

Design of a Multicoupled Loop-Gap Resonator Used for Pulsed Electron Paramagnetic Resonance Measurements

Yoshihiko Sakamoto, Hiroshi Hirata, and Mitsuhiro Ono

Abstract—The purpose of the present paper is to establish a method of design for a multicoupled loop-gap resonator used for pulsed electron paramagnetic resonance measurements. For the design of resonator characteristics, the method has an advantage of a systematic approach without iterative calculations. In this design, the number of loop-gap resonators used is first determined from the pass band required as the specifications of the resonator. To satisfy the specifications, electrical parameters of an equivalent circuit and the dimensions of the resonator are estimated. By the proposed method, a prototype resonator which has the operation frequency of 1.3 GHz is designed and fabricated. For the prototype resonator, the characteristics of the return loss agree with the required ones. As a result, the validity of the design method is experimentally confirmed.

I. INTRODUCTION

A PULSED electron paramagnetic resonance (EPR) method is a spectroscopy for the observation of unpaired electrons [1], [2]. In this spectroscopy, a microwave resonator is used for the supply of magnetic energy in radio frequency to a sample. Moreover, the resonator detects EPR signals such as free induction decay (FID) and electron spin echo (ESE). Fig. 1 illustrates the schematic diagram of a pulsed EPR instrument. In the pulsed EPR measurements, a measured sample is positioned in the loop-gap resonator close to the coupling coil. By applying microwave pulses to the sample, relaxation of magnetization for the sample is observed. The microwave pulses which have durations less than several 10 nsec are usually generated. The broadband characteristics of the resonator are necessary to apply the microwave pulses to the sample. In addition, the resonator should be sensitive to the measurements of the EPR signals. A rectangular cavity which operates in the TE_{102} mode has been widely used for the pulsed EPR measurements in X and K bands [3]. Furthermore, a loop-gap resonator (LGR) has been used for the EPR measurements [3]–[6]. These resonators generally have a high quality factor which is not suitable for transmitting the “short” microwave pulses. It is necessary to reduce the quality factor by inserting a material, which has large dielectric loss, into the resonator. Because of this dielectric loss, the sensitivity of the spectrometer is decreased. To overcome this problem, a multicoupled loop-gap resonator (MLGR) has been proposed [7].

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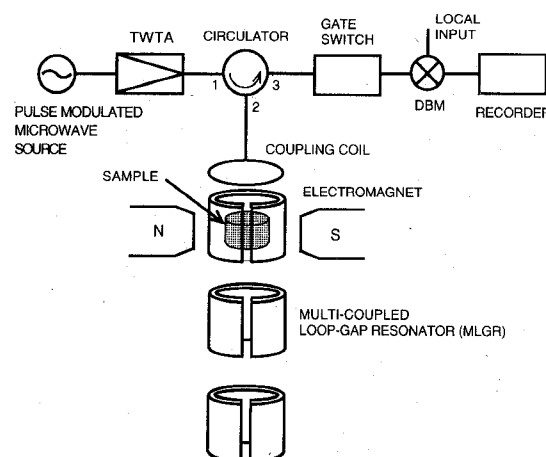


Fig. 1. Schematic diagram of pulsed EPR instruments including the multi-coupled loop-gap resonator (MLGR).

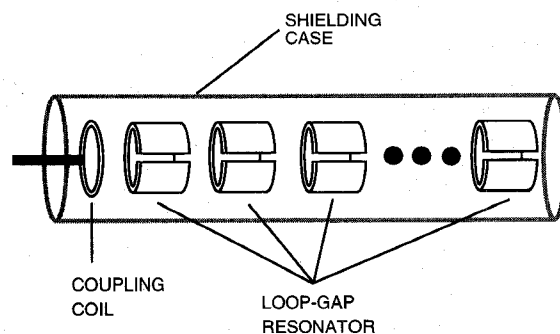


Fig. 2. Scheme of the multicoupled loop-gap resonator (MLGR).

The MLGR has the features of broadband characteristics and low loss. Fig. 2 shows the structure of the MLGR. This resonator consists of the LGR elements which are magnetically connected to each other. The pass band of the MLGR is formed by the superposition of the resonances of the LGR's. To make good use of the MLGR in the pulsed EPR measurements, a method of design for the MLGR is necessary. The characteristics of the MLGR in the frequency domain will be designed by appropriately determining the coupling coefficients among the LGR elements. Although the LGR has been analyzed [8], [9], a practical design method for the MLGR has not been established yet.

The purpose of the present paper is to establish a method of design for the MLGR used for the pulsed EPR measurements.

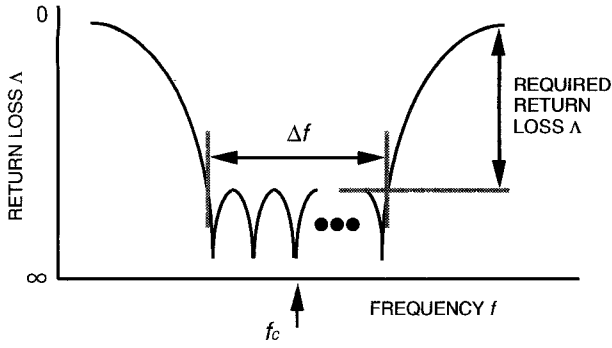


Fig. 3. Characteristics of the return loss at the pass band of the multicoupled loop-gap resonator (MLGR): Λ indicates the required return loss, Δf the bandwidth of the pass band, and f_c the center frequency of the pass band.

First, the structure and the principle of the MLGR are explained. Second, a method for designing the characteristics of the MLGR is described. Next, a prototype resonator designed by the proposed method is fabricated. For the prototype resonator, experimental verification of the design method is carried out. As a result, the validity of the design method will be confirmed.

II. THE PRINCIPLE OF A MULTICOUPLD LOOP-GAP RESONATOR

The LGR elements used for the MLGR are magnetically coupled with each other. As shown in Fig. 2, these elements are shielded by a conductive cylinder which is coaxial with the LGR elements. The MLGR is connected to the spectrometer through a coupling coil. For the LGR, the gap corresponds to a capacitor, and the rounded conductive plate corresponds to an inductor. Consequently, these electrical elements form a resonance circuit. The magnetic coupling of the LGR elements is one thousand times large as the electrostatic coupling of them (For this brief estimation, see Appendix A). Thus, the electrostatic coupling is neglected in this paper. The pass band of the MLGR is formed by the superposition of the resonances of the LGR's. Fig. 3 illustrates a schematic pass band, i.e., the characteristics of the return loss of the MLGR in the frequency domain. In Fig. 3, Λ indicates the required return loss, Δf the bandwidth of the pass band, and f_c the center frequency of the pass band. To supply the microwave pulse to the sample, the input impedance of the MLGR should be matched to that of the transmission line connected to the spectrometer. In other words, the return loss Λ has to be big enough to measure FID or ESE. Moreover, the bandwidth of the pass band Δf should be broad enough to transmit the microwave pulses. This is because the spectra of the pulses are broad.

When the voltage reflection coefficient between the MLGR and the transmission line vanishes, the microwave pulse is efficiently transmitted to the MLGR. Then, the return loss will be infinite because of no reflection. Between the MLGR and the transmission line, the return loss Λ and the voltage reflection coefficient Γ are defined by

$$\Lambda = 20 \log_{10} \frac{1}{\Gamma} \text{ dB}, \quad (1)$$

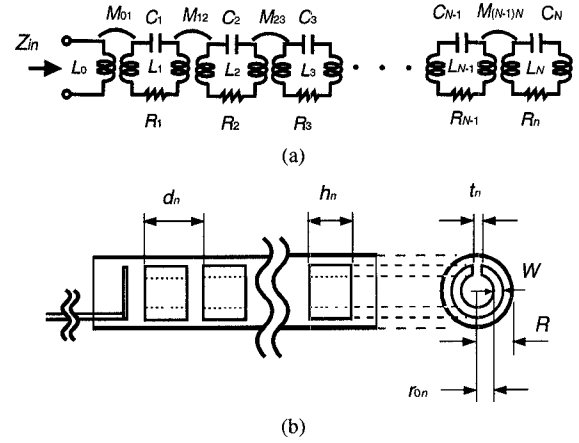


Fig. 4. (a) An equivalent circuit of the multicoupled loop-gap resonator (MLGR). (b) The notation of the dimensions for the MLGR: d_n indicates the distance between the neighboring elements (n th and $n+1$ th), h_n the height of n th loop-gap resonator, t_n the gap distance, W the gap width (the thickness of the plate which forms the LGR), r_{0n} the inner radius, and R the radius of the shielding case.

$$\Gamma = \frac{Z_{in} - Z_0}{Z_{in} + Z_0} \quad (2)$$

where Z_{in} and Z_0 refer to the input impedance of the MLGR and the characteristic impedance of the transmission line, respectively [10]. Fig. 4 illustrates the equivalent circuit and the notation of the dimensions of the MLGR [8], [11]. For this equivalent circuit, the input impedance of the MLGR Z_{in} is given by

$$Z_{in} = j\omega L_0 + \frac{(\omega M_{01})^2}{Z_1 + \frac{(\omega M_{12})^2}{Z_2 + \frac{(\omega M_{23})^2}{Z_3 + \dots + \frac{[\omega M_{(n-1)n}]^2}{Z_n}}} \quad (3)$$

$$Z_n = R_n + j \left(\omega L_n - \frac{1}{\omega C_n} \right) \quad (4)$$

where ω and L_0 are the angular frequency and the inductance of the coupling coil, respectively. Using the coupling coefficient $k_{(n-1)n}$ between the $n-1$ th and n th inductances, L_{n-1} and L_n , the mutual inductance $M_{(n-1)n}$ is denoted by $k_{(n-1)n}(L_{n-1}L_n)^{1/2}$.

For brief comparison of sensitivity of the MLGR to the LGR with lossy dielectric material, the reader may refer to the Appendix B. To design the characteristics of the MLGR, it is necessary to solve the following problems: i) determination of the minimum number of the LGR elements in advance and ii) estimation of the dimensions of the MLGR.

III. METHOD OF DESIGN

A. Goal of Design

Before introducing the design method of the MLGR, the specifications of the resonator should be cleared. Table I lists the parameters given as the specifications. The radius of a shielding case R is limited with the distance between pole pieces of DC electromagnets used in the measurements. The

TABLE I
THE SPECIFICATIONS OF THE MULTICOUPLD LOOP-GAP RESONATOR

Required return loss Λ	30.0 dB
Center frequency f	1300.0 MHz
Bandwidth Δf	0.4 MHz
Radius of a shield case R	15.0 mm
Volume of the LGR element V	5.0 cm ³

TABLE II
THE DIMENSIONS AND THE ELECTRICAL
PARAMETERS OF THE PROTOTYPE RESONATOR

Heights h_1	7.95 mm
h_2	8.77 mm
Inner radii r_{01}	12.7 mm
r_{02}	12.7 mm
Gap distances t_1	4.13x10 ⁻² mm
t_2	4.35x10 ⁻² mm
Thickness of the conductive plate W	0.5 mm
Distances d_1	1.14 mm
d_2	25.6 mm
Coupling coefficients k_{01}	0.1305
k_{12}	7.99x10 ⁻⁴
Unloaded quality factor Q_{0n}	1295

volume of the LGR elements V is taken into account the size of measured samples. The center frequency of the pass band f_c depends on the operation frequency of the spectrometer. The bandwidth of the pass band Δf is dependent on the duration of the microwave pulses generated in the EPR measurements. From these specifications, the goal of design is to determine the dimensions of the MLGR which satisfy the required specifications. Table II shows the parameters of the resonator which is finally determined in this design.

B. Procedure of Design

The design method has to introduce the solution of the two problems by a systematic procedure. To satisfy the required specifications, the dimensions listed in Table II are estimated by the following procedure:

Step 1: The specifications shown in Table I are given.

Step 2: The return loss of the MLGR is estimated from the required signal-to-noise ratio S/N and the characteristics of the spectrometer.

Step 3: The number of the LGR elements N is determined from the bandwidth Δf and the center frequency f_c of the pass band.

Step 4: The dimensions and the coupling coefficients of the LGR elements are estimated to satisfy the return loss characteristics of the pass band.

Step 5: The distances between the LGR elements are determined from the coupling coefficients estimated in Step 4.

The calculation of Step 2 is revealed in the Appendix C, because this estimation is not the scope of this design. The details of each estimation from Step 3 to Step 5 are described in the following.

IV. THE MINIMUM NUMBER OF THE LOOP-GAP RESONATORS

The EPR signals will be buried in the reflection microwave power from the MLGR, if the return loss is too small to detect the signals. Thereby, it is important to design the return loss of the resonator. The minimum number of the LGR elements N which satisfies the required characteristics of the pass band should be determined. To obtain the minimum number N , the return loss is treated as superposition for each element. Moreover, the MLGR is assumed to be matched with the characteristic impedance of the transmission line at the frequencies of $\Delta f/N$ intervals in the pass band. Under these assumptions, the return loss at the center frequency is larger than that value at the edges of the pass band. Hence, the required return loss will be obtained through the pass band, if the required value of the return loss is satisfied at the edges. At the intermediate frequency between 1st and 2nd lower resonance frequencies, the return loss Λ_{edge} is given by

$$\Lambda_{edge} = \zeta \left[\frac{\Delta f}{2(N-1)} \right] + \sum_{i=1}^{N-1} \zeta \left[\frac{(2i-1)\Delta f}{2(N-1)} \right] \quad (5)$$

where $\zeta(\delta f)$ is the function of the return loss at the frequency shifted δf from n th resonance frequency f_{0n} . The function $\zeta(\delta f)$ is obtained from (1)–(4). Using the relation in (5), the minimum number of the LGR elements is determined. In this calculation, the unloaded quality factor of the LGR elements Q_{0n} is necessary to compute the function ζ .

The rough dimensions of the LGR are first determined to estimate the quality factor. A procedure for giving the rough dimensions of the LGR is as follows: 1) The distance of the gap t and the inner radius of the LGR r_0 are assumed. The radius r_0 should be smaller than that of the shield case. 2) The height of the LGR h is computed from the volume V . 3) The resonance frequency of the LGR f_r is calculated by

$$f_r = \frac{1}{2\pi\sqrt{L_n C_n}}, \quad (6)$$

$$L_n = \frac{\pi r_0^2 \mu_0}{h \left(1 + \frac{\Delta h}{h} \right) \left[1 + \frac{r_0^2}{R^2 - (r_0 + W)^2} \right]} \quad (7)$$

$$C_n = \frac{\epsilon_0 W h \left(1 + \frac{\Delta W}{W} \right)}{t} \quad (8)$$

where C_n is the capacitance formed by the gap of n th LGR element, μ_0 the permeability of the vacuum, ϵ_0 the permittivity of the vacuum, Δh the equivalent length extension due to magnetic fringing fields, and ΔW the equivalent gap width extension due to the electric fringing fields. By introducing these parameters, Δh and ΔW , the lumped inductance and capacitance can be treated by only uniform fields without the consideration of the magnetic and electric fringing fields. The value of Δh is obtained from the total energy of the magnetic fringing field at both ends of the resonator. The value of ΔW is calculated from a fringing capacitance of the gap. The reader may refer to the details of the estimations for Δh and ΔW in [9]. 4) When the calculated frequency f_r agrees the center frequency f_c , go to 5). Otherwise, the width of the LGR t

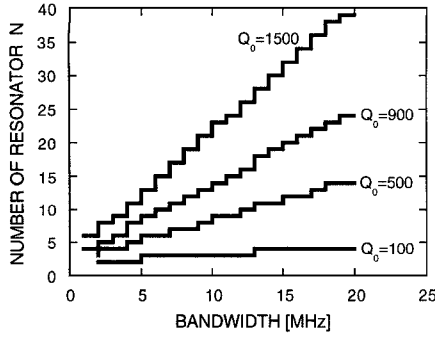


Fig. 5. The minimum number of the loop-gap resonators as a function of the bandwidth at the return loss of 30 dB.

is increased/decreased, and go back to 2). 5) The unloaded quality factor Q_{0n} is calculated by

$$\frac{1}{Q_{0n}} = \frac{1}{Q_s} + \frac{1}{Q_c}, \quad (9)$$

$$Q_s = \frac{r_0}{\delta} \frac{(1 + \rho) \left(1 + \frac{\Delta h}{h}\right)}{1 + \left(1 + \frac{W}{r_0} + \frac{R}{r_0} + \frac{R^2}{U'_{01} h r_0}\right) \rho^2} \quad (10)$$

$$Q_c = \frac{1.7 \times 10^5 t}{f^{3/2} \epsilon_0 W^2 \left(1 + \frac{\Delta W}{W}\right)} \quad (11)$$

where U'_{01} is the lowest root of the Bessel function of first kind and order zero $J'_0(x) = 0$, t the distance of the gap, f the operation frequency, δ the skin depth, and [9]

$$\rho = \frac{r_0^2}{R^2 - (r_0 + W)^2}. \quad (12)$$

For example, Fig. 5 shows the calculated results of the minimum number of the LGR elements. In this calculation, the return loss of 30 dB and the center frequency of 1.3 GHz were assumed. Since the dimensions of the LGR were not taken into account, the value of the quality factor was given as the parameter of this estimation.

V. ESTIMATION OF THE DIMENSIONS AND THE COUPLING COEFFICIENTS OF THE LGR ELEMENTS

To obtain the required pass band, the resonance frequencies and the coupling coefficients of the LGR elements have to be appropriately determined. By Newton–Raphson method, the resonance frequencies f_{0n} and the coupling coefficients $k_{(n-1)n}$ are obtained by solving the simultaneous equations

$$\begin{cases} \text{Re } \Gamma[f_{0n}, k_{(n-1)n}] = 0 \\ \text{Im } \Gamma[f_{0n}, k_{(n-1)n}] = 0 \end{cases} \quad (n = 1 - N). \quad (13)$$

When the input impedance of the MLGR is matched to the transmission line, the voltage reflection coefficient Γ vanishes at the frequencies of f_{0n} . Since the coefficient Γ is a complex number, the real and the imaginary parts of that are zeros, respectively. After solving (13), to satisfy the electrical conditions, i.e., f_{0n} and Q_{0n} , the gap distance t_n and the height h_n are corrected by solving the simultaneous

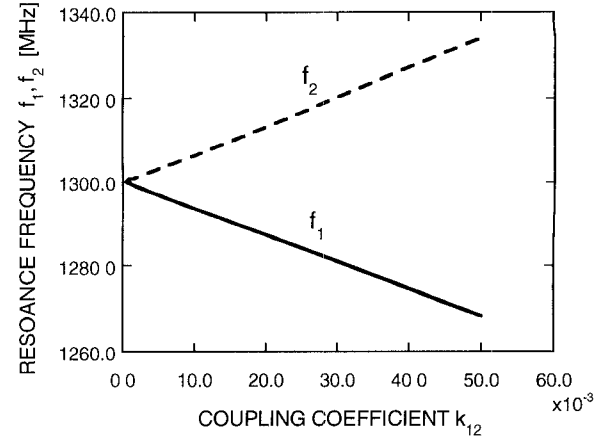


Fig. 6. Relation between the resonance frequencies and the coupling coefficient k_{12} .

equations numerically for (6) and (9). In this correction, Newton–Raphson method is also used as the case of (13). The dimensions of the LGR elements and the coupling coefficients are obtained perfectly by the procedure described here.

VI. THE DISTANCES BETWEEN THE LGR ELEMENTS

To realize the coupling coefficients calculated in the previous section, the distances between the LGR elements have to be determined. To explain the procedure for estimating the distances of each LGR element, it is focused on the MLGR which consists of two LGR elements. The resonance characteristics of that MLGR mainly depend on the coupling coefficient k_{12} between the two elements. Fig. 6 shows an example of the calculated resonance frequencies of the MLGR as a function of the coupling coefficient k_{12} . As shown in Fig. 6, the difference between the resonance frequencies, f_1 and f_2 , is proportional to the coupling coefficient k_{12} . When the resonance frequencies are measured as a function of the distance d_2 , the coupling coefficient k_{12} will be related to the distance d_2 .

The procedure for estimating the distances between the LGR elements is described as follows: 1) After carrying out Steps 1–4, the unloaded quality factor Q_{0n} and the resonance frequency f_{0n} of each element are measured; 2) for the fabricated MLGR formed by the two elements, the resonance frequencies, f_1 and f_2 , are measured as a function of the distance d_2 ; 3) from the relation between the resonance frequencies and the distance, the coupling coefficient k_{12} is calculated by solving (13) by Newton–Raphson method as a function of the distance; 4) to realize the necessary coupling coefficient k_{12} , the distance d_2 is determined from the relation between k_{12} and d_2 . Since the coupling coefficients between the neighboring elements are necessary, this procedure is applicable to the case of more than two elements.

VII. EXPERIMENTAL VERIFICATION OF THE DESIGN METHOD AND DISCUSSIONS

To discuss the validity of the proposed method, a prototype resonator was designed and fabricated. For the prototype resonator, the specifications in Table I were given in advance.

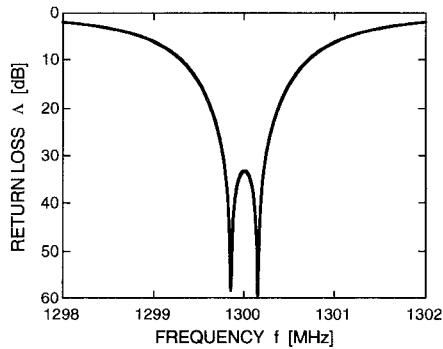


Fig. 7. Numerically calculated characteristics of the return loss for the prototype resonator.

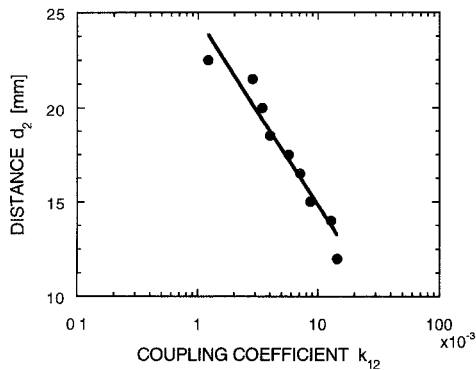


Fig. 8. Relation between the coupling coefficient k_{12} and the distance d_2 : Closed circles denote the coupling coefficients estimated from the experimental results of the resonance frequencies and the distance d_2 . The solid line was drawn by the method of the least square from the experimentally obtained values of the coupling coefficients.

The EPR measurements need more broad characteristics of the pass band in practice. However, the resonator which has a relatively narrow pass band is focused in the present paper. This is because the purpose of this section is to examine the validity of the design method. Table II shows the dimensions and the electrical parameters of the resonator designed by the proposed method. In this design, the number of the LGR elements is estimated to be 2 from Fig. 5. The prototype resonator was made by thin copper plates which is 0.5 mm in thickness. Fig. 7 shows the calculated characteristics of the return loss for the prototype resonator. To obtain the characteristics shown in Fig. 7, it is necessary that the estimated coupling coefficient k_{12} is precisely produced. On the basis of the procedure described in Section VI, the relation between k_{12} and d_2 was obtained. Fig. 8 shows the coupling coefficient k_{12} as a function of the distance d_2 . Closed circles denote the coupling coefficients estimated from the experimental results of the resonance frequencies and the distance d_2 . From the experimentally obtained values of the coupling coefficients, the solid line was drawn by the method of the least square. For the prototype resonator, the distance d_2 was determined from the solid line shown in Fig. 8. The distance d_1 was also estimated by the same way as the case of d_2 .

Fig. 9 indicates the measured characteristics of the return loss for the prototype resonator before and after corrections.

TABLE III
THE DISTANCES BETWEEN THE LOOP-GAP RESONATORS
AND THE COUPLING COIL OF THE PROTOTYPE RESONATOR

Distance	Designed	Adjusted
d_1	1.14 mm	1.0 mm
d_2	25.6 mm	28.5 mm

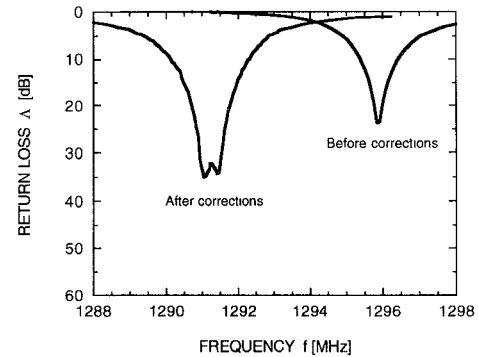


Fig. 9. Measured characteristics of the return loss for the prototype resonator: the center frequency of the pass band f_c is 1291.1 MHz, and the bandwidth which satisfies the return loss of 30 dB Δf 0.628 MHz. The measured return loss before corrections is also shown in addition to the characteristics after corrections.

Since the coupling coefficients determined at Step 4 were not obtained, only the resonance of one element appeared in the return loss characteristics before corrections. Consequently, corrections of the distances between the elements were necessary to obtain the required bandwidth. After adjusting the distances, the center frequency of the pass band f_c was 1291.2 MHz, and the bandwidth of that Δf was 0.628 MHz. The measured bandwidth is broader than that of Fig. 7. This is because the unloaded quality factors of the LGR's used were approximately 960, which is 73% of the theoretically estimated value of those. For this reason, adjustment of the distance was necessary to obtain the required characteristics. Table III shows the designed and adjusted distances between the LGR's and the coupling coil of the prototype resonator. The adjusted distances, d_1 and d_2 , had the errors of approximately 10% from the designed ones. Although there is a slight difference in the bandwidth, the required specifications were obtained in the prototype resonator. From this fact, it follows that the proposed method is applicable to the design of the MLGR.

VIII. SUMMARY

To design the MLGR used for the pulsed EPR measurements, the procedure for estimating the dimensions of the MLGR was described. The proposed method was actually applied to the design of the prototype MLGR. For the prototype resonator, the measured characteristics of the return loss practically agreed with the specifications given in advance. As a result, the validity of the proposed method was experimentally confirmed.

Although the number of gaps is different, the flow of current is circular. Since the flow of current is similar, the magnetic field in the neighborhood of the LGR element is not changed drastically. Thereby, the model described here will be accurate, as long as the electrostatic coupling is negligible in comparison to the magnetic coupling.

APPENDIX A

RELATIVE MAGNITUDE OF THE MAGNETIC COUPLING AND THE ELECTROSTATIC COUPLING

Relative magnitude of the magnetic coupling between the LGR elements is briefly estimated in comparison to the electrostatic coupling of them. Fig. 10(a) illustrates the geometry of two LGR elements. The magnitude of the magnetic coupling is represented by the coupling coefficient of the mutual inductance between these elements. When the LGR element is 26 mm in diameter and 10 mm in height, the self inductances, L_1 and L_2 , become 2.9×10^{-8} H. If the distance between each center of the elements d is 25 mm, the mutual inductance M is 2.1×10^{-9} H. For these values, the coupling coefficient is computed by

$$k = M / \sqrt{L_1 L_2},$$

$$= 7.24 \times 10^{-2}. \quad (14)$$

On the other hand, the magnitude of the electrostatic coupling is very small in comparison to the magnetic coupling. When there is the potential difference of 1 V for the gap of the element 1, the charges $\pm Q$ occur on both the ends of the gap as shown in Fig. 10(b). Although the charges distribute in the ends of the gap, these charges are assumed to be a dipole. The intensity of the electric field generated by the dipole E_{dipole} is calculated by

$$|E_{dipole}| = \frac{Q(t_1/2)}{2\pi\epsilon_0(t_1^2 + d^2)^{3/2}} \quad (15)$$

where t_1 is the gap width, ϵ_0 the permittivity of the vacuum. When the electrode area of the condenser formed by the gap is 5×10^{-6} mm² and the gap width is 0.1 mm, the produced charge Q is 8.58×10^{-13} C. From (15), the electric field intensity E_{dipole} becomes 0.1 V/m at the center of the element 2. When the gap width of the element 2 t_2 is also 0.1 mm, the potential difference at the center of the element 2 becomes 10^{-5} V. When the electrostatic coupling coefficient is defined by the ratio of the potential differences, that coefficient is 10^{-5} in this geometry. As a result, the magnitude of the magnetic coupling is 10^3 times as large as the electrostatic coupling. The effect of the electrostatic coupling is negligible in the MLGR.

APPENDIX B

BRIEF ESTIMATION OF SENSITIVITY FOR THE MLGR AND THE DUMPED LGR

To compare the sensitivities of the MLGR and a LGR having low quality factor, i.e., a dumped LGR, the output voltages of them were calculated. For the MLGR and the dumped LGR, Fig. 11(a) and (b) illustrates the equivalent circuit including the voltage source of the ESR signal. Fig. 11(c) shows the

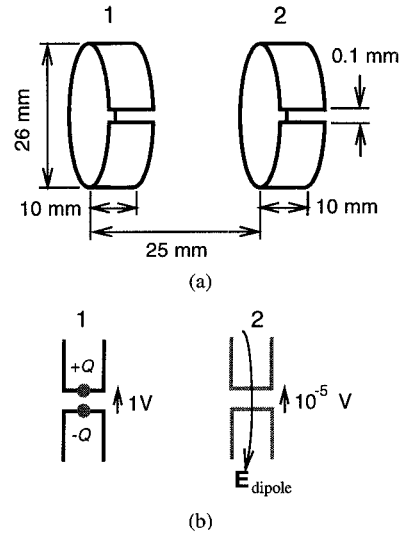


Fig. 10. Calculation model of the magnitudes of the magnetic and electrostatic couplings. (a) Geometry of the loop-gap resonators and (b) dipole model for estimating the magnitude of the electrostatic coupling.

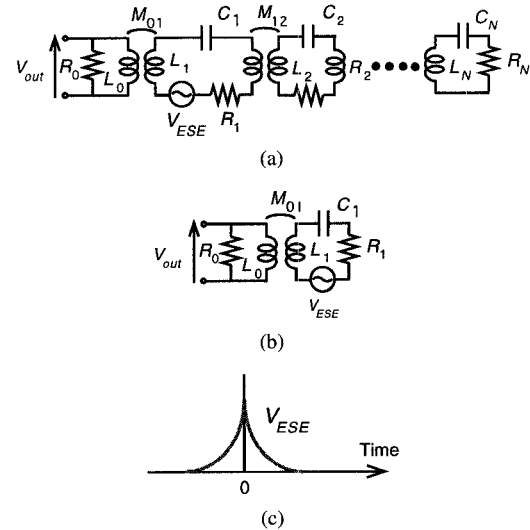


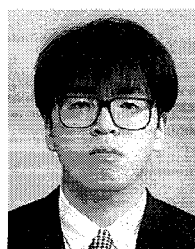
Fig. 11. (a) Equivalent circuit of the multicoupled loop-gap resonator and (b) equivalent circuit of the loop-gap resonator which has low quality factor, and (c) scheme of the voltage source V_{ESE} of electron spin echo.

envelope of the ESR signal which is a function of time t and given by

$$V_{ESE} = \begin{cases} e^{t/\tau} \sin \omega_0 t & (t \leq 0) \\ e^{t/\tau} \sin \omega_0 t & (t > 0) \end{cases} \quad (16)$$

where τ is the time constant of the ESE signal and ω_0 the angular frequency of carrier. For these circuit, the output voltage V_{out} concerned with the voltage source was estimated. The circuit parameters listed in Table IV were used in this calculation. Fig. 12 shows the relative output voltages of the dumped LGR and the MLGR in $n = 1 - 5$. All MLGR have the return loss of 30 dB in the pass band as broad as possible. Moreover, the MLGR was assumed to be constructed by the LGR elements which have the quality factor of 250. On the other hand, it was assumed that the dumped LGR has the quality factor of 100. From Fig. 12, it seems that the MLGR

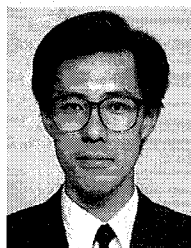
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