Three-loop two-gap resonator simulation in HFWorks

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Electron spin resonance experiments and other measurements of magnetic properties at microwave frequencies require the use of a resonator to produce a strong microwave field. For experiments below say 10 GHz, microwave cavities are too large to be useful with small samples, and planar structures have a low quality factor and do not produce a uniform field over a 3D volume. In order to remedy these issues, the loop-gap resonator was developed in the 1970s for ESR experiments¹. The basic structure is very simple to implement as a tube with a slot cut along its length.

This design presents a variety of issues. Firstly, the mode pattern is that of a magnetic dipole which has severe radiation losses without the presence of an enclosure. Additionally, the mode pattern is not well controlled and is sensitive to nearby metallic objects, presenting significant design challenges. The accessible frequency range of this design is also limited, because in order to increase the resonant frequency the capacitance of the structure must be reduced. This is accomplished by increasing the gap width, but when the gap becomes too large the capacitance cannot be further reduced due to parasitic capacitance in the loop.

To solve these issues, a modification of this design was developed by Wood et al.² In this design, a resonant structure is formed by three holes in a metal block linked by two thin gaps. This three-loop two-gap design has many advantages over the one-loop one-gap design. The magnetic flux return path is confined to a small volume near the resonator rather than being sensitive to the enclosure. The accessible frequency range is also much greater with this design. For example, with a 6mmx11mm sample loop area, the single loop design cannot be pushed past 3.5 GHz, whereas the three-loop design can easily be tuned to frequencies above 5 GHz.

The design of such a device is more challenging, as it is not possible to reliably estimate the resonant frequency using a lumped-element model. It is effective to instead use a finite element method solver such as HFWorks, which has a resonant mode solver that makes it easy to calculate the resonant frequency and mode field patterns for a given geometry.

¹Mehdizadeh, Mehrdad, et al. "Loop-gap resonator: A lumped mode microwave resonant structure." *IEEE Transactions on Microwave Theory* and Techniques 31.12 (1983): 1059-1064.

²Wood, Robert L., Wojciech Froncisz, and James S. Hyde. "The loop-gap resonator. II. Controlled return flux three-loop, two-gap microwave resonators for ENDOR and ESR spectroscopy." *Journal of Magnetic Resonance (1969)* 58.2 (1984): 243-253.

The model as created to run the HFWorks simulation is shown in Fig.1. For my experiment, the resonator must be placed in a ~2" steel tube, so the simulation model consists of a cylinder of air with the resonator model cut out. Due to the symmetry of the structure we can model only half of the cylinder and use the perfect magnetic conductor symmetry boundary condition on the flat plane, which allows more efficient simulation and easier visualization of the field pattern on this plane. Both the resonator body and external faces of the cylindrical cavity are modeled as perfect electrical conductor boundary conditions.



Figure 1 Model of the three-loop two-gap resonator used for HFWorks simulation

The magnetic field magnitude pattern is shown in Fig.2, and the vector pattern is shown in Fig.3. The electric field pattern is shown in Fig. 4. These simulations show the operation of the resonator as desired, with a strong, uniform magnetic field confined to the loops, and an electric field confined to the gaps, reducing dielectric heating of the sample.



Figure 2 Magnitude of the magnetic field in the resonator. Note the uniformity within the gaps and relative amplitudes between the loops corresponding to the ratio of their areas.

A resonator similar to this model has been fabricated and has a resonant frequency of around 4.9 GHz, compared to 5.07 GHz in the HFWorks simulation. This is good agreement; the actual resonator has slightly different dimensions and a coupling loop placed near an outer loop that disturbs the mode field slightly. Simulation in HFWorks has proven to be quite helpful in the design process, as I initially had used equations in Wood et al. for determining the design parameters, but the manufactured resonators had much lower resonant frequencies than expected, perhaps because the equations were applicable only to certain geometries.



Figure 3 Vector field pattern of the resonator, showing the quadrupole pattern of the mode, which is confined well to the loops and uniform within them.



Figure 4 Electric field pattern of the resonator, showing that the E-field is very well confined to the gaps.

With HFWorks I was able to create a model that accurately reproduced my original resonators and figure out the changes necessary to achieve the desired frequency; widening the gaps ended up being the simplest way to tune the frequency up.