions. Thus, NQR captures intricate nuances of molecular arrangements, facilitating the differentiation of substances with similar chemical compositions but disparate structural configurations, a task that other spectroscopic methods often struggle with. NQR’s non-invasive nature further enhances its utility, making it suitable for diverse applications including security screening and medical diagnostics. Additionally, its non-destructive character preserves the integrity of samples and ensures minimal interference with their normal use. This combination of properties underscores NQR’s importance as a precise and powerful analytical tool across diverse fields.

C. QUADRUPOLEAR NUCLEI

A survey of the elements reveals that over 50% of all nuclear species are quadrupolar (i.e., have a spin $> 1/2$) and can thus generate NQR signals. A subset of these nuclear species are suitable for analyzing substances of interest to law enforcement agencies. Notably, nitrogen (^{14}N) and chlorine (^{35}Cl) emerge as prominent candidates due to their prevalence in a wide range of chemical compounds and significant quadrupole moments [25], [26]. ^{14}N is ubiquitous in organic molecules, amino acids, and explosives, while ^{35}Cl is present in chlorinated organic compounds. These nuclei have distinct NQR signatures that provide the basis for efficient and accurate substance detection, particularly in security screening applications for explosives and hazardous materials. Beyond ^{14}N and ^{35}Cl , other quadrupolar nuclei like copper (^{63}Cu) and sodium (^{23}Na) are promising for specific applications [27], [28]. For example, ^{63}Cu is found in

TABLE 2. Common nuclear species detected via NQR and their corresponding spin quantum numbers.

Element	Nuclear Species	Nuclear Spin, I
Chlorine	^{35}Cl	3/2
Chlorine	^{37}Cl	3/2
Nitrogen	^{14}N	1
Sodium	^{23}Na	3/2
Potassium	^{39}K	3/2
Bromine	^{79}Br	3/2
Iodine	^{127}I	5/2
Copper	^{63}Cu	3/2
Oxygen	^{17}O	5/2

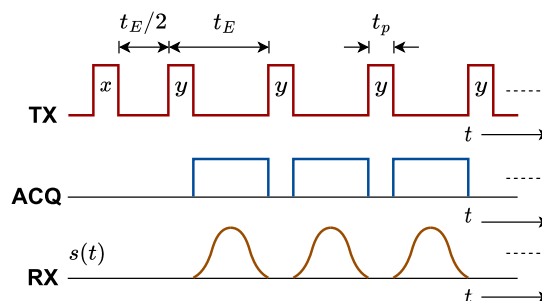


FIGURE 1. Basic spin-locked spin echo (SLSE) pulse sequence used for NQR experiments, and the resulting received signal, $s(t)$.

certain minerals and its detection using NQR can potentially aid in geological analysis. By contrast, ^{23}Na is found in various biological tissues and fluids and its detection opens avenues for medical and biological applications, expanding NQR’s scope into areas such as tissue characterization and physiological studies. A list of the most common quadrupolar nuclei and their spin quantum numbers, I , is listed in Table 2.

D. NQR INSTRUMENTATION AND TECHNIQUES

NQR instrumentation uses several key components and techniques to study samples containing quadrupolar nuclei. Most modern NQR spectrometers operate in pulsed mode. The choice of pulse sequence is critical, with the spin-locked spin echo (SLSE) sequence and the saturation recovery (SR) sequences being commonly employed [29], [30]. In many respects, the SLSE sequence resembles the Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence commonly used in NMR. Like the CPMG, it consists of a single excitation pulse and a series of uniformly-spaced refocusing pulses to minimize the impact of inhomogeneous broadening, as shown in Fig. 1. However, unlike the CPMG, all the pulses have the same flip angle, α . The optimum values of α for maximizing SNR are approximately 120° and 102° for powder samples containing nuclei with spin $I = 1$ and $3/2$, respectively.

Irrespective of the pulse sequence, SNR is maximized when the center frequency of the RF pulses matches the NQR resonance frequency of the nuclei of interest. The pulses are applied via an RF coil that typically encloses the sample and is also series- or parallel-tuned by a capacitive network at the chosen NQR frequency to maximize power transfer efficiency. The applied magnetic field generates a time-varying magnetization within the sample, which constitutes the NQR signal. The latter can be inductively detected

by either the same RF coil, or a separate receiver coil. Alternatively, it can be detected by sensitive magnetic field sensors such as superconducting quantum interference devices (SQUIDs) or atomic magnetometers. Regardless of the type of detector, the received NQR signals are subsequently amplified, filtered, and digitized. Data processing, often involving Fourier transformation, converts the time-domain free induction decay (FID) or spin echo (SE) signals into frequency-domain NQR spectra [31]. The resulting data is analyzed to extract crucial information about quadrupolar interactions and the local chemical environment of the nuclei, providing valuable insights into sample properties. Modern NQR instruments are typically computer-controlled, with dedicated software for data acquisition and analysis that enhances the precision and efficiency of NQR experiments.

Various techniques and strategies have been created to enhance sensitivity and specificity in substance detection. One approach involves employing multi-frequency NQR, where multiple excitation frequencies are used to detect different NQR-active nuclei simultaneously, increasing specificity by identifying unique resonance frequencies for distinct substances [32]. Composite RF pulses, such as adiabatic pulses or pulse trains, can improve the excitation bandwidth for a given peak RF power level and thus minimize spectral distortion. Measuring the decay rates of NQR signals, which are quantified by the relaxation time constants T_1 and T_2 , provides insights into sample characteristics and can aid in their differentiation [33]. Two-dimensional NQR (2D-NQR) techniques offer additional information by detecting correlations between the multiple NQR resonance frequencies of a given nuclear site. These correlations help to 1) distinguish between substances with overlapping NQR spectra, and 2) separate NQR signals from external RF interference (RFI) [34].

Dynamic NQR techniques, such as saturation recovery and spin-locking, also aid in substance identification [35], [36]. Isotopic enrichment and cryogenic cooling can increase the NQR signal amplitude for target isotopes, enhancing sensitivity. Advanced data processing techniques, including active noise cancellation and machine learning algorithms, can analyze complex NQR spectra in the presence of RFI, thus enabling the detection and classification of substances with greater accuracy. Lastly, applying external constraints like temperature or pressure can alter NQR parameters and reveal substance-specific signatures, further enhancing specificity in NQR-based substance detection. Collectively, these techniques and strategies offer a versatile toolkit for improving both sensitivity and specificity in NQR-based substance identification.

III. COMPARISONS BETWEEN ANALYTICAL TECHNIQUES

In the realm of substance detection, various spectroscopic techniques offer a diverse array of tools for identifying and characterizing materials. NQR stands as a distinct player among other well-established techniques like Nuclear Magnetic Resonance (NMR), Near-Infrared Spectroscopy

(NIR), Raman Spectroscopy, and Mass Spectrometry (MS). Each technique has its unique strengths and weaknesses, which dictate its utility in different scenarios. This section will compare and contrast some of the current analytical techniques available on the market.

A. NMR SPECTROSCOPY

NQR and NMR spectroscopy are two well-known analytical techniques often compared with each other due to their common origin in nuclear energy levels (hyperfine structure) [37]. However, a closer look reveals distinctive features that steer them towards distinct applications.

One of the foremost disparities between NQR and NMR revolves around sensitivity. NMR is a bulk technique that requires a large number of nuclei within the sample to yield a discernible signal, a challenging feat when dealing with trace-level analyses [38]. However, the SNR of an NMR experiment increases with the amount of Zeeman splitting between nuclear energy levels induced by an external magnetic field (known as B_0), which in turn is proportional to the field strength. Thus, NMR practitioners can improve the SNR for a given sample volume by using a stronger magnetic field, which has driven the development of ultra-high-field magnets. SNR can be further improved by using various hyper-polarization methods, such as dynamic nuclear polarization (DNP) that increase the degree of nuclear polarization beyond its thermal equilibrium value. By contrast, NQR utilizes the splitting between quadrupolar energy levels in the local EFG. The latter is determined by the sample's physical and chemical structure and is independent of external fields. Thus, the SNR per nucleus of an NQR experiment is an intrinsic property of the sample and cannot be improved by applying external fields. Moreover, it is generally lower than for an NMR experiment at typical B_0 field strengths ($> 0.5T$). Hyper-polarization methods for NQR are also less effective than for NMR. The most popular approach relies on adiabatic polarization transfer from nearby non-quadrupolar nuclei, typically protons [39]. However, the resulting gains in SNR are highly sample-dependent and typically modest (less than $10\times$).

Specificity marks another important contrast between the two techniques. As for any spectroscopic method, the specificity of an NMR or NQR spectrum is a decreasing function of both the resonant frequency shift (which is a measure of accuracy) and the line width (which is a measure of precision). The specificity of an NMR spectrum is degraded by many line broadening and coupling mechanisms, including field inhomogeneities, susceptibility gradients, chemical shift anisotropy, and spin-spin coupling (including dipolar coupling, J-coupling, and quadrupolar coupling). Some of the same mechanisms impact NQR spectra, but several field-dependent mechanisms are absent since the measurement is ideally performed at zero fields ($B_0 = 0$). On the other hand, the fact that NQR resonances arise from coupling with the EFG tensor introduces new

line-broadening mechanisms, including EFG inhomogeneity due to crystal structure. Thus, the question of whether NMR or NQR has greater specificity has no unique solution: the answer is sample-dependent. Broadly speaking, nuclear species with relatively small (but non-zero) quadrupolar coupling constants, such as ^{14}N and ^{35}Cl , tend to generate highly-specific NQR spectra with narrower line widths than obtainable using NMR.

Sample preparation emerges as yet another dimension where NQR and NMR diverge. Typical sample preparation for NMR spectroscopy entails dissolving the sample in an organic or inorganic solvent and then housing it within a specialized NMR tube — a process that can be both time-consuming and costly [40]. By contrast, NQR streamlines the sample preparation procedure. In most cases, little to no special preparation is required, which ultimately makes it a more straightforward and cost-effective choice for many substance detection applications.

While NQR and NMR share a common origin in nuclear energy levels, they differ in terms of sensitivity, specificity, and sample preparation, as discussed above. NMR benefits from the use of strong external magnetic fields to improve SNR, which can often be further enhanced by implementing hyper-polarization methods. NQR, on the other hand, provides intrinsic specificity due to its dependence on the local EFG, while requiring minimal sample preparation. Despite its generally lower sensitivity compared to NMR, NQR's zero-field operation eliminates several line broadening mechanisms, making it suitable for applications such as remote or non-contact detection of concealed substances.

Additionally, NQR is particularly useful in environments where applying a strong magnetic field is impractical or unsafe, such as during field detection of explosives or narcotics. However, NQR's lower sensitivity can be a significant drawback in applications requiring detailed structural analysis where NMR's higher sensitivity is advantageous. NQR is also limited to nuclei with quadrupole moments, whereas NMR can be applied to a wider range of nuclei, including those prevalent in organic compounds, such as hydrogen (^1H) and carbon (^{13}C). This limits the scope of NQR in organic chemistry and biochemistry, areas where NMR is widely used for structural elucidation.

B. NIR SPECTROSCOPY

Comparing near-infrared (NIR) spectroscopy with NQR unveils intriguing facets of their analytical properties, shedding light on their distinctive attributes and applications.

A prominent contrast between NQR and NIR revolves around their specificity. The excellent specificity of ^{14}N or ^{35}Cl NQR positions it as the “go-to” choice for discerning minute differences between compounds sharing analogous structures, a challenge that often befuddles alternative methodologies. By contrast, NIR spectroscopy provides insights into a sample's chemical composition by measuring its absorption, reflection, or transmission within the

near-infrared range of the electromagnetic spectrum. While NIR is a non-destructive and swift technique, it typically has lower specificity than NQR of popular quadrupolar nuclei (such as ^{14}N or ^{35}Cl). Fundamentally, this is because the NIR spectrum consists of high-order overtones (harmonics) of molecular vibration lines with fundamental frequencies in the mid-infrared (MIR) range. The profusion of harmonics and their numerous overlaps results in broad spectra with relatively low specificity.

These two spectroscopic techniques can also be distinguished by their sensitivity. The optical transitions utilized by NIR spectroscopy have much larger energies than the RF transitions utilized in NQR. The result is much higher intrinsic SNR per unit sample volume, which allows NIR spectroscopy to detect trace-level constituents and renders it a potent tool for analyzing substances in minute doses. Specifically, the limit of detection (LOD) for typical NIR acquisition times (a few seconds) is at the milligram level. By contrast, NQR spectroscopy has much larger LOD values (typically, several grams) for similar acquisition times.

The physical form of the sample introduces yet another dimension where NQR and NIR diverge. NIR spectroscopy minimizes the rigors of sample preparation and accommodates a diverse range of samples that includes solids, liquids, and gases. NQR spectroscopy is also undemanding in terms of sample preparation, as noted earlier. Additionally, it is a bulk technique that is largely unaffected by surface coatings and encapsulants. By contrast, optical analysis methods such as NIR spectroscopy are easily blocked by opaque surface layers, such as plastic capsules. On the other hand, NQR spectroscopy is fundamentally limited to solids since the NQR signal is averaged out by the random molecular motion within fluids.

NIR spectroscopy provides rapid and non-destructive analysis capabilities, particularly in identifying organic compounds and monitoring industrial processes. It excels in providing real-time data and requires minimal sample preparation. However, NIR is less specific than NQR, as it primarily measures overtone and combination vibrations of molecules, leading to broader, less distinct spectra. While NIR is advantageous for quick screening and quantitative analysis, NQR offers superior specificity in identifying compounds with quadrupolar nuclei, making it more suitable for detailed structural analysis. Moreover, NIR's performance can be affected by water content and sample homogeneity, limiting its applicability in certain scenarios. NQR, unaffected by these factors, can provide reliable and precise information even in complex matrices. This makes NQR an excellent choice for forensic and security applications where accurate identification of specific substances is crucial. However, the lower sensitivity of NQR compared to NIR can be a limitation in scenarios requiring rapid, high-throughput screening. Additionally, NQR's applicability is restricted to nuclei with quadrupole moments, thus reducing its versatility compared to NIR, which can be applied to a wide range of materials.

C. RAMAN SPECTROSCOPY

Raman spectroscopy is an optical analysis method with many similarities to NIR spectroscopy. Both methods measure the vibrational spectra of molecules. However, NIR spectra are measured via absorption, reflection, or transmission of a broadband optical source (such as an LED), while Raman spectra are measured via inelastic scattering of a narrowband optical source (typically, a laser). Additionally, NIR spectra are complex due to overlaps between the high-order harmonics of the fundamental vibrational lines, as noted earlier. The result is broad lines with relatively low specificity. By contrast, Raman spectra have narrow lines with high specificity, making it preferable for sample identification and quantification. However, the inelastic scattering process that underlies Raman spectroscopy is relatively weak, which reduces the intrinsic SNR of the spectrum. Additionally, Raman spectrometers are more expensive and harder to integrate due to their use of a laser. Thus, the choice between traditional NIR and Raman spectroscopy is sample- and application-dependent.

The choice between NQR and Raman spectroscopy presents a similar set of trade-offs as between NQR and NIR. Broadly speaking, NQR and Raman have comparable specificity (typical fractional line widths of 10^{-4} or less) for many samples of interest to law enforcement. However, Raman has much higher sensitivity, with typical LOD values in the milligram range (compared to several grams for NQR). On the other hand, Raman spectra are highly impacted by surface properties since the typical optical penetration depth is less than 1 mm. By contrast, NQR spectra are largely unaffected by surface properties, including the presence of encapsulants and/or non-metallic packaging. Usable spectra can even be measured from samples within metallized packages, such as blister packs, as long as they do not form a complete Faraday shield.

Raman spectroscopy is highly effective in identifying molecular vibrations, making it a powerful tool for characterizing chemical compositions and molecular structures. It is particularly suitable for studying inorganic compounds, crystalline structures, and materials with symmetrical molecules. However, Raman spectroscopy can be limited by fluorescence interference and requires careful sample preparation. In contrast, NQR's specificity and ability to analyze substances without external magnetic fields or sample preparation make it a robust choice for detecting quadrupolar nuclei in various materials, even in the presence of complex mixtures. Furthermore, Raman spectroscopy's sensitivity to laser-induced damage and the need for clean and smooth sample surfaces can be restrictive. NQR's non-invasive nature and ability to work with heterogeneous samples provide significant advantages in fields such as pharmaceuticals and homeland security, where maintaining sample integrity is essential. Nevertheless, NQR's generally lower sensitivity compared to Raman spectroscopy means it may not be the best choice for detecting low-concentration substances or for applications requiring high spatial resolution. Additionally,

NQR is limited to substances containing quadrupolar nuclei, while Raman spectroscopy can analyze a broader range of substances, including those without quadrupolar nuclei.

D. MASS SPECTROMETRY

NQR and mass spectrometry (MS) present an interesting contrast in terms of their detection mechanisms, specificity, sensitivity, and sample preparation requirements. Unlike resonant techniques such as NQR, NIR, and Raman spectroscopy, the analytical basis of MS is the measurement of mass-to-charge ratios of ions. The result is a mass spectrum that allows the molecular composition of a sample to be quantified.

In general, both NQR and MS spectra have excellent specificity (in terms of fractional linewidth). However, they measure completely different physical properties. Thus, the resolution offered by these analytical methods is a complex function of multiple factors, including the method, the sample, and the property to be measured.

Another distinction between NQR and MS is sensitivity. MS has excellent sensitivity, with typical LOD values in the femtogram (10^{-15} gram) range. As a result, MS is widely used for trace-level analyses of contaminants and other substances in minute quantities. By contrast, NQR has LOD values in the gram range, as noted earlier, which largely limits its applicability to bulk samples.

Sample preparation introduces a final layer of contrast between NQR and MS. The range of samples that can be analyzed using MS is relatively broad, and includes solids (after dissolution in a solvent), liquids, and gases. However, MS is a destructive technique and typically demands a significant amount of sample preparation, which often includes a pre-separation process such as ion mobility spectrometry (IMS), gas chromatography (GC), or liquid chromatography (LC). By contrast, NQR is limited to solids but is non-invasive, non-destructive, and generally requires little sample preparation.

Mass spectrometry stands out for its unparalleled sensitivity and ability to provide molecular weight information and structural details of compounds. It is widely used in proteomics, metabolomics, and pharmaceutical analysis due to its accuracy and precision. However, MS requires ionization of the sample, often leading to fragmentation, and involves complex instrumentation and data interpretation. NQR, while less sensitive, does not alter the sample and provides specific information about the local environment of quadrupolar nuclei. This makes NQR a complementary technique for situations where non-destructive analysis and specificity are paramount. Additionally, the high cost and maintenance of MS equipment, along with the need for highly trained personnel, can be prohibitive for routine analysis. NQR's relatively straightforward setup and operation offer a cost-effective alternative for continuous monitoring and quality control in various industries. Its capability to operate *in situ* without altering the sample's state makes it particularly valuable in scenarios where preserving the sample's integrity

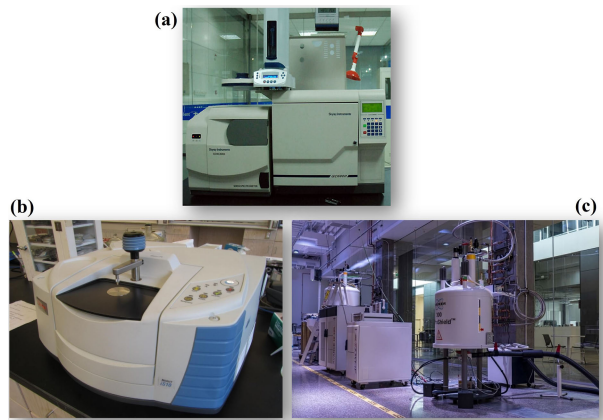


FIGURE 2. Different types of commercialized spectrometers available on the market: (a) GC-MS 6800 Gas Chromatograph Mass Spectrometer (GC-MS) system; (b) Thermo Nicolet iS10 Fourier Transform Infrared (FTIR) spectrometer; and (c) Bruker Avance II 300 MHz NMR spectrometer.

is important, such as in historical artifact analysis or screening of mail packages.

However, NQR's lower sensitivity and the requirement for quadrupolar nuclei limit its applicability compared to the broad usage of MS across different types of compounds and elements. Furthermore, NQR signal acquisition can be time-consuming, making it less suitable for high-throughput analyses where MS excels. Thus, while NQR is advantageous for specific, non-destructive analysis, its limited sensitivity, scope, and longer acquisition times compared to MS's broad applicability, high sensitivity, and rapid analysis are significant weaknesses.

Table 3 compares the advantages of various spectroscopic techniques for sample analysis, including NQR, NMR, NIR, and Raman spectroscopy. The main comparison metrics include economic feasibility, robustness, measurement resolution, sensitivity, quantitative nature, sample preparation requirements, and measurement speed.

IV. CHALLENGES AND LIMITATIONS OF NQR-BASED SUBSTANCE DETECTION

A variety of existing applications have demonstrated the powerful impact of NQR on substance detection and authentication. Nevertheless, while NQR holds promise as a sophisticated technique for substance identification, it is accompanied by a set of inherent drawbacks that must be carefully navigated. These issues are further discussed below.

A. SIGNAL-TO-NOISE RATIO (SNR)

One of the most notable drawbacks of NQR is its relatively low signal-to-noise ratio (SNR), which plays a pivotal role in the quality and reliability of NQR measurements [41]. The SNR in NQR is influenced by multiple factors, including the inherently weak nature of NQR signals and the susceptibility of these signals to various forms of noise. As discussed in the previous section, the relatively weak interaction between quadrupolar nuclei and their local electric field gradients makes NQR signals much weaker than for optical

spectroscopy or MS. These weak signals are frequently corrupted by external RFI, thus further reducing the SNR.

The SNR of an NQR experiment is proportional to the total number of nuclei within the sample, and thus to the density of nuclear spins for a given sample volume. The limitations imposed by low SNR are particularly evident when detecting nuclei within complex molecules, which tend to have low spin densities due to their high molecular weights. Additionally, spin density is proportional to the fractional concentration of the compound of interest within a mixture. Thus, low SNR also limits the ability to analyze samples with inherently low concentrations, such as trace impurities and contaminants.

External electromagnetic interference (known as RFI) can disrupt NQR signals, overwhelming the weak resonances of interest and rendering them challenging to distinguish from the background noise. Efforts to improve the SNR of NQR spectra therefore often involve sophisticated signal processing techniques, noise reduction algorithms, and hardware optimizations [42]. Additionally, careful consideration of experimental conditions, shielding from electromagnetic interference, and minimization of noise sources can contribute to enhancing the SNR. However, despite these efforts, achieving a favorable SNR remains a significant challenge in NQR, particularly in real-world scenarios featuring complex sample geometries and multiple noise sources.

B. TEMPERATURE DEPENDENCY

An inherent drawback in NQR lies in the sensitivity of the resonance frequencies to sample temperature, an effect that can significantly impact the accuracy and repeatability of NQR measurements [43]. Temperature fluctuations cause thermal expansion of the crystal lattice, which drives resonance frequency shifts by altering the EFG tensor. The resulting deviations from the expected NQR frequencies poses a challenge for sample identification, i.e., reduces the specificity of NQR spectra. The dependence of NQR signal properties on temperature further extends to relaxation times, which dictate the decay rate of NQR signals after excitation. Temperature variations influence relaxation times via changes in $J(\omega)$, the spectrum of lattice vibrations and molecular motion exhibited by the sample. These changes subsequently affect the signal amplitude and SNR [44]. Such temperature-dependent variations in NQR signal amplitude complicate accurate data interpretation and can potentially undermine the reliability of substance detection.

Efforts to mitigate the impact of temperature sensitivity in NQR measurements involve maintaining a stable temperature during data acquisition. Temperature-controlled environments, such as environmental chambers, are often employed to minimize temperature-induced variations in NQR signals. Additionally, using calibration samples with known NQR frequencies at different temperatures and referencing the acquired signals against these standards can help to compensate for temperature-induced shifts.

TABLE 3. Comparing the advantages of spectroscopic techniques for sample analysis.

Technique	Specificity	Sensitivity	Sample Preparation	Analysis Depth
NQR	High	Low	Minimal, but limited to solids	Bulk, entire sample
NMR	High	Medium	Often requires sample dissolution	Bulk, entire sample
NIR	Low	High	Minimal	Surface, < 1 mm
Raman	Medium	High	Minimal	Surface, < 1 mm
Mass Spectroscopy	Medium	Very high	Significant	N/A (destructive method)

C. LIMITS ON SAMPLE FORM

The last challenge that limits NQR in substance detection lies in the fact that it can only detect crystalline solids (either single crystals or powders), i.e., is unable to directly detect liquids or gases. This limitation stems from the underlying principles of NQR, which relies on the interactions between quadrupolar nuclei and their local EFG [45], [46]. In solids, these interactions are well-defined due to the ordered lattice structure, enabling the generation of distinguishable NQR signals. However, in liquids, the dynamic molecular motion and lack of a stable lattice arrangement result in significant line broadening and reduced coherence times, causing the NQR signals to be weak and difficult to detect.¹ This inherent restriction narrows the scope of NQR applications considerably, particularly in situations where the target substance exists in liquid form or where the analysis of liquid samples is essential. The inability of NQR to directly detect liquids hampers its potential for sample detection and analysis. In particular, it prevents NQR from detecting explosives or drugs in liquid, semi-solid, or amorphous form. Moreover, it restricts its use in quality control processes where the assessment of liquid-based products is essential.

D. IMPACT OF NQR LIMITATIONS

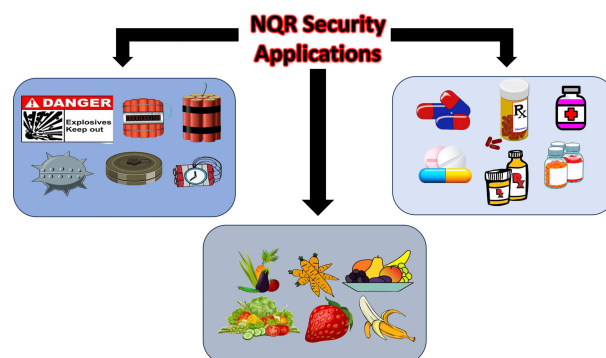
1) NANOCRYSTALS

Nanocrystals are nanoscale particles that exhibit unique properties due to their small size and high surface area. These properties make them valuable in a wide range of applications, including pharmaceuticals, material science, and security. Because of their critical roles, precise and reliable detection methods are essential for nanocrystals.

Theoretical and experimental studies have shown that NQR line widths increase rapidly for nanocrystals that contain less than ~ 10 atomic layers [47]. Such small particles are dominated by their surface layers, which suffer from additional line broadening due to their broken chemical bonds. The result is reduced specificity, which makes NQR spectroscopy ineffective for detection and analysis of samples containing such small nanocrystals.

The reduced specificity of NQR in nanocrystals can be an issue for security screening applications, which are often required to detect contraband substances in various physical forms. Similarly, in the pharmaceutical industry, precise detection of nanocrystal drug formulations is essential for quality assurance and regulatory compliance. In this case, reduced specificity can lead to inadequate characterization

¹Liquid crystals are an exception. Their long-range order enables NQR spectra to be measured in certain cases.

**FIGURE 3.** NQR's diverse detection power: Unveiling medicine, explosives, and food.

and quality control, in turn affecting the efficacy of nanocrystal-based medications.

2) SENSITIVITY AND LOD

As discussed earlier, the term LOD refers to the minimum quantity of a substance that can be reliably detected using a given analytical technique. Achieving high sensitivity, and thus a low LOD, is crucial for practical applications such as security and substance detection. However, the inherently low sensitivity of NQR limits its LOD, making it challenging to detect and/or quantify small quantities of substances.

In security and screening applications, the high LOD of NQR limits its effectiveness in detecting small quantities of explosives or narcotics. For example, the inability to detect low levels of concealed substances reduces the overall reliability and effectiveness of NQR technology for airport screening or border control. Similarly, in the pharmaceutical industry, the accurate detection of trace impurities and counterfeit drugs is essential. A high LOD restricts the ability of NQR to identify low-level contaminants or to authenticate drugs with high precision, posing a challenge for quality control and regulatory compliance.

V. APPLICATIONS OF NQR

A. EXPLOSIVES DETECTION

NQR has played a significant role in modern security screening, as summarized in Fig. 3. Its unique ability to target specific nuclei with quadrupole moments sets it apart as a powerful tool for identifying and differentiating explosive materials. NQR's contribution to security screening goes beyond conventional techniques, offering enhanced accuracy and reliability in identifying concealed or well-disguised explosive substances. One of NQR's prime applications in security is the detection of explosives such as TNT

(trinitrotoluene) and RDX (cyclotrimethylenetrinitramine). These compounds contain nitrogen nuclei that are amenable to NQR analysis. Unlike metal detectors or X-ray scanners, which mainly focus on the device's physical components, NQR directly detects the chemical presence of explosive materials themselves. This attribute provides a higher level of specificity, enabling security personnel to pinpoint the actual threat rather than relying solely on indirect indicators. Another critical aspect of NQR's utility in security screening is its potential to detect explosives within complex environments. Explosives can be concealed within a variety of objects or materials, making their detection and identification difficult. Fortunately, NQR's ability to identify explosives based on their unique chemical signatures enables it to identify hidden threats even in such scenarios. Thus, many experiments on detection of explosives have been discussed in the NQR literature [48], [49].

Next, we briefly discuss some the proposed applications of NQR for explosive detection. For example, the authors in [50] outline the design of a sensing system that uses ^{14}N NQR to remotely detect explosives containing nitrogen-based compounds. Existing remote NQR detection faces significant RFI challenges since the samples are not shielded (e.g., within a solenoidal coil), thus resulting in more pronounced RFI. To address this issue, the research group designed their sensing system to include two key components: 1) active noise cancellation (ANC) to counter external RFI; and 2) a Q -switch circuit to reduce the recovery time of the RF probe. The ANC system consists of three key parts: the primary coil used for NQR detection, two auxiliary coils for sensing RFI, and digital signal processing for RFI cancellation. The first auxiliary coil is dedicated to cancelling RFI in the analog domain, i.e., before it reaches the NQR console. This ANC loop utilizes an amplifier with gain auto-regulation, a tunable phase shifter, and a signal subtractor. The second auxiliary coil uses an additional amplifier and a digital receiver for cancelling RFI in the digital domain. Additionally, a lossy Q -switch circuit is used to shorten the ring-down time of the probe after each high-power RF pulse, i.e., improve the dynamic response of the probe by reducing its recovery time. Importantly, the Q -switch is turned off during signal acquisition, such that measurement sensitivity and SNR are unaffected.

In other work, a research group at Kings College, London, developed an affordable and easily transportable NQR device designed specifically for detecting explosives [12]. This device consists of several key components, including a power supply, an NQR control unit, a transceiver, and the RF coil used for sensing and excitation. The system is designed to be portable: it has relatively low power consumption (3.1-6.6 W) and can be powered by lightweight Li-ion batteries. To keep costs down, the system employs a readily available FPGA board for control and signal processing. The spectrometer uses a planar RF coil to allow detection of large samples in a "single-sided" configuration and a digital quadrature detection method for signal acquisition. The geometry of the

RF coil was optimized to utilize a gradiometer configuration for reducing external RFI while maintaining good detection sensitivity. The article also highlights several contributions to advancing existing technology, including the development of 1) a series-resonant probe in transmit mode (tuned to the desired NQR resonance frequency of ~ 3.41 MHz) to eliminate the need for a high voltage (HV) power supply; 2) a power-efficient dual-supply class-D power amplifier utilizing GaN MOSFETs to maximize battery life; and 3) a noise-matched trans-impedance amplifier (I - V converter) to minimize receiver noise figure (NF).

To prove the effectiveness of their application, the team loaded different sized targets with varying amounts of the explosive HMT (50 g, 100 g, and 200 g), which is used within anti-personnel landmines. Detection performance was characterized at distances of 10 cm and 5 cm from the planar RF coil. The measured signal amplitudes were normalized to a reference value to facilitate comparison, as shown in Fig. 4. The results show that the signal amplitude is proportional to quantity of sample, as expected. Additionally, the amplitude decreases by 3.7-4.6 \times when the distance to the coil increases from 5 cm to 10 cm. Such rapid decay of sensitivity with distance, which is unavoidable for single-sided coil geometries, ultimately limits the useful operating range of remote NQR detectors.

The integration of NQR spectroscopy into modern security protocols and systems provides a novel approach to substance detection with distinct advantages over traditional methods. The non-invasive nature of NQR ensures the safety of both individuals being screened and operators conducting the scans, as it eliminates the need for harmful ionizing radiation (such as X-rays). Moreover, the technique's high specificity in targeting nuclear resonances of specific substances significantly reduces false positive rates, thereby enhancing the accuracy of threat identification. The ability of NQR to detect substances concealed within various materials aids security personnel in identifying hidden threats that might otherwise evade conventional methods. Unlike imaging technologies that raise privacy concerns, NQR focuses on chemical composition, thus mitigating potential infringements to personal privacy and fostering a balanced approach to security screening.

B. AUTHENTICATION OF PHARMACEUTICALS

Apart from explosives detection, researchers have incorporated NQR into other substance detection applications. A good example is the use of NQR in ensuring the security of the pharmaceutical supply chain. Recent years have witnessed a rapid growth in counterfeit/adulterated medicines, and the Food & Drug Administration (FDA), law enforcement, and other government officials have struggled to de-escalate this growing epidemic with the detection systems currently available on the market. NQR is emerging as a key technology for addressing this challenge. Specifically, the widespread availability of NQR is expected to disrupt the circulation and trading of falsified drugs by

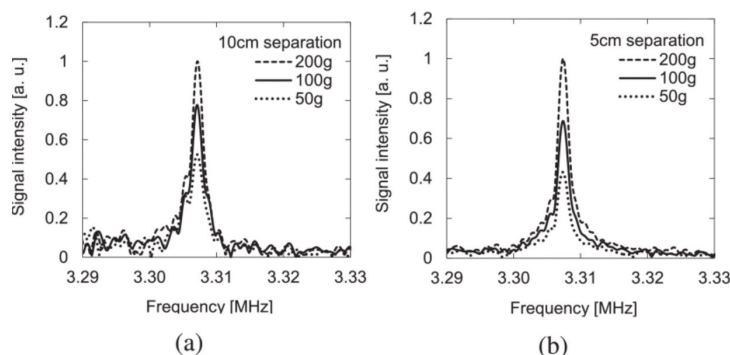


FIGURE 4. Signals emitted by 50 g, 100 g, and 200 g of HMT, as detected by the proposed NQR spectrometer at two different distances from the detection coil: (a) 10 cm, and (b) 5 cm. Each scan used a free induction decay (FID) detection sequence. Signals were accumulated over 4,000 scans, resulting in an acquisition time of ~ 200 sec. Figure reproduced from [12].

enabling non-invasive authentication of medicines at different stages of the supply chain.

The dietary supplement market is estimated to generate \$57 billion in revenue by 2024, while counterfeit pharmaceuticals are also a billion-dollar industry [51], [52]. The authors in [16] proposed a robust NQR-based authentication approach to ensuring the legitimacy and quality of dietary supplements at different points in the supply chain. In particular, the research team authenticated supplements from various manufacturers using NQR spectroscopy combined with machine learning (ML). Pulsed NQR measurements were conducted using the SLSE sequence, and the following parameters extracted from the resulting echoes: initial amplitude (A), frequency-domain line-width (Δf), and decay time constant ($T_{2,eff}$). These features were then used to train a supervised learning algorithm such as a support vector machine (SVM). The trained SVM was used for inference, i.e., classifying dietary supplements from different manufacturers. Experimental results demonstrated the effectiveness of combining NQR spectroscopy with SVM-based classification for authenticating dietary supplements. Samples from different manufacturers are accurately distinguished. The study also evaluated other classification algorithms, with SVMs achieving the highest accuracy. Furthermore, the authors examined the impact of temperature fluctuations on NQR measurements and classification accuracy. Temperature-related changes in NQR parameters like amplitude and decay time constant were indeed observed, but the SVM classifier remained robust within a specific temperature range. Thus, the proposed authentication method is insensitive to minor environmental fluctuations.

As previously stated, NQR is insensitive to the presence of non-conductive packaging. One of the most commonly used portals to transport and distribute counterfeit/illicit narcotics throughout the United States is the postal network. The logistics of the postal network includes multiple stages, which range from origin post offices to national distribution centers. Each step often involves limited authentication, especially

for international shipments. The authors in [17] focused on the potential of ^{14}N NQR spectroscopy to detect drugs within different mailing packages. As an example, they demonstrated the detection of benzocaine, which is a topical analgesic found in various over-the-counter medications and has raised concerns due to its association with a blood disorder named methemoglobinemia. In addition to a conventional enclosed detector (a solenoid coil), the authors also developed an open-geometry planar coil to allow larger packages to be scanned. Data from both enclosed and open detectors was compared to study their relative sensitivity. Experiments were also conducted to study the effect of different packaging materials, including cardboard, bubble wrap, paper envelopes, plastic envelopes, blister packages, and electrostatic discharge (ESD)-protected mailers. The results shown in Fig. 5 indicate that NQR is insensitive to the presence of such non-conductive packaging, as expected. Conductive packaging, such as blister packs with aluminum foil, does present challenges for NQR detection due to partial shielding of the RF field during both transmission and reception. Nevertheless, the measured NQR signal can still be used to quantify sample properties. For example, a linear relationship can be derived between NQR signal amplitude and the weight of an active pharmaceutical ingredient (API), with different fitting parameters for each type of package. Such a model enables non-invasive quantification of the API from NQR measurements of packaged samples.

C. AUTHENTICATION OF FOOD & CONSUMABLES

As human civilization progresses, the demand for high-quality food continues to grow [53]. However, the global food supply chain is increasingly subject to quality control and security concerns. Food adulteration or substitution has become common at different stages of the supply chain. The typical goal of food fraud is to achieve some form of economic gain by tampering with food ingredients and labels and/or making misleading statements about products [54], [55], generally with no intent to directly harm the consumer.

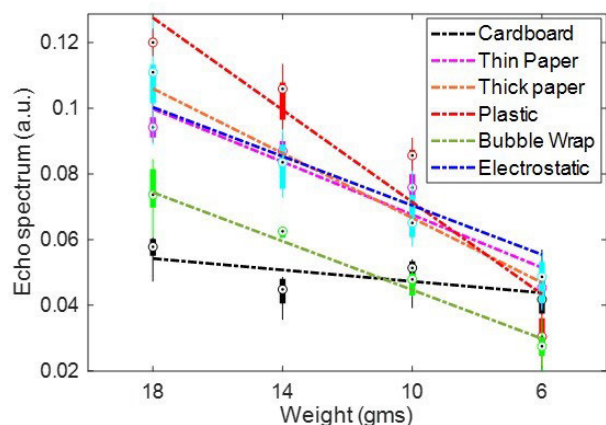


FIGURE 5. Comparison of ^{14}N NQR signal amplitudes obtained from the psychoactive drug Benzocaine when the sample was enclosed within different types of packaging materials.

There has been a recent surge of interest in addressing this issue by applying NQR-based detection to authenticate food items.

The authors in [11] present a novel approach to improve the security and integrity of the food supply chain using NQR spectroscopy. The paper proposes an authentication and traceability approach that relies on applying NQR spectroscopy to authenticate the contents of packaged food products. The authors highlight the benefits of NQR, including its non-invasive, non-destructive, and quantitative nature, as well as its sensitivity to subtle features of the solid-state chemical environment. These features make NQR a promising tool for substance detection applications, particularly in cases where other analytical spectroscopic techniques such as NIR or Raman spectroscopy may not be effective. The authors also propose a SVM-based classification approach in which the classifier is trained using measured NQR parameters and then used to authenticate food products. This approach again shows that ML techniques can extract subtle differences between substances from NQR data. The authors also note that sensitivity and specificity can be further improved by optimizing the instrumentation, which highlights the importance of continued research and development in this area. Overall, this paper demonstrates the potential of NQR spectroscopy in detection and authentication of consumables in complex supply chains.

The authors in [56] present a novel solution to the problem of counterfeiting in the consumables industry. The paper focuses on the authentication of consumables using NQR spectroscopy and chemical fingerprinting. The paper also provides detailed information on the fundamentals of NQR-based authentication, feature extraction, and ML-based classification. The paper also introduces the concept of extrinsic tagging and analyzes its security properties, including entropy functions, thus providing valuable insights into the use of NQR spectroscopy for authentication purposes.

Lastly, the same research team proposed the novel concept of material biometrics for authenticating individual products [57]. The method involves modifying objects via

programmable additive manufacturing of built-in chemical “tags” that generate signatures depending on their chemical composition, quantity, and location. These signatures can be non-invasively read out using NQR spectroscopy, which is insensitive to packaging, opacity of the material, surface roughness, and other physical characteristics. The authors demonstrated their material biometrics concept by integrating it within an additive manufacturing process flow for creating arbitrary plastic objects. For this purpose, raw plastic pellets were mixed with a small amount of NQR-sensitive chemical (NaClO_3 in this case) to create custom tagged filaments. A filament extrusion system was used to form the mixture into cylindrical filaments that can be fed into a 3D printer. A dual-nozzle printer was loaded with both the modified (i.e., tagged) filament and a normal (i.e., un-tagged) filament. The device was then used to 3D-print objects containing unique chemical signatures that can be detected using ^{35}Cl NQR spectroscopy.

VI. CONSIDERATIONS AND CHALLENGES IN NQR-BASED SAMPLE ANALYSIS

A. POLYMORPHS

NQR is highly sensitive to the local environment of quadrupolar nuclei, making it an effective tool for distinguishing between different physical forms of a substance. Polymorphs, which are different crystal structures containing the same molecule, thus exhibit distinct NQR signals [58]. However, the practical challenge lies in the complexity of accurately identifying and differentiating polymorphs in mixtures. This requires sophisticated signal processing techniques and extensive reference databases to interpret the NQR spectra accurately.

B. REGULATORY REQUIREMENTS

Implementing NQR-based systems in real-world applications also involves navigating various regulatory requirements. For instance, NQR systems used in security for detecting explosives or narcotics must meet stringent standards set by government agencies. These standards ensure the accuracy, reliability, and safety of the technology. Compliance with these regulations often requires extensive testing and certification processes, which can be time-consuming and costly. Furthermore, the use of high-power RF pulses by NQR spectrometers raises concerns about electromagnetic interference (EMI) with other electronic devices, necessitating careful design and shielding of NQR equipment to comply with regulatory limits on EMI emissions.

VII. FUTURE RESEARCH DIRECTIONS

Emerging trends in NQR-based substance detection are paving the way for improved security and quality control in various applications. The use of NQR to detect and identify explosives and narcotics is becoming more refined, thus enabling more accurate and non-invasive substance detection at airports, borders, and critical infrastructure. The pharmaceutical industry is also exploring the potential of NQR for rapid quality control, ensuring drug authenticity and reducing

the risk of counterfeit medications entering the market. In summary, NQR substance detection is poised to shape the security landscape, offering precise and versatile solutions to complex supply chain challenges in multiple domains. In this section, we briefly discuss research directions with the potential to further improve the performance of analytical devices based on NQR spectroscopy.

A. ENHANCEMENT OF SIGNAL PROCESSING TECHNIQUES

Future development in NQR applications can significantly benefit from the advancements in signal processing techniques. One area of focus involves refining algorithms to effectively mitigate noise, thus improving SNR of NQR measurements. Novel de-noising methods based on wavelet transforms, adaptive filtering for active noise cancellation, or ML can be explored to suppress background noise while preserving NQR signals' integrity.

Additionally, efforts can be directed towards developing spectral de-convolution algorithms aimed at enhancing spectral resolution. These algorithms can help in resolving complex multiplet structures and overlapping peaks, facilitating precise identification and quantification of NQR resonances. Techniques such as non-negative matrix factorization (NMF) and sparse signal decomposition hold promise in this regard.

Lastly, the implementation of real-time processing capabilities within NQR instrumentation can significantly enhance its practical utility. By deploying efficient signal processing pipelines on FPGA or GPU platforms, researchers can achieve high-speed data analysis without compromising accuracy. Such real-time processing capability is crucial for enabling rapid decision-making in time-sensitive applications such as security screening.

B. DEVELOPMENT OF PORTABLE NQR SYSTEMS

Advancements in miniaturization and instrumentation are key to unlocking the full potential of NQR, particularly in field applications where portability and rapid deployment are paramount. Future research can focus on developing portable NQR systems tailored for on-site detection.

One avenue for development involves leveraging emerging technologies to miniaturize NQR instrumentation without compromising performance. This includes exploring compact magnet designs, such as electromagnets or permanent magnets, that offer sufficient magnetic field strength for significantly improving the SNR of NQR signals via polarization transfer from nearby protons [39] while also minimizing the overall size and weight of the system. Innovations in RF coil design, front-end electronics, and packaging can further contribute to compact system architectures, facilitating ease of transportation and deployment in field environments.

Furthermore, efforts can be directed towards integrating auxiliary components, such as power sources and data acquisition systems, into portable NQR platforms to enable standalone operation in remote or resource-limited settings. This may involve exploring alternative power options, such

as rechargeable batteries or solar panels, to provide sufficient energy for sustained operation without relying on external power sources. Similarly, the development of ruggedized data acquisition units capable of capturing and processing NQR signals in real-time can enhance the system's autonomy and reliability in field conditions.

C. USE OF CLOUD DATABASES

IoT-enabled "smart" NQR devices can benefit from the advantages of cloud-based data storage, which include accessibility, quality control, and long-term archiving. By securely uploading NQR data to the cloud, researchers can easily access historical data and share it with colleagues and organizations, fostering collaborative research efforts. The real-time collaboration enabled by a cloud database transcends geographical boundaries, allowing researchers to collectively analyze and work on NQR data, promoting a collaborative and interconnected research ecosystem. Furthermore, user-friendly web and mobile interfaces will play a pivotal role in making NQR technology more accessible. Intuitive dashboards and data visualization tools will make it easier for both experts and non-experts to interact with and gain insights from NQR data. Equally critical is the emphasis on data security for maintaining the integrity and confidentiality of NQR data. Researchers must also focus on implementing robust data encryption, authentication mechanisms, and access control to protect sensitive information, ensuring that the capabilities of NQR spectroscopy are coupled with robust security measures.

VIII. CONCLUSION

This review paper has delved into the wide array of substance detection applications enabled by NQR spectroscopy. From its inception as a niche analytical technique to its burgeoning role in fields such as security, medicine, and materials science, NQR has showcased its potential for non-invasive, selective, and sensitive detection. With ongoing advancements in instrumentation, signal processing, and ML, the future of NQR-based substance detection promises further advances. As we continue to unravel the intricacies of NQR measurements, its adoption in real-world applications is poised to make significant strides in enhancing our ability to detect concealed substances, diagnose medical conditions, and improve material analysis, ultimately contributing to a safer, healthier, and more innovative world.

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