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Simulation of nuclear quadrupole resonance for sensor probe optimization

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ABSTRACT

A simulation method to estimate the detection efficiency of nuclear quadrupole resonance (NQR) was proposed for optimizing a sensing probe operating at radio frequencies (RFs). It first calculates the transmitted magnetic field from the probe coil to the target sample. The nuclei make quadrupole resonance by it. We considered this nonlinear reaction to estimate NQR emission by the nuclei. Then the received NQR signal intensity from the sample at the probe coil. We calculated the efficiency by testing two different probe types (solenoid and gradiometer) and by changing the relative positions of the probe and sample. The simulation results were in good agreement with the experimental results.

1. Introduction

Nuclear quadrupole resonance (NQR) is a nuclear magnetic resonance phenomenon that can be used to identify materials present in samples. Unlike nuclear magnetic resonance (NMR), NQR has the advantage of not requiring a static magnetic field. NQR can be used in fields such as the detection of narcotics [1–4] and explosives [4–9]. Because NQR does not require an external static magnetic field, the device can be much smaller than that required for NMR, and stand-off detection is also easy. For efficient detection by NQR, the probe must be optimized for various parameters such as the inspection environment, the sample position, the probe size, *etc*. The overall sensitivity is affected greatly by the probe design. Many types of probes have been proposed, including gradiometer [10], helical surface [11], two-spiral flat [12], and meanderline surface types [13].

Nowadays there are many commercially available simulators for electromagnetic fields that allow the transmitted electromagnetic fields from the coils to be easily calculated. For simulation of the NQR signal detection, however, the magnetic radiation from the nucleus is excited by a radio frequency (RF) pulse, and its reception at the probe must also be modeled. Therefore, we have developed the simulator including all the processes from the RF pulse transmission to the NQR signal reception at the probe, while considering the nuclear excitation efficiency. Our method includes not only calculation of the transmitted magnetic field but also the received NQR signal from the excited samples. The developed simulator was evaluated by comparing its calculation results with the experimental results for the two cases of a solenoid probe and a gradiometer probe.

2. Basic theory of NQR signal detection by a probe coil

The NQR signal can be observed after the excitation of the quadrupolar nucleus if the nuclear spin number $I_S \geq 1$. The quadrupolar nucleus is excited by an RF pulse at the resonance frequency. A nucleus with $I_S=1$ such as ^{14}N has three resonance frequencies corresponding to the gaps between quadrupole energy levels. The NQR quantization axis is determined from consideration of the quadrupole principle axis system (QPAS) defined by the electric field gradient tensor at the quadrupolar nucleus [14–20]. The QPAS of a nucleus with $I_S=1$ is expressed in a manner such that three possible transitions are associated with each of the three orthogonal axes [21]. The quadrupolar nucleus is excited depending on the projections of RF pulses on the QPAS axis, and the RF magnetic field generated by the NQR transition is radiated along the same QPAS axes. The NQR signal is observed in the interlinkage direction against the RF field on the receiver coil. A probe coil can be made to serve as both the RF pulse transmitter and the NQR signal receiver when the divider circuits, such as the $\lambda/4$ circuit, are used. The coil is required to be light and small in order to be used in many configurations while inspecting the environment. This is the reason why the single coil antenna was used to transmit and receive the RF electromagnetic field in our simulator.

An outline of our simulation sequence is as follows. First the RF magnetic field was calculated at the sample position transmitted from the probe coil. Next, the quadrupolar nuclei in the sample were considered to be excited depending on the direction and magnitude of the RF magnetic field from the probe coil. Then, the RF magnetic field transmitted from the nuclei to the probe coil was estimated. Finally, the NQR signal received at the probe coil was calculated, where the NQR radiation field came from the interlinkage direction.

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2.1. RF magnetic field transmitted from a probe coil

The RF magnetic fields for causing transitions between the quadrupole energy levels of a nucleus were calculated by the Biot–Savart law. The magnetic field contribution $\Delta\vec{B}$ at a position $\vec{r}$ due to a segment $\Delta\vec{s}$ of a wire with current I is generally given by Eq. (1). In the case of a single loop coil as shown in Fig. 1, the current unit vector $\Delta\vec{s}$ at point P and the displacement vector $\vec{r}$ from point P to point Q are expressed by Eqs. (2) and (3), respectively, where R is the radius of the loop coil, and φ is the angle from the X-axis to the projection of vector $\vec{r}$ onto the X–Y plane. The magnetic field $\Delta\vec{B}$ at point Q from the segment $\Delta\vec{s}$ is derived in Eq. (4). The total magnetic field $\vec{B}$ at point Q induced by the current I is obtained from an integral of Eq. (4) along the complete current path. Thus the components of magnetic field along the X, Y, and Z directions at point Q from the loop coil are derived in Eqs. (5)–(7). For numerical calculation of these equations, the magnetic field contributed from the sufficiently small segments dividing the loop coil into small angle steps were calculated, and then were added together. The results defined the vector of the RF magnetic field transmitted from the coil.

$$\Delta\vec{B} = \frac{\mu_0 I}{4\pi}\frac{\Delta\vec{s}\times\vec{r}}{r^3} \tag{1}$$

$$\Delta\vec{s} = R\mathrm{d}\varphi(-\sin\varphi, \cos\varphi, 0) \tag{2}$$

$$\vec{r} = (x - R\cos\varphi, y - R\sin\varphi, z) \tag{3}$$

$$\Delta\vec{B}(x,y,z) = \frac{\mu_0 I}{4\pi}\frac{R\mathrm{d}\varphi}{\{(x-R\cos\varphi)^2+(y-R\sin\varphi)^2+z^2\}^{\frac{3}{2}}} \times \begin{pmatrix} z\cos\varphi \\ z\sin\varphi \\ R - x\cos\varphi - y\sin\varphi \end{pmatrix} \tag{4}$$

$$B_X(x,y,z) = \frac{\mu_0 I}{4\pi}\int_0^{2\pi}\frac{Rz\cos\varphi}{\{(x-R\cos\varphi)^2+(y-R\sin\varphi)^2+z^2\}^{3/2}}\mathrm{d}\varphi \tag{5}$$

$$B_Y(x,y,z) = \frac{\mu_0 I}{4\pi}\int_0^{2\pi}\frac{Rz\sin\varphi}{\{(x-R\cos\varphi)^2+(y-R\sin\varphi)^2+z^2\}^{3/2}}\mathrm{d}\varphi \tag{6}$$

$$B_Z(x,y,z) = \frac{\mu_0 I}{4\pi}\int_0^{2\pi}R\frac{R - x\cos\varphi - y\cos\varphi}{\{(x-R\cos\varphi)^2+(y-R\sin\varphi)^2+z^2\}^{3/2}}\mathrm{d}\varphi \tag{7}$$

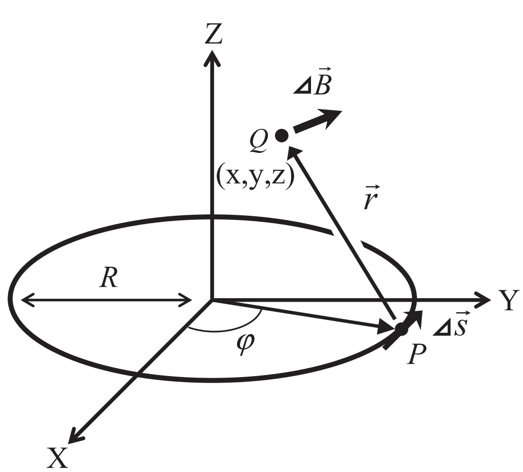

Fig. 1. Model for RF magnetic field calculation of a single loop coil. The magnetic field contribution $\Delta\vec{B}$ at point Q from the small element carrying current I at point P.

2.2. NQR magnetization in a powder sample

The quadrupolar nucleus can be excited by the projection of the RF magnetic field on the QPAS axis. Assuming that a quadrupolar nucleus is excited with an RF magnetic pulse having an intensity of B along the QPAS axis, the nuclear magnetization M_S is given by

$$M_s = C\sin(\gamma B\tau) \tag{8}$$

where γ is the gyromagnetic ratio of the nuclear spin, and τ is the duration time of one RF pulse, and C is the nuclear magnetization (J/T) from the N nuclei at thermal equilibrium, which is expressed by Eq. (9)

$$C = N\frac{\gamma h}{3}\left(\frac{h\nu}{kT}\right) \tag{9}$$

where h is Planck's constant, ν the resonance frequency, k is the Boltzmann factor, T is the temperature.

When the QPAS axis and the magnetic field form an angle θ, the nucleus magnetization M_S is given by Eq. (10), in which the nuclei excitation depends on the projection of the field on the QPAS axis.

$$C\sin(\gamma B\tau\cos\theta) \tag{10}$$

However, in many cases, hidden narcotics and explosives are found as powder in security checks. Each nuclear magnetization vector of the myriad nitrogen atoms in the powder sample has a random direction. We must take into account the summation of magnetizations of each nitrogen atom over all directions defined by the electric field gradient in the nucleus because the powder has no unique direction. Given that the QPAS axes of the spin are tilted by angles of θ' and ϕ' in polar coordinates, the total NQR magnetization M_T from the nitrogen atoms in a powder sample is given by the following Eqs. [14, 18–20, 22, 23]:

$$M_T = C\int_0^{\pi}\mathrm{d}\theta'\int_0^{2\pi}\mathrm{d}\phi'\sin\theta' C\sin[\gamma B\tau\cos\theta'] = C\sqrt{\frac{\pi}{2\gamma B\tau}}J_{3/2}(\gamma B\tau) \tag{11}$$

where $J_{3/2}$ is the Bessel function of order 3/2. From Eq. (11), magnetization of the powder sample is dominated by the Bessel function which depends on the magnetic field from the coil. In addition, the NQR magnetization in a small volume of a powder sample can reduce to a uniformly magnetized single dipole along the RF field direction from the coil [22].

2.3. NQR signal detected at a probe coil

The NQR magnetization field in a small volume of a powder sample is consistent with a single dipole field, the direction and magnitude of which depend on the transmitted magnetic field from a probe coil. The magnetization vector $\vec{M}_T$ has the same direction as the transmitted field. The NQR signal is related to the magnetic field received at the same probe coil from the dipole in the sample. The magnetic field $\vec{B}_D$ at a certain position is expressed using Eq. (12) as

$$B_D(M_T, r) = \frac{\mu_0}{4\pi r^3}(3(M_T,\hat{r})\hat{r} - M_T) \tag{12}$$

where r is the absolute value of the position vector $\vec{r}$ from the dipole, and $\hat{r}$ is the position unit vector.

The NQR signal received at the probe coil is regarded as an integrated value of the z-component of the magnetic field over the area inside the loop as shown in Fig. 2. In this simulation, the NQR signal received at the probe coil was numerically obtained by dividing the area inside the loop into small elements, calculating the magnetic field contributions from the dipole at each of the