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RESEARCH OF THE NUCLEAR QUADRUPOLE RESONANCE METHOD AND ITS APPLICATION FOR PRECISION TEMPERATURE MEASUREMENT AND OTHER RELEVANT FIELDS

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Annotation. This article describes the concept, essence, and application areas of nuclear quadrupole resonance. The purpose of this paper is to study the method of nuclear quadrupole resonance in devices for accurate temperature measurement. Special attention is paid to the study of the linear and nonlinear regions of this method temperature-frequency response. The simulation of a nuclear quadrupole thermometer in the *LabView* environment is performed. The results of the study to determine the accuracy of the measured temperature and recommendations for its improvement are given.

Keywords. Nuclear quadrupole resonance, precision temperature measurement, spectral line, spectroscopy, thermometer.

Nuclear quadrupole resonance (NQR) is the resonant absorption of radio waves based on the interaction of the electric field gradient of the crystal lattice of a substance and the nuclear quadrupole moment of the nucleus. This interaction causes the precession of the nuclei, the frequency of which depends on the gradient of the crystal lattice field, which in turn depends on the temperature.

Based on the NQR method, a cryostatic, broadband, fast-scanning VHF-band NQR spectrometer has been developed for use in the field of magnetic resonance imaging (MRI) [1]. In recent years, the NQR method has been increasingly used in various measuring equipment. On the basis of this method, sensors of temperature, magnetic field and pressure are manufactured. The high absolute accuracy of temperature measurement of 0.001 °C makes them indispensable for precision measurements. NQR thermometers do not require periodic verification and calibration and can be used as temperature standards, as well as on long-term orbiting space stations and in technological processes.

The essence of the NQR is as follows. The nuclear quadrupole moment is a value that shows the degree of deviation of the charge distribution over the surface of the nucleus from the spherical symmetry. A large number of periodic system nuclei possess such quadrupole moments. When the nuclear quadrupole interacts with the electric field of the electron shells of the molecules in the crystals, the orientation of the nuclear spins in a certain direction occurs. This orientation [2] is shown in Fig. 1 (b). If a radio frequency field is applied orthogonally to this direction, the frequency of which coincides with the frequency of transitions between levels, then the absorption of radio frequency power can be observed [2], as shown in Fig. 1 (c). The occurrence of the nuclear quadrupole moment [3] is shown in Figure 1 (a).

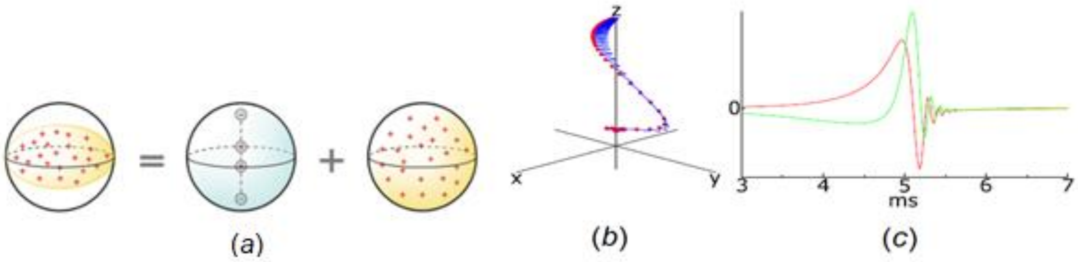


Figure 1 - The occurrence of the quadrupole moment (a), the precession of the nuclei (b), and the absorption of radio frequency power (c)

The ellipsoid distribution of the positive charge (left) can be considered as the sum of the quadrupole distribution (center) and the spherical distribution (right) [3]. The frequency of core precession and radio frequency power absorption is determined by the formula

$$f_{nqr} = eQq_{zz} \div (2 \times h), \tag{1}$$

where e is the electron charge;

Q – quadrupole moment of the core;

q_{zz} – components of the electric field gradient tensor;

$h = 6{,}62607015 \times 10^{-34} J \times s$ – Planck's constant.

KClO3 is usually used as a thermosensitive substance for temperature measurement using the NQR. However, its use in the temperature range above 300 °C is associated with some difficulties: the decomposition temperature of KClO3 is 370 °C; when using KClO3, its toxicity and explosion hazard should be taken into account; nonlinear nature of the temperature dependence of the 35Cl NQR frequency in KClO3. To increase the range of measured temperatures, as well as for more accurate measurements, Cu2O copper oxide will be used, which has a lower temperature coefficient and a higher stability than KClO3. To study the spectral line of the NQR of 65Cu nuclei, an NQR thermometer has been modeled in the *LabVIEW* simulation environment, the block diagram of which is shown in Figure 2.

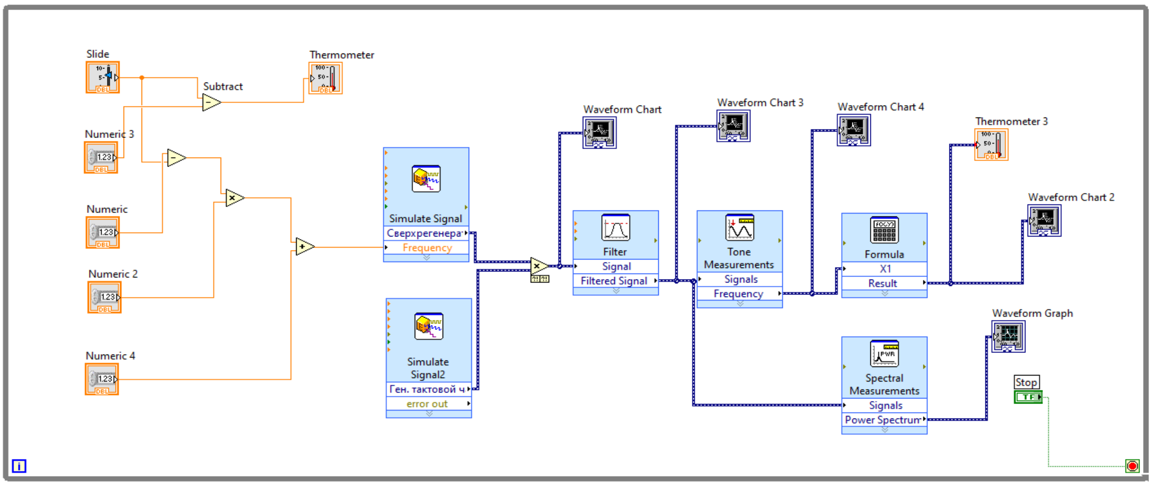


Figure 2 – Block diagram of an automatic NQR thermometer in the *LabVIEW* simulation environment

Figure 3 shows the shape of the NQR spectral line for 65Cu nuclei in Cu2O at T = 298 K.

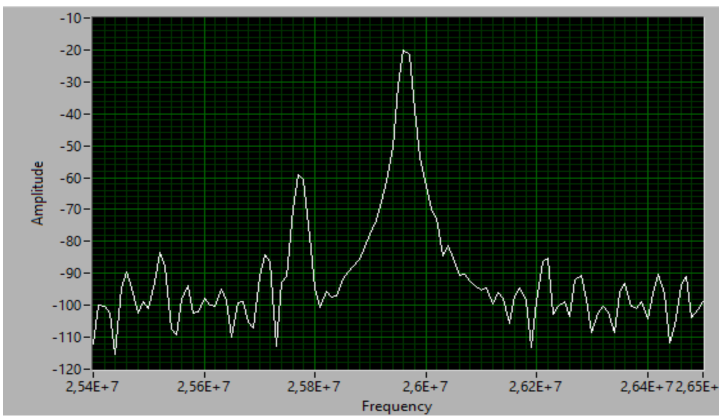
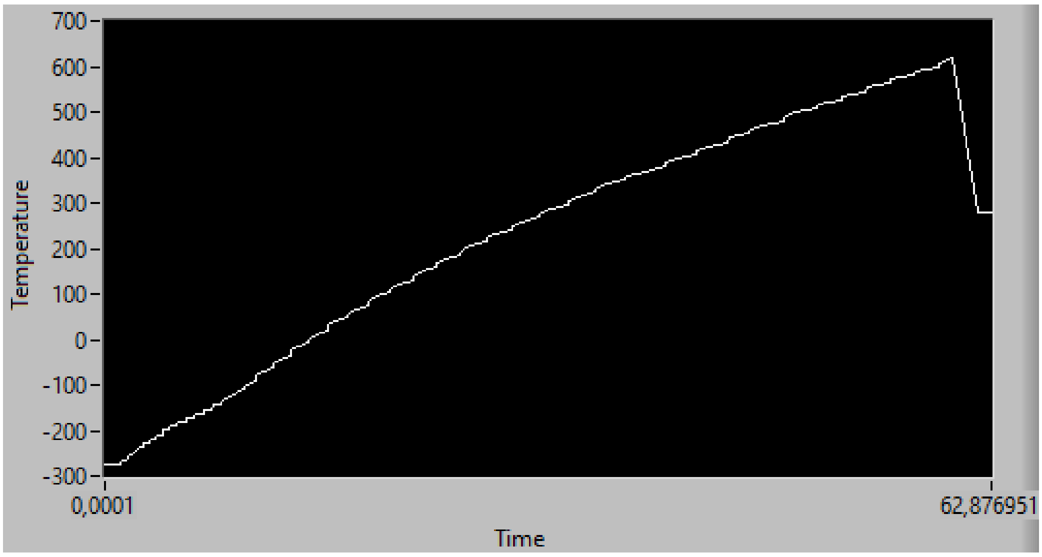


Figure 3 - The spectral line of the NQR for 65Cu nuclei

The figure shows that for the sample under study, the frequency of the NQR is approximately 26 MHz. Based on the block diagram from Fig. 2, a temperature-frequency response (TFR) has been constructed, covering the temperature range from 0 to 900 K. The constructed TFR is shown in Figure 4.



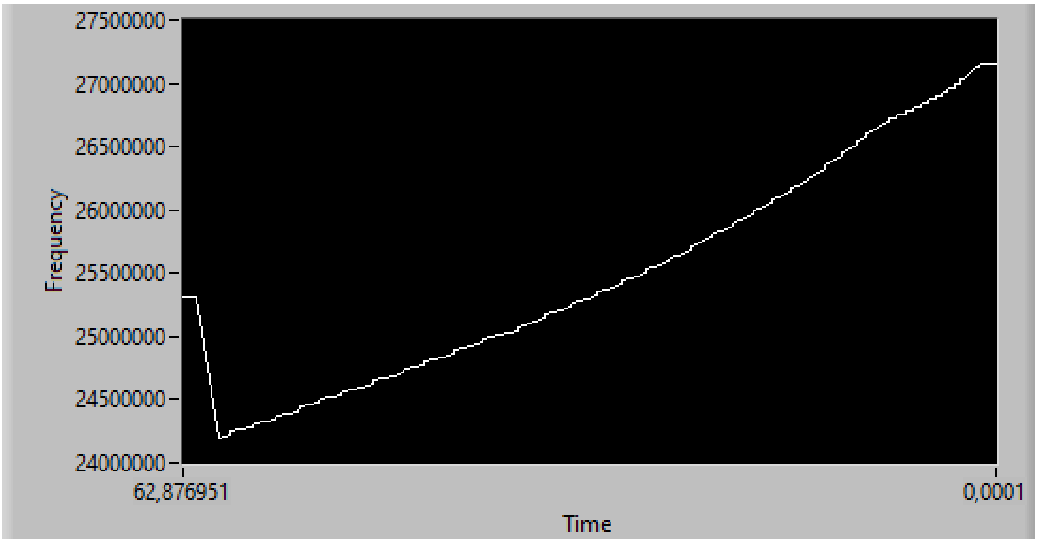


Fig. 4 – Temperature-frequency response for 65Cu cores in Cu2O

The graphs show that the TFR is almost linear in the temperature range from -273.15 °C (0 K) to 617.66 °C (890.816 K). With a further increase in temperature, a decrease in the characteristic is observed. To prevent the decline, it is proposed to apply a more advanced algorithm for converting frequency to temperature and using a more accurate bandpass filter. Also, to reduce the measurement error, it is proposed to transfer the super-regenerator to the regenerative mode.

References

1. *Scharfetter, H. A cryostatic, fast scanning, wideband NQR spectrometer for the VHF range / H. Scharfetter, M. Bödenler, D. Narnhofer // Journal of Magnetic Resonance. – 2018. – №286. – P. 148–157.*

2. *Hibe, Y. Rapid survey of nuclear quadrupole resonance by broadband excitation with comb modulation and dual-mode acquisition / Y. Hibe, Y. Noda, K. Takegoshi, K. Takeda // Physical Chemistry Chemical Physics. – 2020. – Vol.22, iss.1. – P. 1-22.*

3. *Miller, J. B. Explosives detection with nuclear quadrupole resonance / J. B. Miller, G. A. Barrall // American Scientist. – 2005. – Vol.93. P. 50–57.*