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Ways to high performance EPR (Electron Paramagnetic Resonance) resonators

PC ⚡ DC
Physikalische Chemie und Didaktik der Chemie

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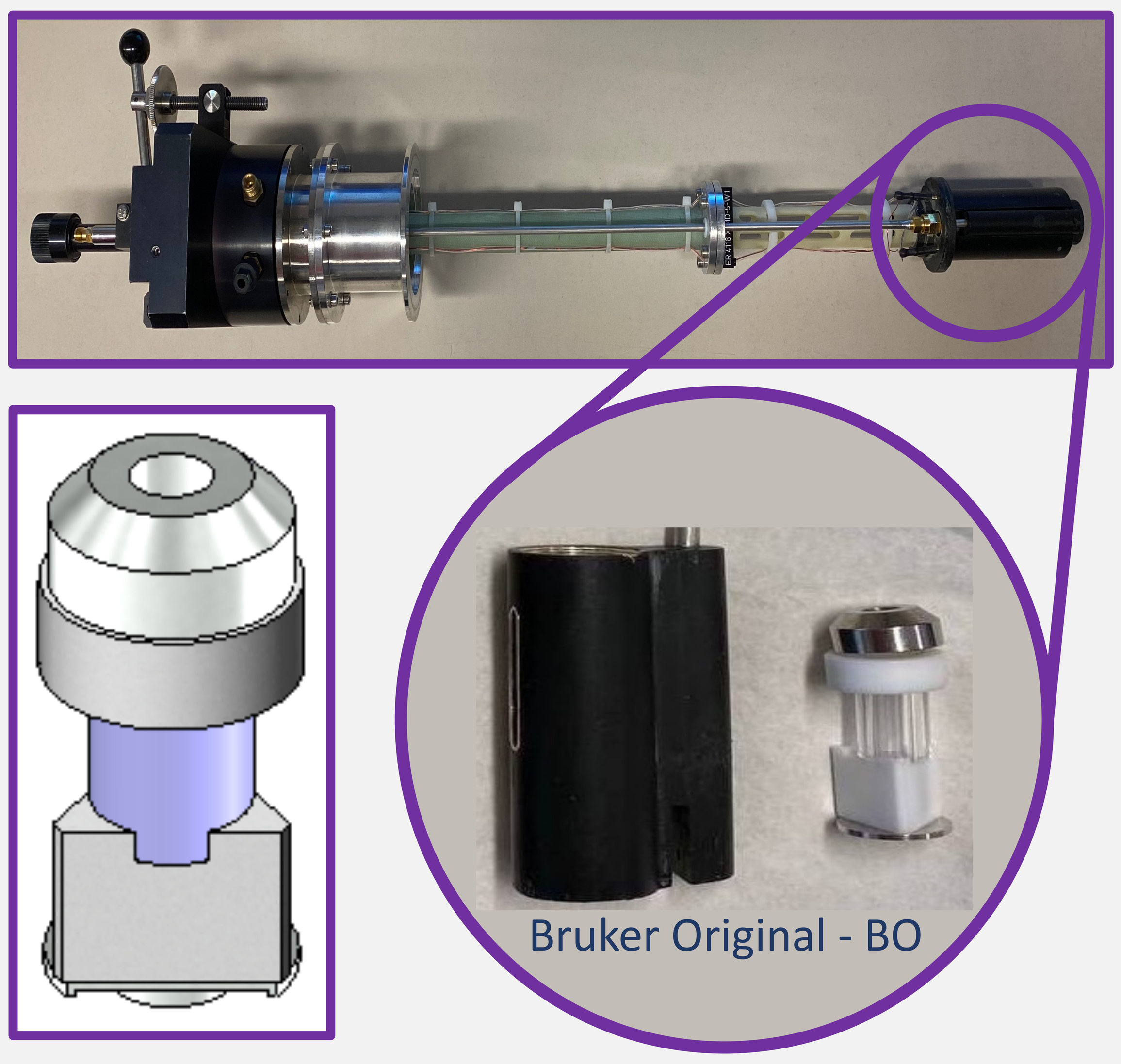
Abstract

Microwave (MW) resonators in Electron Paramagnetic Resonance (EPR) concentrate the MW magnetic field (B_1) at the sample of interest and separate the MW electric field from the sample to prevent overheating. There are numerous experimental methods in EPR spectroscopy (e.g. CW, transient EPR, pulse EPR) which all impose different requirements on MW resonators, like high quality factors, large MW conversion factors or homogeneous B_1-fields.

Commercial spectrometers already offer good standardized MW resonators for a broad application range. Newly emerging highly specialized research fields push these spectrometers to or beyond their sensitivity limits. Optimizing the MW resonator offers a direct approach to increase the sensitivity.

Here, we present three low-cost optimization methods for a commercially available X-band MW resonator (**Bruker Original, BO**) for three experimental purposes. At first we examined the symmetry and holders of the dielectric resonator to enhance the MW conversion factor (**Symmetric Long, SL**). Afterwards, we switched towards the dielectric resonator and its length for CW purposes (**Short cylinder, SC**) and its shape for B_1-field homogeniety (**Symmetric Diabolo, SD**). [1]



Three pathways to performance optimization

Symmetric teflon holders & metal caps

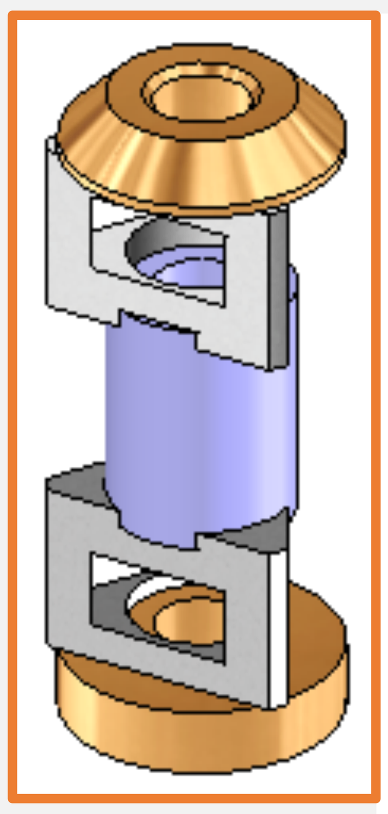
- Reduction of teflon volume provides higher Q-factors
- Cu caps superior to Ag coated Ni, due to lower skin depth [2]
- Conversion factors measured with pentacene illuminated at 532 nm [3]
  ⟶ SL best suitable option for TR-EPR

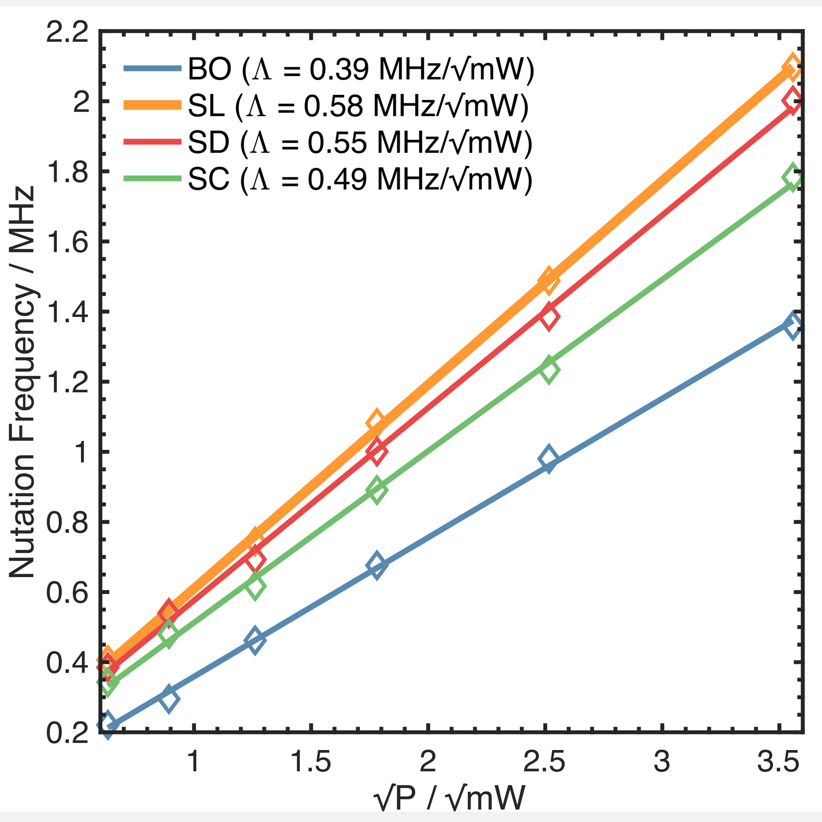
B_1-field homogeniety

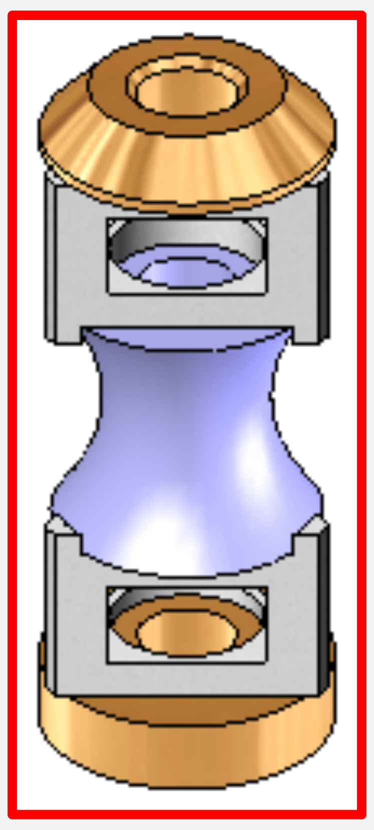
- Syriamina et al. proposed an extended homogeneous B_1 field distribution for a biconcave shape [4]
- BDPA as a point sample was positioned throughout the resonator to probe the B_1 field distribution
- Biconcave shape provides a larger homogeneous B_1 field range

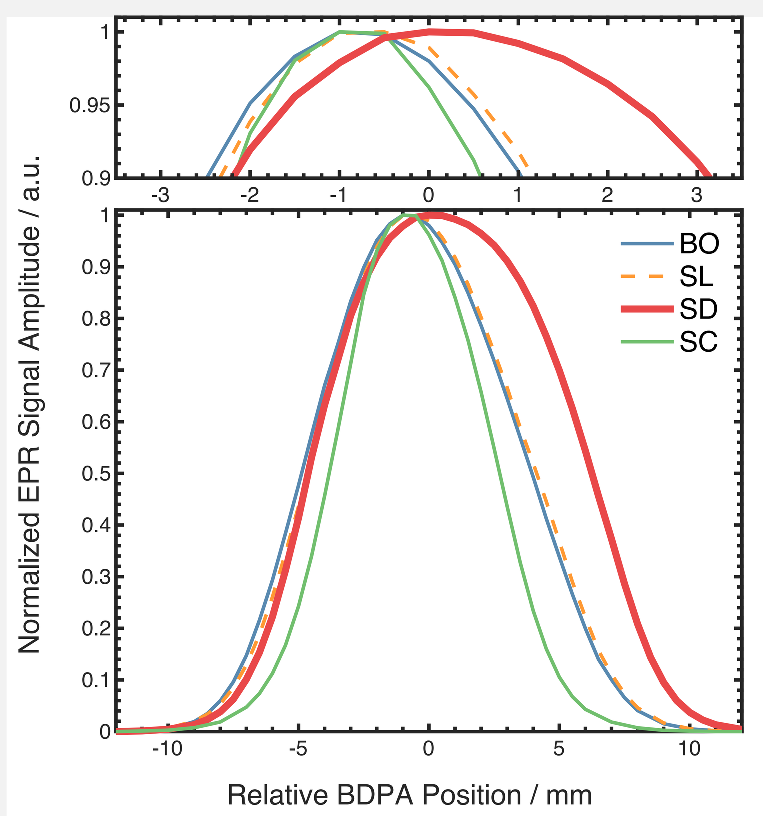
Length of dielectric resonator

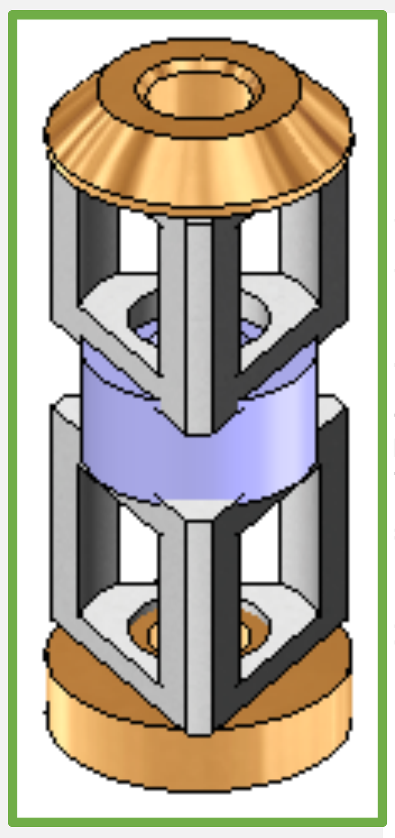
- Smaller dielectric resonators are advantegeous for small samples
  ⟶ Higher SNR
- Performance is characterized by pulse EPR, using a γ-irradiated quartz (eprime)
- Spin echo indicates that SC possesses the strongest B_1 field
  ⟶ SC best suitable option for CW EPR

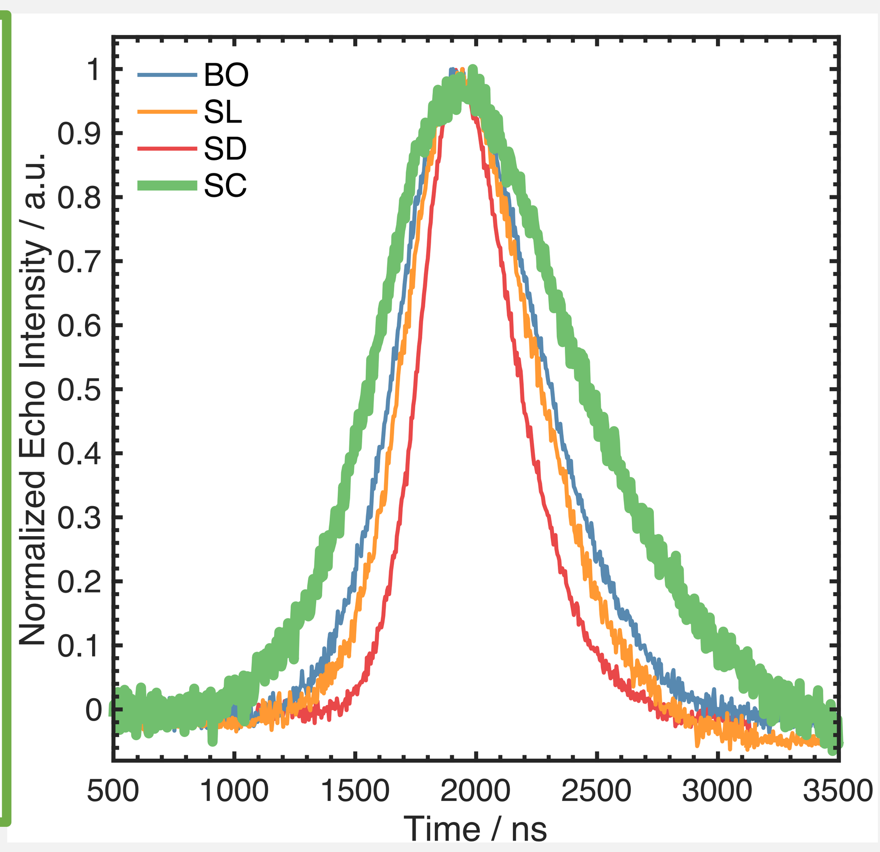








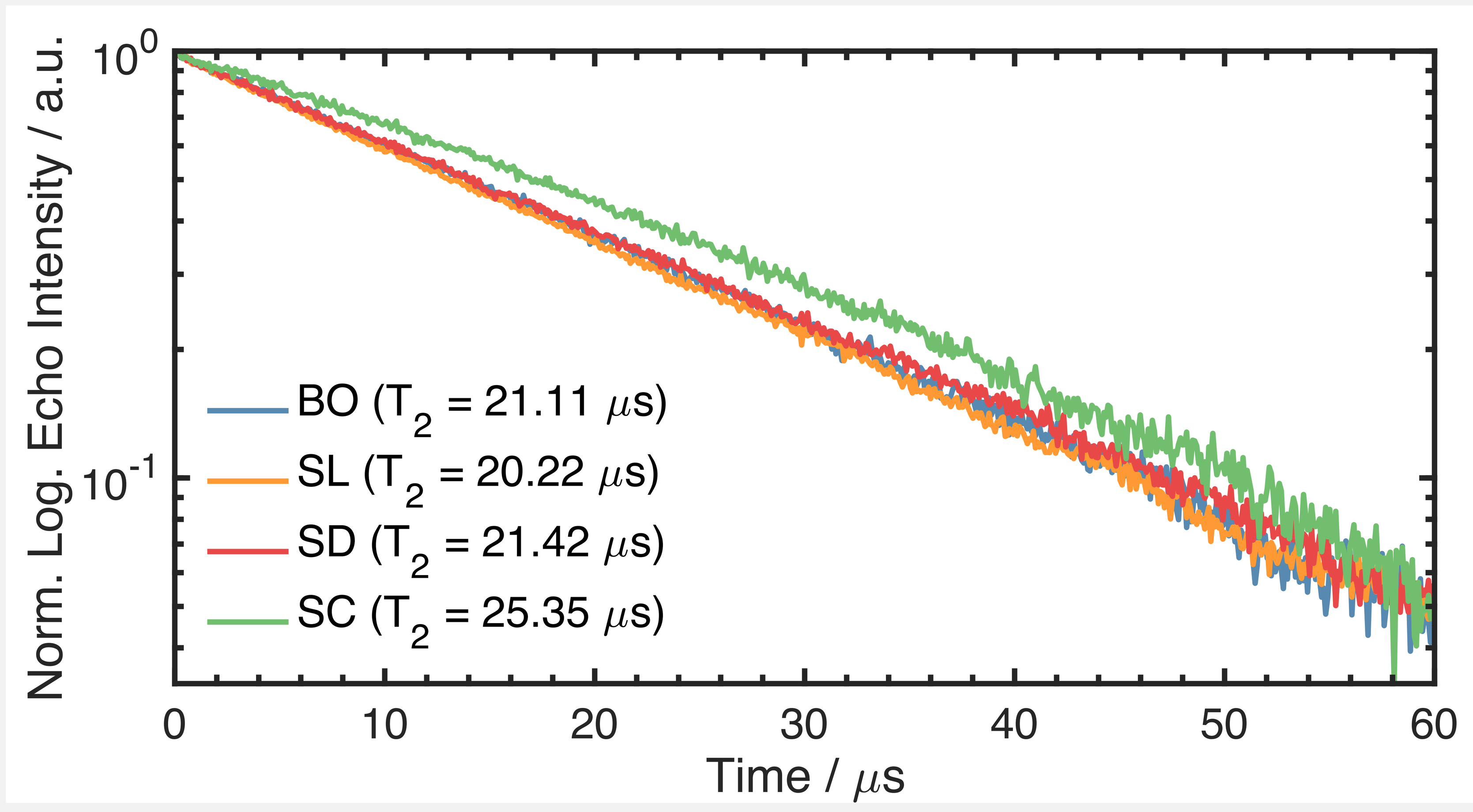




Conclusion and outlook

- Three optimized MW resonators could be developed and were characterized by means of CW, TR- and pulse EPR
- All three resonators can be implemented in commercial pulse EPR measurement setups
- **SL** features the best conversion factor and good CW properties
- **SC** provides the highest SNR and is the best option for point samples in CW EPR
- **SD** produces the narrowest echo and has promising pulse EPR (e.g. DEER, ENDOR) abilities

⟶ Further analysis on the behaviour of B_1-field conversion of MW inside the resonator can lead to higher performances



References

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[3] M. Schröder, D. Rauber, C. Matt, *Appl. Magn. Reson.*, **2021**, 1–10.
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