COMSOL CONFERENCE
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ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Swissto12
terahertz applications

RF MAGNETIC FIELD SIMULATION OF A NOVEL PLANAR DNP-NMR COIL

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Outline

- Introduction (NMR and DNP)
- Planar Probe and Simulation Model
- RF Simulation Results
- Microwave Simulation Results
- Conclusions

Introduction - NMR

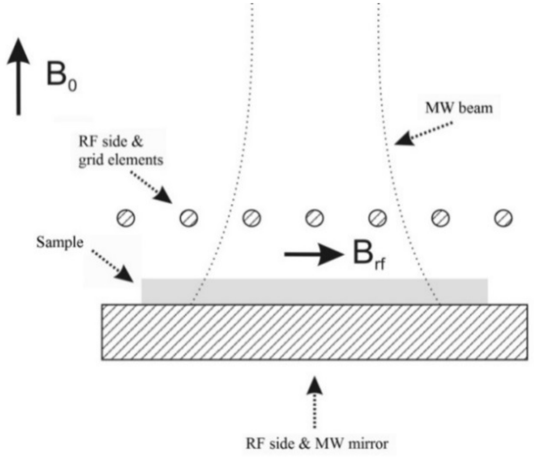
- NMR: Nuclear Magnetic Resonance spectroscopy.
- Magnetic properties of atomic nuclei: determination of physical/chemical properties of the containing molecules.
- Information about: structure, dynamics, reaction state, and chemical environment of the molecules.
- Fundamental sensitivity limitation: long acquisition times for complex structures (e.g. biomolecules).

Introduction - DNP

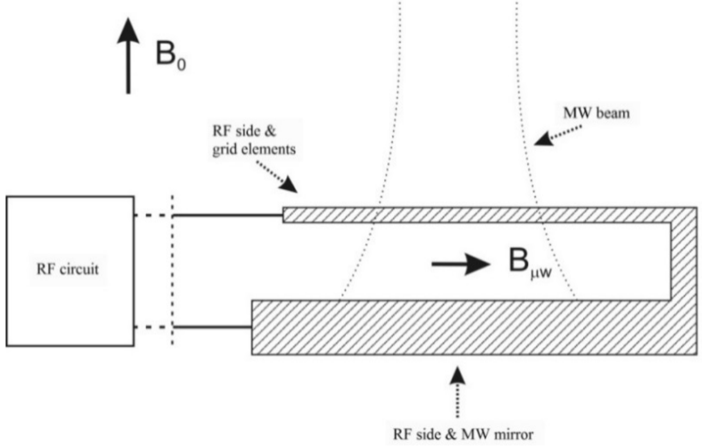
- DNP: Dynamic Nuclear Polarization.
- Goal: To improve the sensitivity of NMR by transferring the polarization of electron spins to bulk nuclei.
- Electron paramagnetic resonance (EPR) transitions excited with high-power microwave radiation (e.g. gyrotrons).
- DNP enhancement factor mainly defined from the average magnetic field values in the sample region.

Planar Probe - Concept

- Single-turn coil, formed by a polarizer and a ground plane.
- Goal: Minimization of sample heating due to MW power.



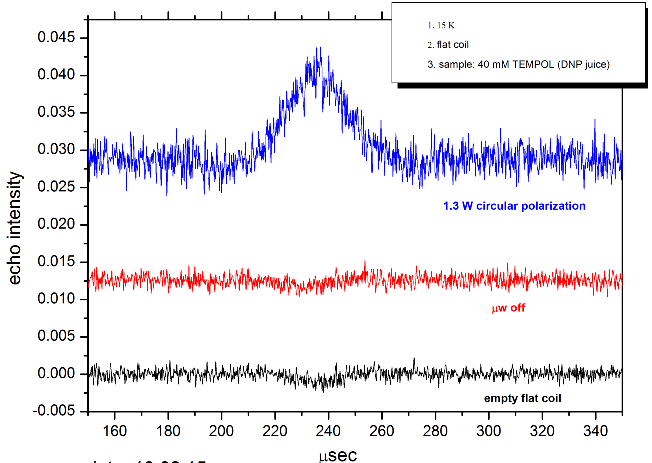
Front view

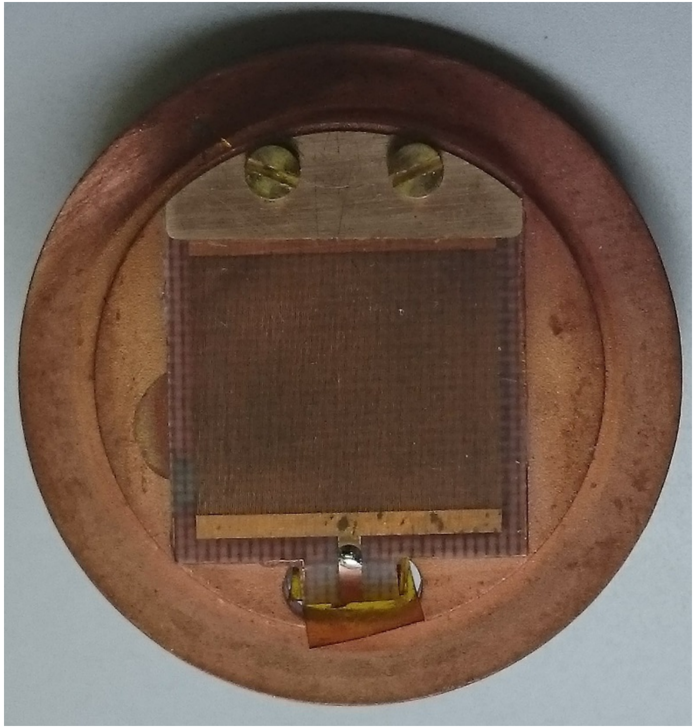


Side view

Planar Probe - First Implementation

- Grid fabricated on a thin PCB.
- Big enhancement factor obtained, but impossible to quantify (signals from glue).
- RF field homogeneity not great.



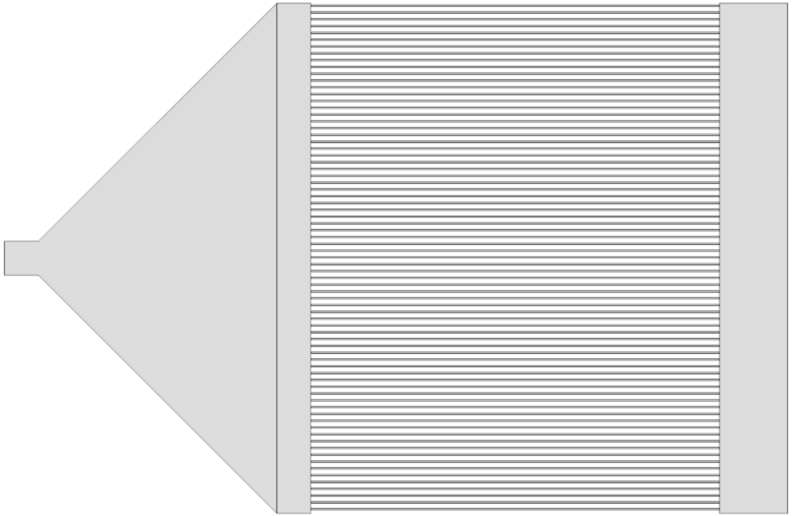


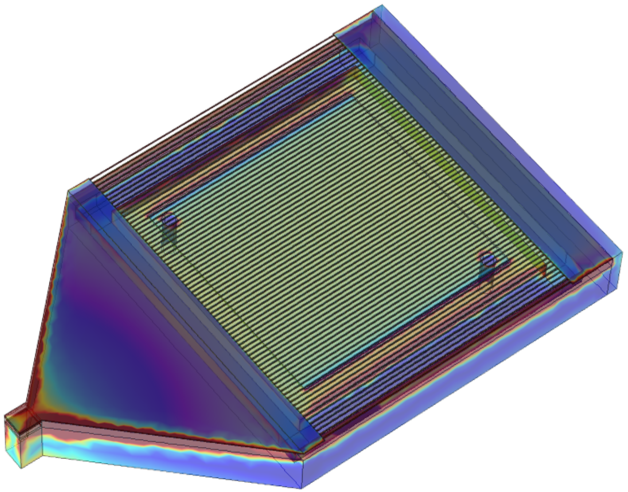
RF Design Model - Implementation

- Simulations performed with AC/DC module, Magnetic Fields interface (solution of Ampère's law).
- Impedance boundary conditions applied to copper surfaces, magnetic insulation to limit the computational domain.
- Lumped port used as an excitation, to model the coaxial connector feeding the device.
- Similar COMSOL Tutorial: Modeling of a 3D Inductor.

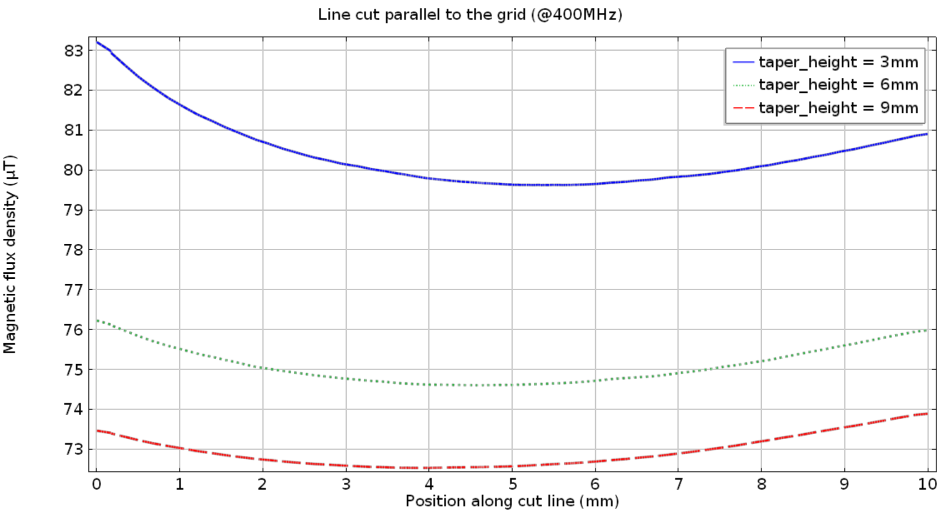
RF Design Model - Visualization

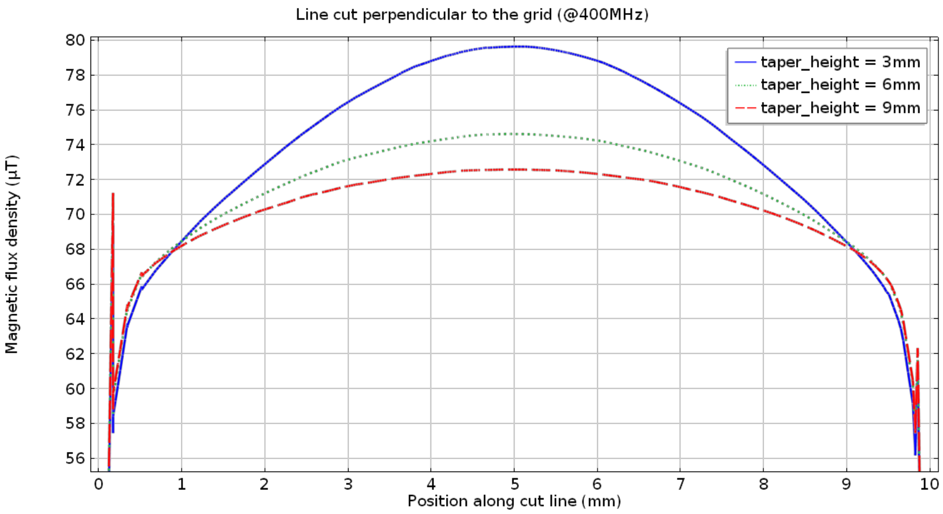
Top-view of wire grid





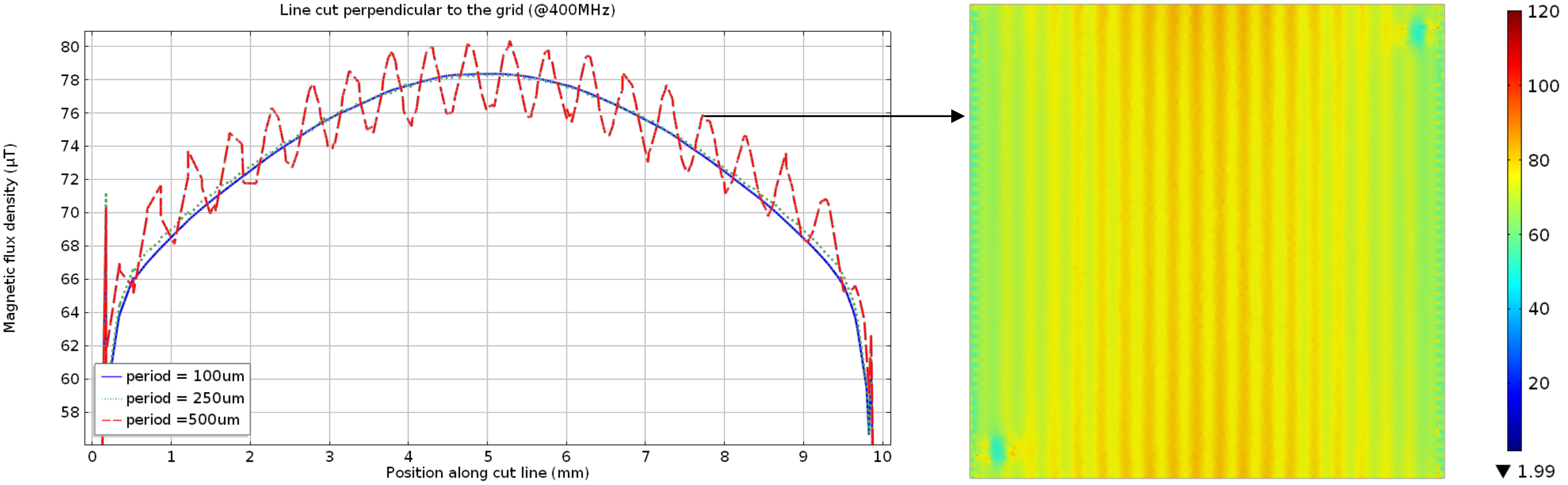
RF Simulation Results - Taper Height





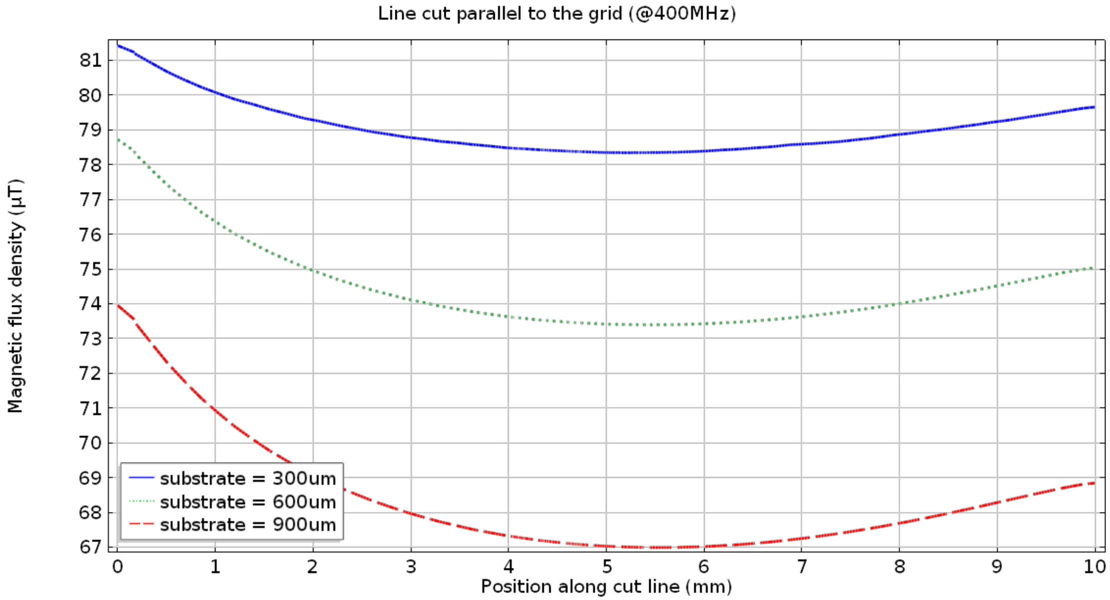
- Lower but more homogeneous RF magnetic field distribution for longer tapered sections (more homogeneous surface current distribution).
- Maximum value restricted from the available space in magnet's bore.

RF Simulation Results - Periodicity



- Small periodicity is required to ensure RF magnetic field homogeneity.
- Related to the transparency of the grid with respect to the MW wave.

RF Simulation Results - Substrate Height

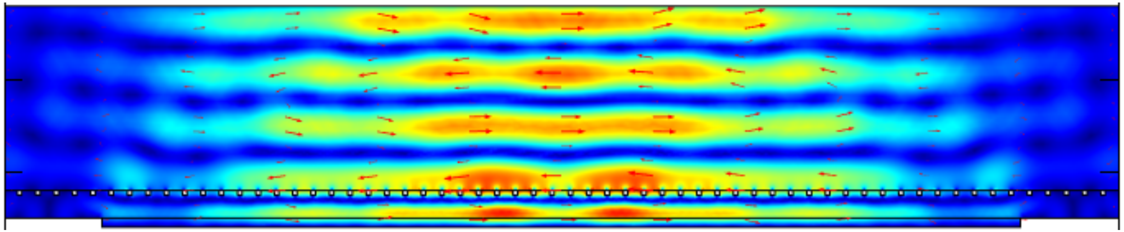


- Thicker substrate → lower and more inhomogeneous RF magnetic field in the sample.
- Thicker substrates are easier to fabricate and manipulate during the experiments.
- Compromise needed.

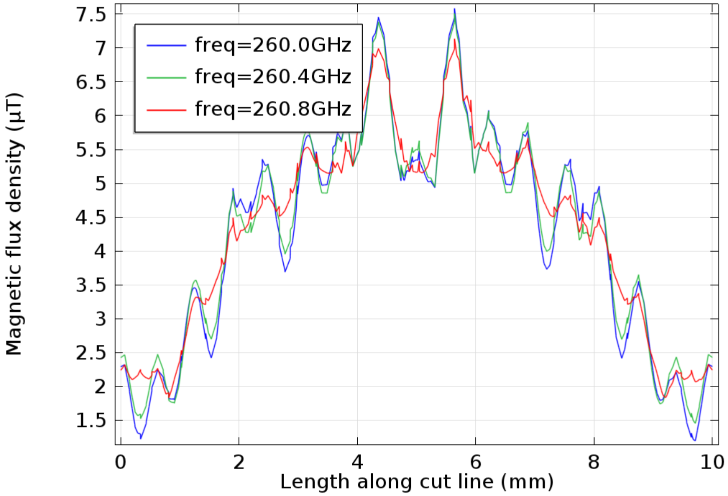
MW Simulation Results

- 2D model with Gaussian beam excitation (beam waste of 4.8mm) at frequencies between 260GHz-261GHz.

Electric field magnitude @260GHz



Variation of magnetic field in the sample



- Optimal wire size of 50umx50um (for a periodicity of 100um).

Conclusions

- Improved RF magnetic field homogeneity due to the introduction of a tapered region.
- Height of the substrate and periodicity of the wires also affect significantly the magnetic field values.
- The dimensions of the wires are determined from a 2D microwave simulation for different sample materials.
- First experimental results are expected soon.

Thank you for your attention!!

Any questions?