NANO HIGHLIGHT
Materials authentication using nuclear quadrupole resonance spectroscopy

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Counterfeit, substandard, and/or contaminated pharmaceuticals, dietary supplements, and food items have emerged as a major worldwide health problem. High-value items such as packaged medicines, which are often sold online through untrusted supply chains, are particularly prone to fraud. The trade in such illicit medicines is worth tens of billions of dollars annually, and these products now account for about 20% of all illegal goods seized at national borders. This project is developing spectroscopy, data analysis, and machine learning techniques that exploit the nanoscale structure of materials in the solid state for authenticating their chemical composition. The overall goal is to enable users throughout the supply chain to reliably verify the identity and source of consumables (medicines, supplements, and food items) using portable and low-cost devices. The adoption of such authentication technology is expected to eventually have a major positive impact on public health by enhancing the security of the supply chain for consumables.

About 50% of all the atoms in the periodic table contain so-called quadrupolar nuclei that generate nuclear quadrupole resonance (NQR) spectra. These include common nuclei such as nitrogen (^{14}N) and chlorine (^{35}Cl and ^{37}Cl). The proposed authentication approach takes advantage of the sensitivity of such NQR spectra to the electric field gradient (EFG) tensor in the neighborhood of the quadrupolar nucleus, which in turn is primarily determined by the spatial distribution of valence electrons in the crystal lattice. Thus, such spectra are highly sensitive to chemical composition and physical properties, i.e., act as unique “chemical signatures” that are difficult to emulate or falsify. Our work has focused on i) understanding the fundamental physical principles that underlie the generation of such signatures; and ii) optimizing the sensors, measurement protocols, data analysis methods, and classification techniques to improve sensitivity and specificity, and thus the precision with which such signatures can be measured. Many of the resulting innovations are currently being commercialized by industrial partners.

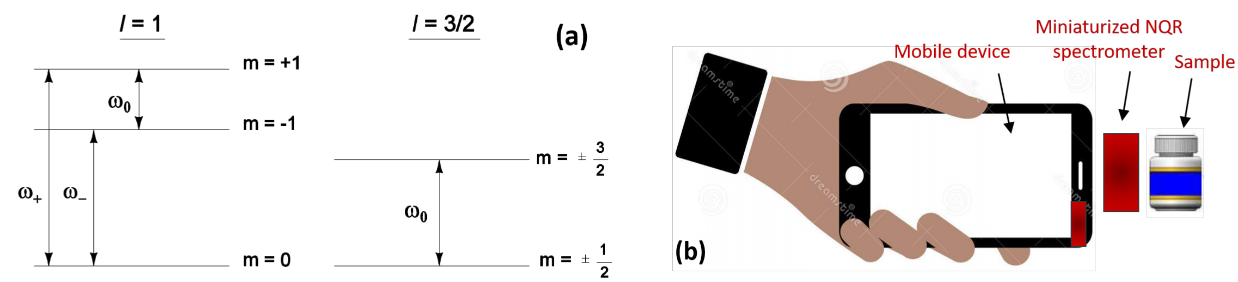

Figure 1: (a) Energy levels for quadrupolar nuclei (spins I = 1 and 3/2); NQR spectra are generated when an external magnetic field induces resonant transitions (coherences) between these stationary states. (b) Block diagram of a miniaturized device that uses the proposed NQR-based materials authentication approach.

References

[1] For further information about this project, visit https://sites.google.com/site/casecirc or email sxm833@case.edu.
[2] C. Chen, F. Zhang, J. Barras, K. Althoefer, S. Bhunia, and S. Mandal, Authentication of medicines using nuclear quadrupole resonance spectroscopy, *Trans. Computational Biology & Bioinformatics*, Vol. 13:3, pp. 417-430, 2016.
[3] C. Chen, F. Zhang, S. Bhunia, and S. Mandal, Broadband Quantitative NQR for Authentication of Vitamins and Dietary Supplements, *Journal of Magnetic Resonance*, Vol. 278, pp. 67-79, 2017.