S-band electron spin resonance spectroscopy using a short-circuited coplanar waveguide resonator

Subhadip Roy 1, Pronoy Das and Chiranjib Mitra 1  

Department of Physical Sciences, Indian Institute of Science Education And Research Kolkata, India 1  
These authors have contributed equally to the work.  
E-mail: chiranjib@iiserkol.ac.in  

Keywords: coplanar waveguide, optical lithography, electron spin resonance, planar resonator

Abstract

In this work, we study the development of a coplanar waveguide (CPW) resonator and its use in an electron spin resonance (ESR) spectrometer. The CPW resonator is designed to operate in S-band (2–4 GHz), with a short circuit configuration leading to miniaturization. It is so constructed such that it has a characteristic impedance of 50 ohms. The resonator supports quasi-TEM mode of propagation owing to its uniplanar nature, demanding detailed electromagnetic simulation. The design parameters and the electromagnetic field distribution are obtained from the simulation. The resonator is fabricated using optical lithography with a rapid prototyping technique. The characteristic response of the resonator is measured by coupling it to a Vector Network Analyzer (VNA). The ESR absorption spectrum of free radical 2,2-diphenyl-1-picrylhydrazyl (DPPH) is captured by using this resonator in reflection geometry. The microwave magnetic field distribution at the sample position is investigated. The ascertained value of Lande g-factor is consistent with that reported in the literature. Spin sensitivity of the order of $10^{15}$ spins/ gauss is achieved upon using this resonator at room temperature. The quality factor of this resonator is found to be low and this makes it suitable for use in a Pulsed ESR spectrometer.

1. Introduction

Planar microwave resonators have versatile applications ranging from their use in dielectric measurement setup [1, 2], magnetic resonance experiments [3–6] and as gas sensors [7, 8]. These resonators are generally based on two popular varieties of the planar transmission line, namely, microstrip line [9, 10] and coplanar waveguide (CPW) [11]. For magnetic resonance experiments, CPW based resonators are quite suitable. Localized resonant microwave magnetic field concentrating structures based on the need of the experiment, can be easily realized by using this planar transmission line technology [12].

A CPW resonator, being a uniplanar structure [13], is easier to fabricate as compared to a microstrip line resonator. CPW resonators can be made compact by either meandering or short-circuiting. In particular, it is easier to short-circuit the signal to the ground in a CPW resonator, whereas the substrate has to be drilled and metallic vias have to be used in case of microstripline resonator [14]. Rapid PCB prototyping technology can be easily applied for fabricating such resonators [15]. These resonators can be suitably designed for integration into any type of cryostat including the closed cycle cryostats [12]. Superconducting microwave resonators can also be fabricated based on CPW transmission line [16, 17].

A CPW transmission line supports quasi-TEM mode of propagation [18], which necessitates detailed electromagnetic simulation for extracting fabrication parameters for a CPW resonator as closed form design equations are non-existent. The simulation setup for designing a CPW based resonator is not very well documented in existing literature. In this work, we elaborately describe the simulation process used for making the short-circuited CPW resonator. Further we show that the structure can be well adapted for rapid prototyping [10]. The designed short-circuited CPW resonator is characterized and used in a custom-built room temperature ESR spectrometer. The spectrometer is used to record the ESR spectrum of a standard free radical.
2. The short-circuited CPW resonator

2.1. Geometry
The planar resonator is based on an ungrounded coplanar waveguide transmission line. An ungrounded CPW transmission line consists of a dielectric of thickness $h$ and three conductive traces of thickness $t$ on top of it without any metallization on the bottom surface. The central conductive trace is the signal line of width $s$, and the other two traces are ground lines which are at separation $w$ with respect to the signal trace. The cross-sectional view of an ungrounded CPW transmission line is shown in Figure 1.

In the resonator design, the signal and ground traces have been short-circuited. The length of the resonator $l$ is chosen so that $l \approx \frac{\lambda}{4}$, where $\lambda$ is the guided wavelength corresponding to the resonance frequency $f_0$ of the resonator. A short-circuit resonator, being quarter wavelength, is shorter than a open-circuit resonator which is half-wavelength. Therefore, a short circuit resonator leads to miniaturization. The gap $g$ separates the resonator and the feed line. The degree of coupling of the resonator to the external microwave source is controlled by $g$.

Figure 2 depicts the top view of the resonator.

2.2. Simulation
The electromagnetic simulation of the resonator has been carried out with CST Microwave Studio (MWS) and ANSYS High Frequency Structure Simulator (HFSS) software. The resonator is designed to resonate at $f_0 = 3.5\ \text{GHz}$. The microwave laminate used is AD1000 (Rogers Corporation) which has a dielectric constant of 10.7 and loss tangent of 0.0023 at 10 GHz. The conductor is modelled as 17.5 $\mu$m thick copper, with electrical conductivity value as predefined in the simulation software [19].

Analytical expressions were evaluated to obtain the initial values for the design parameters [20]. Parameter tuning was done in CST MWS initially to extract the design specifications. The length $l$ was tuned to achieve $f_0$. The parameters $s$ and $w$ were optimized to obtain the characteristic impedance of 50 $\Omega$. The coupling gap $g$ was...
adjusted to obtain a reasonable quality factor. The structure was excited by a waveguide port centered about the signal trace. The waveguide port was square in shape and had a side length of $k$, where $k = 3(s + 2w)$. Open boundary condition is used on the side of the port, while radiating open (add space) boundary condition is used on all other sides of the resonator. The final design parameters were extracted from CST MWS and are tabulated in Table 1. These parameters are used in fabrication. A comparative simulation of the resonator was setup in HFSS using the parameters listed in Table 1. The structure was excited by a waveguide port similarly as that has been described for CST MWS. The simulated response of the resonator obtained from both the simulation software has been compared with that of measured response in Section 2.3. While a time domain solver has been used in CST MWS, HFSS uses a frequency-domain solver, leading to a slight difference in results.

Table 1. Final design parameters.

| Parameter                  | Value  |
|----------------------------|--------|
| Length of resonator ($l$)  | 8.25 mm|
| Coupling Gap ($g$)         | 0.33 mm|
| Signal trace Width ($s$)   | 0.9 mm |
| Gap between signal and ground traces ($w$) | 0.5 mm |
| Length of the feedline     | 3 mm   |

Figure 5. Laser printed photomask used in the fabrication.
Figure 6. Fabricated short-circuited CPW resonator.

Figure 7. Comparison of simulated and measured $S_{11}$ responses for 10 dBm input port power.

Figure 8. Simulated and measured frequency sweeps of the resonator on the Smith chart.
distribution of the microwave electric field and magnetic field of the resonator for port power of 10 dBm obtained from the CST MWS simulation has been shown in figures 3 and 4.

2.3. Fabrication and characterization
The resonator has been fabricated on the microwave laminate using optical lithography, followed by chemical etching. The photomask is printed on tracing paper using a standard 1200 DPI Laser printer [10]. A solution of de-ionized water, concentrated hydrochloric acid (35%) and hydrogen peroxide (30%), mixed in the ratio of 7:2:1, is used as a fast etchant. The overall process is cheap and fast, allowing for rapid prototyping and testing. Figures 5 and 6 show the used photomask and fabricated resonator, respectively. A vector network analyzer (VNA) (ZVA24, Rohde Schwarz) is used to measure the reflection coefficient response of the fabricated resonator in dB. The frequency response circle is recorded on the Smith chart. The measured responses are compared with the simulation results in figures 7 and 8. The measured response of the fabricated resonator is found to be closer to critical coupling and is sharper when compared to simulated results.
3. Continuous wave electron spin resonance spectroscopy

The fabricated resonator is used as a component of a custom-built electron spin resonance (ESR) spectrometer. The resonator is coupled to the VNA port using semi-rigid transmission line and is placed at the center of an electromagnet (GMW 3473-70). The electromagnet provides the Zeeman field, \( B_0 \). The placement of the resonator is done such that the external magnetic field is perpendicular to the resonator’s microwave magnetic field. The magnetic field is controlled using a programmable power supply (Sorensen SGA60X83D). Calibration of the external magnetic field against the supplied current is done using a gaussmeter (DTM-151, GMW Associates). The illustration of the room temperature ESR setup is shown in figure 9.

3 mg of powder sample 2,2-diphenyl-1-picrylhydrazyl (DPPH) wrapped in Teflon tape is placed near the shorted end of the resonator, which is the region of the maximum magnetic field as deduced from the simulation. Figures 2 and 10 indicate the sample placement region and the magnetic field distribution in that region respectively. The power supply of the magnet and the VNA is synchronously controlled through a custom designed digital interface. An averaging of 25 and port power of 10 dBm are set in the VNA. The ESR signal is manifested as a change in the resonant dip of the S11 response of the resonator loaded with sample, while the \( B_0 \) field is swept at room temperature. A plot of this resonant dip as a function of \( B_0 \) yields the ESR spectrum as shown in figure 11. Spectral acquisition time is 17 minutes.

4. Results

The measured resonance frequency of the resonator is 3.424 GHz which slightly differs from the simulations. The simulation run in CST MWS predicted a resonance frequency of 3.494 GHz and that in HFSS indicated a resonance frequency of 3.46 GHz. The \( S_{11} \) response is sharper for the fabricated resonator when compared to the simulated results. The fabricated resonator has a quality factor of 70. The calculated g-factor of DPPH is 2.05, which is consistent when compared with ESR spectrometers which use planar resonators [17]. Measured ESR linewidth is 4.6 Gauss. The line shape of the spectrum is Lorentzian. The signal to noise ratio (SNR) of the custom-built spectrometer for DPPH sample is 437 [21].

Spin sensitivity is defined [22–24] as

\[
\text{Sensitivity (spins/ gauss)} = \frac{\text{No. of spins present in the sample}}{\text{SNR} \times \text{linewidth}}
\]

3 mg of DPPH sample has \( 4.59 \times 10^{18} \) spins [25]. The achieved spin sensitivity at room temperature is \( 2.3 \times 10^{15} \) spins/ gauss.

5. Conclusion

The ESR spectrometer based on this resonator captures the spectra of the free radical DPPH with a good SNR and decent spin sensitivity. A detailed electromagnetic simulation procedure has been described which can be adapted for any kind of CPW based resonators. The rapid prototyping technique employed here can be used to fabricate different planar transmission line based resonators with reasonable accuracy. The low Q factor of the resonator makes it suitable for use in Pulsed ESR spectrometer.

\[\text{Figure 11. ESR spectrum of DPPH. Redline denotes the Lorentz fit.}\]
Acknowledgments

Authors acknowledge Ministry of Human Resource Development (MHRD), Government of India & Science and Engineering Research Board (SERB) (grant no. - EMR/2016/007950) for funding this work. S. R. acknowledges Council of Scientific & Industrial Research (CSIR), India for research fellowship. The authors thank Prof. Bhaskar Gupta, Department of Electronics & Telecommunication Engineering, Jadavpur University for providing simulation facilities. The authors are grateful to Rogers Corporation, USA for free samples of the microwave laminate.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

ORCID iDs

Subhadip Roy @ https://orcid.org/0000-0002-0815-590X
Chiranjib Mitra @ https://orcid.org/0000-0003-3067-2548

References

[1] Sofin R G S and Aiyer R C 2005 Measurement of Dielectric Constant using a Microwave Microstrip Ring Resonator (MMRR) at 10GHz irrespective of the type of overlay Microwave Opt. Technol. Lett. 47 11–4
[2] Peterson R I. and Drayton R F 2002 A CPW T- resonator technique for electrical characterization of microwave substrates IEEE Microwave Wireless Compon. Lett. 12 90–2
[3] Narkowicz R, Suter D and Stonies R 2005 Planar microresonators for EPR experiments J. Magn. Reson. 175 275284
[4] Clausen C, Dressel M and Scheffler M 2015 Optimization of coplanar waveguide resonators for ESR studies on metals Journal of Physics: Conf. Series 592 012146
[5] Glowinski H, Schmidt M, Goscianska I, Ansermet J-P and Dubowik J 2014 Coplanar waveguide based ferromagnetic resonance in ultrathin film magnetic nanostructures: impact of conducting layers J. Appl. Phys. 116 053901
[6] Zhang S, Oliver S A, Israeloff N E, Widom A and Vittoria C 1997 Ferromagnetic resonance of micrometer-sized samples J. Appl. Phys. 81 4307
[7] Bailly G, Harrabi A, Rossignol J, Michel M, Stuerga D and Pribetich P 2017 Microstrip spiral resonator for microwave-based gas sensing IEEE Sensors Letters 1 4500404
[8] Draganoma M, Gremier K, Dubuc D, Bary L, Planas R, Fourn E and Flahaut E 2007 Millimeter wave carbon nanotube gas sensor J. Appl. Phys. 101 106103
[9] Maloratsky L G 2000 Reviewing the basics of microstrip lines Microwaves & RF 39 79–88
[10] Roy S, Saha S, Sarkar J and Mitra C 2020 Development of planar microstrip resonators for electron spin resonance spectroscopy Eur. Phys. J. Appl. Phys. 90 31001
[11] Wen C 1969 Coplanar waveguide: a surface strip transmission line suitable for nonreciprocal gyromagnetic device applications IEEE Trans. Microwave Theory Tech. 17 1087–90
[12] Rahim M J, Leibleiter T, Bothner D, Krellner C, Krellner C, Kleiner R, Dressel M and Scheffler M 2016 Metallic coplanar resonators optimized for low-temperature measurements J. Phys. D: Appl. Phys. 49 395501
[13] Hettak K and Stubbs M G 2001 The use of uniplanar technology to reduce microwave circuit size Phys. J. 4302–16
[14] Gopinath A 1979 A comparison of coplanar waveguide and microstrip for GaAs monolithic integrated circuits Microwave Journal of Physics: Conf. Series 592 012146
[15] PETLE Woven Fiberglass
[16] Bailly G, Harrabi A, Rossignol J, Michel M, Stuerga D and Pribetich P 2017 Microstrip spiral resonator for microwave-based gas sensing IEEE Sensors Letters 1 4500404
[17] Martin S Z, Rostas A M, Heidinger L, Spengler N, Meissner M V, MacKinnon N, Schleicher E, Weber S and Korvink J G 2016 A microwave resonator integrated on a polymer microfluidic chip J. Magn. Reson. 270 106–75
[18] Assenheimer H M 2013 Introduction to Electron Spin Resonance (Berlin: Springer Science+Business Media, LLC) pp. 74–6
[19] Blank A, Twig V and Ishay Y 2017 Recent trends in high spin sensitivity magnetic resonance J. Magn. Reson. 280 20–9
[20] Yang X, Babakhani A and Single-Chip A 2015 Electron Paramagnetic Resonance Transceiver in 0.13-μm SiGe BiCMOS IEEE Trans. Microwave Theory Tech. 63 3727–35
[21] Silitia M A and Suleiman Y M 1975 The use of DPPH as a standard for the measurement of G-values Radiat. Eff. 27 111–2

IOP Publishing IOP SciNotes 1 (2020) 035202 S Roy et al