The International Journal of E-Learning and Educational Technologies in the Digital Media (IJEETDM) 2(2): 73-79
The Society of Digital Information and Wireless Communications (SDIWC), Apr - 2016 (ISSN: 2410-0439)

Modeling of Compositional Analysis for Liquid Solvents in Microfluidic Channel Using Split Ball Resonator

Tahir Ejaz, Hamood Ur Rahman, Adnan Masood, Tahir Zaidi, Muhammad Naveed
National University of Sciences and Technology (NUST),
Islamabad, Pakistan.
tahir.ejaz@ceme.nust.edu.pk, hamood@ceme.nust.edu.pk, am34029@yahoo.com,
tahirzaidi@ceme.nust.edu.pk, naveednust@gmail.com

ABSTRACT

A novel structure to determine volume fraction of liquids present in microfluidic channel/tube with high accuracy is being presented. Such determination also known as compositional analysis is widely used in chemical, bio-medical, pharmaceutical and other applications/industries. Monitoring/measuring volume fraction of liquid in mixture through conventional methods is a time consuming task. Some quantity of liquid is also wasted in this process. Microwave technique using resonance method has eased such a task. Proposed split ball resonator structure removes these problems. Proposed structure can detect/sense complex permittivity of liquid mixture in microfluidic channel/tube. Basing upon this structure a model is being proposed to determine volume fraction of liquids. This model utilizes measured electrical quantities i.e. resonant frequency and quality factor of proposed structure. Compositional analysis of liquids can be done within fraction of a second without wasting time and material through proposed system.

KEYWORDS

Compositional analysis, complex permittivity, microfluidic channel, split-ball resonator, volume fraction.

1 INTRODUCTION

Microwave techniques to determine/sense permittivity of materials are well established. Determination of permittivity is essential in processing of food, rubber, plastic, ceramic etc [1]. Food grading [2], design improvement, quality and control of products [3], study of microwave effects on biological tissues [4] are some other application areas where knowledge regarding permittivity is important. Numerous microwave techniques [3], [5], [6] are available for such characterization. These techniques can be classified amongst reflection, transmission and resonant methods [3], [5]-[7]. These classes are further grouped under numerous methods. Each of these methods can characterize materials of certain class depending upon loss factor of material [3], [8].

Resonant methods provide most accurate information regarding permittivity of low loss materials [1], [3], [7]. Resonators of different types have been utilized for this purpose [6]. Dielectric resonator, coaxial surface-wave resonator and split resonators are different resonant methods [6], [9] and employ various structures/arrangements for measurements. Compositional analysis of liquids and material characterization has been performed with high accuracy while utilizing split-ring resonator [10]-[14]. Split-ball resonator (SBR) [15], [16] possesses high quality (Q) factor which is an important parameter for permittivity measurement. In this work a novel structure based upon SBR has been proposed for compositional analysis of liquid solvents in microfluidic channel/tube. Resonant frequency and Q factor of structure can be measured with the help of vector network analyzer (VNA). A mathematical model is also introduced to determine volume fraction of liquids in mixture.

2 COMPLEX PERMITTIVITY OF LIQUID SOLVENTS

Dielectric materials have a tendency to store energy when placed in electric field [17]-[19]. This energy storage capability is known as permittivity. When it is compared with free space it is known as relative permittivity. Relative permittivity (ε_r^*) or permittivity of a material is a complex quantity and comprises of two parts. Real part ($\varepsilon_r^{'}$) signifies energy storage capability of material whereas imaginary part ($\varepsilon_r^{''}$) represents lossy part of permittivity. These parameters are dependent upon temperature, frequency, relative humidity etc [9]. Complex permittivity of material is represented as:

$$\varepsilon_r^* = \varepsilon_r^{'} - j\varepsilon_r^{''} \quad (1)$$

Value of imaginary part signifies rate at which stored energy is dissipated. Depending upon value/nature of imaginary part materials are classified amongst low, medium and high loss. Ratio between $\varepsilon_r^{''}$ and $\varepsilon_r^{'}$ is known as loss tangent, tan delta or dissipation factor *D* and given as [8], [9]:

$$\tan\delta = D = \frac{1}{Q} = \frac{\varepsilon_r^{''}}{\varepsilon_r^{'}} \quad (2)$$

When a dielectric material is subjected to alternating electromagnetic field, its electric dipoles interact with applied field. This response is known as dielectric relaxation [9]. Due to this material behavior both $\varepsilon_r^{'}$ and $\varepsilon_r^{''}$ show variation against frequency. Such behavior has been modeled by researchers and represents material behavior with changing frequency of applied field [6], [9]. Simplest is known as Single-Debye response [6], [9] and is given as:

$$\varepsilon_r^* = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + j\,{}^{f}/{}_{f_r}} \quad (3)$$

where ε_s is known as static permittivity (value of $\varepsilon_r^{'}$ at very low frequencies) while ε_∞ is known as high-frequency permittivity limit (value of $\varepsilon_r^{'}$ at very high frequencies), f_r is relaxation frequency and f is frequency of applied electromagnetic wave.

When a liquid mixture is prepared, resultant permittivity or effective permittivity ε_{eff} can be predicted keeping in view various factors. These include chemical and physical properties of solvents, volume fraction of each solvent, environmental conditions, microstructure details, material polarizability etc. A lot of work has been produced to model effective permittivity [6], [20]-[22]. Some simple formulas based upon volume fraction of two solvents/composites [6] are presented below:

Looyenga's formula:

$$\varepsilon_{eff}^{\frac{1}{3}} = f_1\varepsilon_1^{\frac{1}{3}} + (1 - f_1)\varepsilon_0^{\frac{1}{3}} \quad (4)$$

Beer's formula:

$$\varepsilon_{eff}^{\frac{1}{2}} = f_1\varepsilon_1^{\frac{1}{2}} + (1 - f_1)\varepsilon_0^{\frac{1}{2}} \quad (5)$$

Lichtenecher's formula:

$$\ln\varepsilon_{eff} = f_1\ln\varepsilon_1 + (1 - f_1)\ln\varepsilon_0 \quad (6)$$

where permittivity of host and inclusion materials are given by ε_0 and ε_1 respectively with volume fraction f_1 of inclusion material. Other worked out formulas using parameters described above are also available [20]-[22].

3 SPLIT BALL RESONATOR STRUCTURE

Side and top view of a spherical SBR is shown in Figure 1. Spherical ball can be made using any good conducing metal. Gap of ball serves as capacitance whereas body acts as inductance. It acts as resonator with a specific resonant frequency f_0 value of which will depend upon radius/diameter (r or d) of spherical ball and gap (t). Resonator will also exhibit Q factor which will depend upon material properties and dimensions of SBR. For its utility it has to be placed within some enclosed metallic structure i.e. cavity/shield [23]-[25] over a loss-less base [26]. Shield not only provides means for utilizing SBR but also enhances Q factor besides reducing effects of external noise/interference [26], [27]. SBR enclosed in a spherical shield with air in-between is shown in Figure 2.

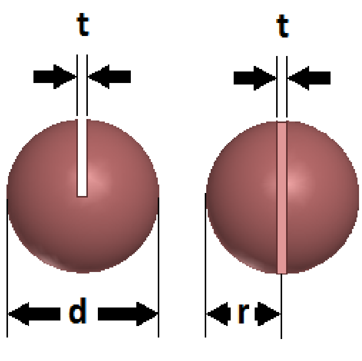


Figure 1. Side and top view of split-ball resonator

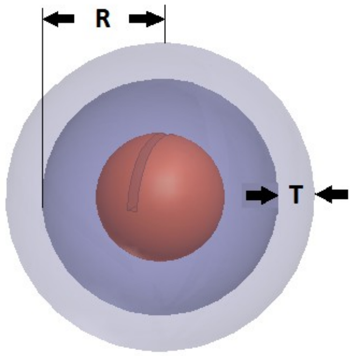


Figure 2. SBR enclosed in spherical shield.

In Figure 2 a suitable metallic shield [28] of internal radius R and thickness T has been utilized to enclose SBR. Structure of different dimensions was simulated in Ansoft HFSS [29] to find output parameters i.e. resonant frequency and Q factor. SBR was fabricated using copper while shield was made of aluminum [28]. Simulation was designed in two phases. In first phase, SBR dimension r was varied from 11 mm to 18 mm with 1 mm step size and t from 1.5 mm to 3.5 mm with 0.2 mm step size, while shield dimensions R and T were kept fixed at 30 mm and 7 mm respectively. In second phase, shield dimension R was varied from 20 mm to 30 mm with step size 1 mm and T was varied from 7 mm to 12 mm with step size 1 mm, while SBR dimension *r* and *t* were kept fixed at 13 mm and 2.3 mm respectively. This was done to study effects of dimensional variations on output parameters [27] and obtain an optimized design. It yielded a total of 88 and 66 simulations in first and second phase respectively. Table 1 shows few results of these simulations pertaining to extreme values of SBR and shield radii.

Table 1. SBR Simulation

Dimensions (mm)				**Resonant Frequency (GHz)**	**Q Factor**
r	11	t	1.5	4.444	10206.20
r	11	t	1.9	4.332	8521.02
r	11	t	2.3	4.373	9817.77
r	11	t	2.7	4.279	9004.88
r	11	t	3.1	4.342	9867.69
r	11	t	3.5	4.278	9431.91
r	18	t	1.5	3.331	3746.99
r	18	t	1.9	3.329	3739.29
r	18	t	2.3	3.326	3751.81
r	18	t	2.7	3.325	3742.71
r	18	t	3.1	3.324	3732.04
r	18	t	3.5	3.322	3733.10
R	20	T	7	4.144	6821.86
R	20	T	8	4.167	6752.82
R	20	T	9	4.116	6735.57
R	20	T	10	4.182	7045.48
R	20	T	11	4.128	6949.44
R	20	T	12	4.132	6868.36
R	30	T	7	3.557	12419.37
R	30	T	8	3.548	11910.12
R	30	T	9	3.551	11856.09
R	30	T	10	3.567	11720.68
R	30	T	11	3.551	11793.08
R	30	T	12	3.554	12266.15

It was observed that highest Q factor was achieved for SBR dimensions r = 13 mm and t = 2.3 mm and shield dimensions R = 30 mm and T = 7 mm. However, resonant frequency of shield itself was found to be very close to SBR structure which could result in interference/distortion. Furthermore thickness of shield in this case was relatively low to reject external noise. Therefore simulated data was explored to finalize a design with reasonably high Q factor and minimum distortion. Final design parameters of SBR structure had dimensions r = 13 mm, t = 2.3 mm, R = 23 mm and T = 12 mm. This yielded resonant frequency of 3.930 GHz and 8000.22 as Q factor.

4 PERMITTIVITY SENSING CAPABILITY – SBR STRUCTURE

Simulation was designed to study permittivity sensing capability of the designed SBR structure. A microfluidic channel in shape of glass tube was utilized. This tube was meant to accommodate liquid mixture within SBR gap. External diameter of tube was kept 2 mm whereas 1.6 mm was internal diameter. Length of tube was 40 mm with one end closed. Tube was placed 2 mm above base of SBR gap where electric field intensity was maximum. SBR structure containing air inside microfluidic channel was simulated. It yielded resonant frequency of 4.015 GHz with Q factor measuring 9236.56.

Microfluidic channel was filled with a test liquid for studying permittivity sensing capabilities of structure. A SBR structure with test liquid in microfluidic channel is shown in Figure 3. Real part of permittivity was linearly varied from 1 to 90, whereas loss factor was logarithmically varied from 0.001 to 10. Patterns for permittivity sensing capability were obtained through a 450 solutions simulation.

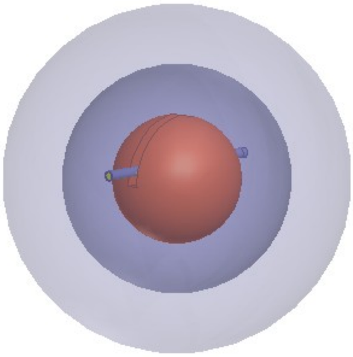
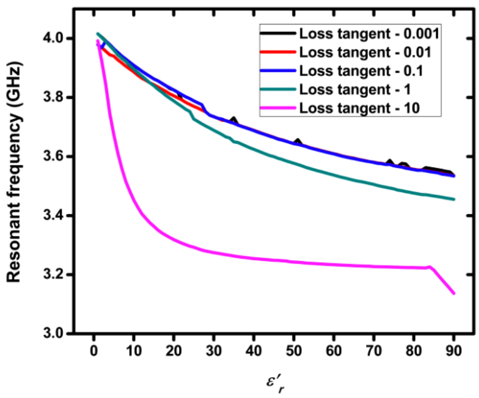
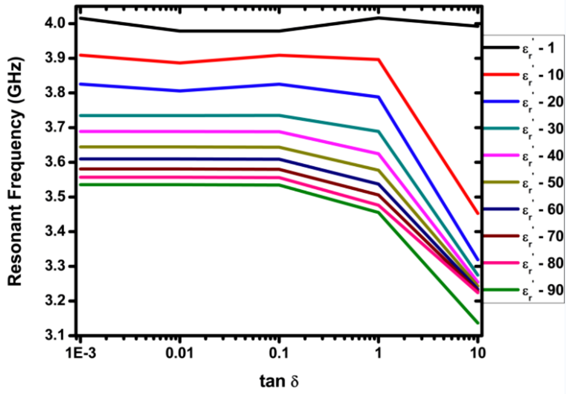


Figure. 3. SBR structure with test liquid in microfluidic channel.

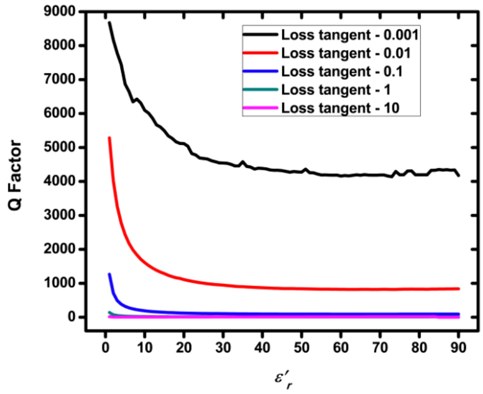
Figure 4 shows system response when permittivity of test liquid was varied. Figure 4a shows that resonant frequency of SBR structure varied gradually within entire range of ε_r' for low loss material, whereas it initially varied sharply against ε_r' for high loss material and changed gradually thereafter. Figure 4b shows that resonant frequency remained almost unaffected when loss factor was varied up-to a value of 1. However, resonant frequency changed as loss factor was varied beyond this value. Figure 4c shows that high values of Q factor was obtained for low loss materials within entire range of ε_r' whereas medium and high loss materials yielded low values of Q factor with very small variations. Figure 4d showed that Q factor varied over larger ranges of loss factor for lower values of ε_r' whereas such variation was noticed within limited range for higher values of ε_r'. It was also observed that resonant frequency and Q factor were very sensitive for low values of ε_r' and loss factor. All of these observations lead to conclude that such a structure could perform high resolution compositional analysis of low loss liquid solvents contained in microfluidic channel.



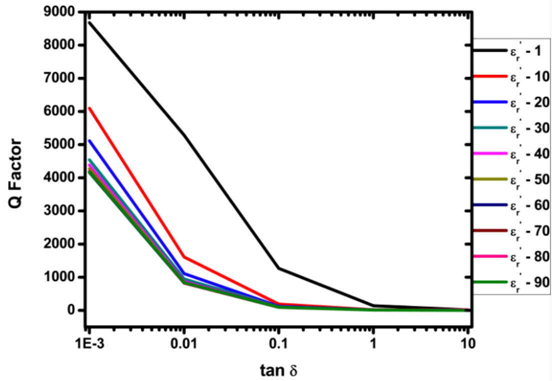
(a) Resonant frequency versus ε_r'



(b) Resonant frequency versus loss factor



(c) Q factor versus ε_r'



(d) Q factor versus loss factor

Figure. 4. Permittivity sensing by SBR structure

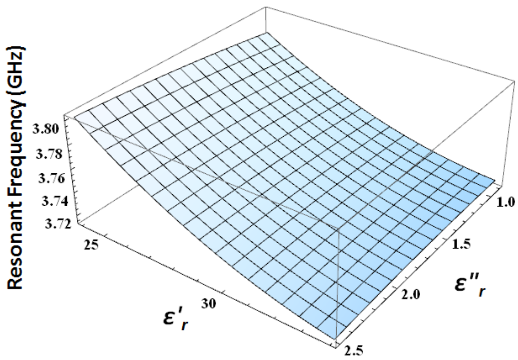
5 MODELING

A model depicting compositional analysis was finally designed utilizing SBR structure as described above. Ethanol and methanol were selected for developing a model. Permittivity of ethanol and methanol were found to be 24.86 - j2.46 and 33.60 - j0.99 respectively at 0.1 GHz [30]. These two liquids when mixed could yield resultant permittivity depending upon volume fraction and other properties of liquids in mixture. System response in terms of resonant frequency and Q factor were essential for analysis. For depicting compositional analysis of these two liquids, permittivity of test liquid inside microfluidic channel was varied. During simulation real part (ε_r') was varied from 24 to 34 with step size 1 whereas imaginary part (ε_r'') was varied from 0.9 to 2.5 with step size 0.1. This yielded 187 solutions. Response of both parameters i.e. resonant frequency and Q factor were observed. Data was exported for evaluation with Wolfram's Mathematica [31]. System response is shown in Figure 5. Second order equations derived for calculating responses using both parts of permittivities are given as:

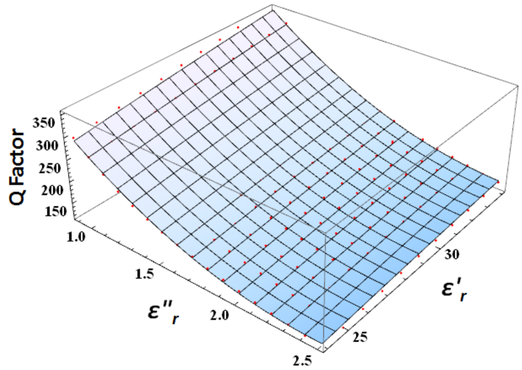
$$f_0(\mathrm{GHz}) = 4.334040 - 0.036621\varepsilon_r' + 0.000541{\varepsilon_r'}^2 + 0.056842\varepsilon_r'' - 0.003155{\varepsilon_r''}^2 - 0.001440\varepsilon_r'\varepsilon_r'' \quad (7)$$

$$Q = 310.979108 + 12.026181\varepsilon_r' - 0.065011{\varepsilon_r'}^2 - 310.368586\varepsilon_r'' + 75.329186{\varepsilon_r''}^2 - 2.340377\varepsilon_r'\varepsilon_r'' \quad (8)$$

These equations depict a model to predict expected value of output parameters when liquid mixture is prepared in any volume fraction. Conversely it can be used to determine both parts of permittivity with the help of measured values of resonant frequency and Q factor by solving equations (7) and (8) simultaneously. Volume fraction of liquids can then be determined by using formulas given as equations (4) to (6) or similar. This method is presented below as a working example.



(a) Resonant frequency versus real and imaginary parts of permittivity.



(b) Q factor versus real and imaginary parts of permittivity.

Figure. 5. System response depicting compositional analysis.

6 WORKING EXAMPLE

A working example is being presented to calculate volume fraction of liquids in a given mixture. This working example utilizes measured values of resonant frequency and Q factor, simultaneous solution of equations (7) and (8) [31] and formula determining effective permittivity, e.g. equations (4) – (6). For using this method it is necessary to determine effective permittivity accurately by studying physical, chemical and other properties of liquids being used. Example utilizes equation (4) considering that it provides accurate value of effective permittivity for liquid mixture containing volume fraction of ethanol and methanol. Table 2 presents assumed measured values of resonant frequency and Q factor and other calculated values [31]. Assumed values were selected to produce expected volume fraction in multiples of 0.1. Degree of precision for these values indicates that model is highly sensitive. Conversely it can be deduced that small variations in volume fraction can lead to considerable changes in measured values causing effective permittivity of liquid mixture to change. Volume fraction (VF) has been calculated as:

$$\mathrm{VF}_{\mathrm{methanol}} = \frac{\varepsilon_{\mathrm{eff}}^{\frac{1}{3}} - \varepsilon_{\mathrm{ethanol}}^{\frac{1}{3}}}{\varepsilon_{\mathrm{methanol}}^{\frac{1}{3}} - \varepsilon_{\mathrm{ethanol}}^{\frac{1}{3}}} \quad (9)$$

$$\mathrm{VF}_{\mathrm{ethanol}} = 1 - \mathrm{VF}_{\mathrm{methanol}} \quad (10)$$

TABLE 2. Working Example

Measured Values		Effective permittivity ε_{eff}		Volume fraction of ethanol	
f_0 (GHz)	Q Factor	ε_r'	ε_r''	Actual	Calculated
3.79067	119.00	24.86	2.46	1.0000	1.00000
3.77951	124.00	25.66	2.27	0.9000	0.90000
3.76912	134.45	26.47	2.09	0.8000	0.80000
3.75955	149.53	27.30	1.92	0.7000	0.70000
3.75085	168.51	28.15	1.77	0.6000	0.60000
3.74306	190.71	29.01	1.62	0.5000	0.50001
3.73624	215.50	29.90	1.47	0.4000	0.40000
3.73044	242.34	30.79	1.34	0.3000	0.30000
3.72570	270.72	31.71	1.22	0.2000	0.20000
3.72208	300.21	32.65	1.10	0.1000	0.10000
3.71962	330.38	33.60	0.99	0.0000	0.00000

7 CONCLUSION

A model for compositional analysis of liquid solvents has been presented. System is based upon a SBR containing microfluidic channel. Permittivity of test liquid was varied through simulation for ranges of ethanol and methanol mixtures. These results were used to develop a model. Some assumed values of resonant frequency and Q factors were presented to this model for validation. Effective permittivity was calculated using these values. Finally volume fraction was determined and compared with expected values. It was observed that calculated values of volume fraction were very close to expected values. Maximum relative error in this case was 0.002 percent. This shows that compositional analysis of liquid mixture has been performed with high degree of accuracy. It can also be observed that model utilizes very precise values which indicate that highly sensitive compositional analysis can be performed using this structure and model.

8 REFERENCES

1. Application Note, “Basics of measuring the dielectric properties of materials.”Agilent Technologies, 2006.
2. M. S. Venkatesh, and G. S. V. Raghavan. “An overview of microwave processing and dielectric properties of agri-food materials.” Biosystems Engineering, vol. 88, no. 1, pp. 1-18, 2004.
3. M. T. Jilani, M. Z. Rehman, A. M. Khan, M. T. Khan and S. M. Ali. “A brief review of measuring techniques for characterization of dielectric materials.” Int. Journal of Information Technology and Electrical Engineering, vol. 1, no. 1, 2012.
4. A. M. Campbell, “Measurements and analysis of the microwave dielectric properties of tissues”, PhD dissertation, University of Glasgow, Oct. 1990.
5. O. V. Tereshchenko, F. J. K. Buesink, and F. B. J. Leferink. “An overview of the techniques for measuring the dielectric properties of materials." In XXXth URSI General Assembly and Scientific Symposium, pp. 13-20, 2011.
6. L. F. Chen, C. K. Ong, C. P. Neo, V. V. Varadan, and V. K. Varadan. “Microwave electronics: measurement and materials characterization.” John Wiley & Sons, 2004.
7. C. Tsipogiannis, “Microwave materials characterization using waveguides and coaxial probe”, Master’s Thesis, Lund University, Lund, Sweden.
8. S. Begley, “Electromagnetic properties of materials: Characterization at microwave frequencies and beyond.” Agilent Webinar, 2010.
9. NPL, “A Guide to characterisation of dielectric materials at RF and microwave frequencies”, London, UK: The Institute of Measurement and Control-National Physical Laboratory, 2003.
10. A. Masood, O. Castell, D. A. Barrow, C. Allender and A. Porch, “Split ring resonator technique for compositional analysis of solvents in microcapillary systems.” Proc. of MicroTAS 2008 Conference, San Diego, pp.1636- 1638, Oct. 2008.
11. D. J. Rowe, S. Al-Malki, A. A. Abduljabar, A. Porch, D. A. Barrow, and C. J. Allender. “Improved split-ring resonator for microfluidic sensing.” IEEE Transactions on Microwave Theory and Techniques, vol. 62, no. 3, pp. 689-699, 2014.
12. T. Chretiennot, D. Dubuc, and K. Grenier, “A microwave and microfluidic planar resonator for efficient and accurate complex permittivity characterization of aqueous solutions.” IEEE Transactions on Microwave Theory and Techniques, vol. 61, no. 2, pp. 972-978, 2013.
13. A. A. Jabita, “Design of singly split single ring resonator for measurement of dielectric constant of materials using resonant method.” Master’s Thesis, University of Gavle, Sweden, 2013.
14. T. Ejaz, A. Sami, H. U. Rahman, T. Tauqeer, M. Naveed, A. Masood, and T. Zaidi, “Compositional analysis of liquid solvents in micro-capillary system using optimized split-ring resonator” unpublished.
15. A. I. Kuznetsov, A. E. Miroshnichenko, Y. H. Fu, V. Viswanathan, M. Rahmani, V. Valuckas, Z. Y. Pan, Y. Kivshar, D. S. Pickard, and B. Lukiyanchuk. “Split-ball resonator as a three-dimensional analogue of planar split-rings.” Nature communications, vol. 5, 2014.
16. A. I. Kuznetsov, A. E. Miroshnichenko, D. S. Pickard, V. Valuckas, V. Viswanathan, M. Rahmani, B. Lukiyanchuk, Y. Kivshar, and Y. H. Fu. "Split-ball resonator." Nature Communications, vol. 5, no. arXiv: 1309.7106: 3104, 2013.

17. S. O. Nelson. “Dielectric properties measurement techniques and applications.” Transactions of the ASAE, vol. 42, no. 2, pp. 523-529, 1999.
18. C. A. Balanis, “Advanced engineering electromagnetics.” vol. 20, New York: Wiley, 1989, pp. 41-48.
19. A Guide to the Characterisation of Dielectic Materials at RF and Microwave Frequencies. Institute of Measurement and Control, 2003.
20. P. Wang, and A. Anderko. “Computation of dielectric constants of solvent mixtures and electrolyte solutions.” Fluid Phase Equilibria vol. 186, no. 1, pp. 103-122, 2001.
21. L. O. Salmazo, F. S. Bellucci, A. E. Job, and M. A. L. Nobre. “Dielectric Permittivity Analysis of Mixtures of Polar Liquids by Impedance Spectroscopy.” 11th Int. Conf. on Advanced Material, Rio De Janerio, Brazil, 2009.
22. H. G. Wang, and C. H. Chan. “Mixture effective permittivity simulations using IMLMQRF method on preconditioned EFIE.” Progress In Electromagnetics Research, vol. 57, pp. 285-310, 2006.
23. W. Froncisz and J. S. Hyde, “The loop-gap resonator: A new microwave lumped circuit ESR sample structure,” Journal of Magnetic Resonance, vol. 47, pp. 515-521, 1982.
24. M. Mehdizadeh, T. K. Ishii, J. S. Hyde and W. Froncisz, “Loop-gap resonator: A lumped mode microwave resonant structure,” IEEE Transactions on Microwave Theory and Techniques, vol. 31, no. 12, pp. 1059-1064, Dec. 1983.
25. M. Mehdizadeh and T. K. Ishii, “Electromagnetic field analysis and calculation of the resonance characteristics of the loop-gap resonator,” IEEE Transactions on Microwave Theory and Techniques, vol. 37, no. 7, pp. 1113-1118, Jul. 1989.
26. T. Ejaz, H. U. Rahman, T. Zaidi, T. Tauqeer, and A. A. Shah, “Analysis, simulation and experimental verification of split-ring resonator,” Microwave and Optical Techmology Letters, vol. 57, no. 10, pp. 2358-2363, 2015.
27. T. Ejaz, A. A. Shah, H. U. Rahman, T. Zaidi, “Improved shield design for split-ring resonator”, Proc. of 3rd Int. Conf. on Technological Advances in Electrical, Electronics and Computer Engineering, Beirut, Lebanon, 29 Apr. – 1 May 2015.
28. T. Ejaz, H. U. Rahman, and T. Tauqeer, “Shield optimization and formulation of regression equations for split-ring resonator,” Mathematical Problems in Engineering, vol. 2016, Article ID 4754192, 10 pages.
29. Ansoft HFSS software: http://ansoft.com/Products/Simulation+Technology/Electronics/Signals+Integrity/ANSYS+HFSS
30. A. P. Gregory and R. N. Clarke. “Tables of the complex permittivity of dielectric reference liquids at frequencies up to 5 GHz.” National Physical Laboratory Report MAT 23, published by NPL, Teddington UK., 2012.
31. Wolfram Research, Inc., Mathematica, Version 9.0, Champaign, IL 2013.