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Simplified THz Instrumentation for High-Field DNP-NMR Spectroscopy

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Abstract

We present an alternate simplified concept to irradiate a nuclear magnetic resonance sample with terahertz (THz) radiation for dynamic nuclear polarization (DNP) experiments using the TE_{01} circular waveguide mode for transmission of the THz power and the illumination of the DNP sample by either the TE_{01} or TE_{11} mode. Using finite element method and 3D electromagnetic simulations we demonstrate that the average value of the transverse magnetic field induced by the THz radiation and responsible for the DNP effect using the TE_{11} or the TE_{01} mode are comparable to that generated by the HE_{11} mode and a corrugated waveguide. The choice of the TE_{11}/TE_{01} mode allows the use of a smooth-walled, oversized waveguide that is easier to fabricate and less expensive than a corrugated waveguide required for transmission of the HE_{11} mode. Also, the choice of the TE_{01} mode can lead to a simplification of gyrotron oscillators that operate in the TE_{0n} mode, by employing an on-axis rippled-wall mode converter to convert the TE_{0n} mode into the TE_{01} mode either inside or outside of the gyrotron tube. These novel concepts will lead to a significant simplification of the gyrotron, the transmission line and the THz coupler, which are the three main components of a DNP system.

1 Introduction

Dynamic Nuclear Polarization (DNP) is a technique that utilizes the vastly larger polarization of the electron spin reservoir to provide a large sensitivity boost for nuclear magnetic resonance (NMR) experiments by several orders of magnitude [1–5]. The large Boltzmann polarization of unpaired electrons is transferred to the nuclear spin reservoir by microwave radiation of the sample at the electron paramagnetic resonance (EPR) transition frequency of the paramagnetic polarizing agent.

In DNP-enhanced solid-state NMR experiments signal intensities can typically be increased by factors of $>10^2$. Hence, acquisition times can be reduced by factor $\gg 10^4$ and experiments that would normally require a month of acquisition time could be performed in just a few minutes with DNP [6–14]. In addition DNP enables experiments that previously would be extremely difficult to perform such as NMR studies of surfaces in which the DNP effect is used to selectively enhance NMR signals from the surface or bulk atoms of interest [15].

DNP is certainly not a new technique; the method was initially proposed by Albert E. Overhauser in the 1950s [1] and later experimentally confirmed by Carver and Slichter [3]. However, while NMR spectroscopy was being extended to higher magnetic fields to increase resolution and sensitivity, the lack of rapid development in high power microwave and millimeter wave technology necessary relegated DNP as an exotic method, and stymied

its acceptance in routine NMR spectroscopy. However, recent advances in millimeter wave and THz technology spurred by defense and plasma heating applications have benefited the application of these technologies in DNP and EPR [16, 17]. Today DNP-enhanced NMR experiments can in principle be performed at all magnetic fields at which NMR spectroscopy is routinely performed (300–900 MHz for ^1H , 197–591 GHz for e^-).

The key component in all DNP experiments is a microwave/THz source capable of delivering sufficient power (several tens of watts) to excite/saturate the EPR transitions of the polarizing agent.¹ At frequencies below 100 GHz (140 MHz ^1H Larmor frequency) a number of devices are available such as solid-state sources and klystrons [18, 19]. At higher frequencies, particularly in the millimeter wave and THz frequencies, the gyrotron is the only demonstrated device capable of reliably generating sufficient power to efficiently drive the DNP process for magic-angle-spinning (MAS) solid-state NMR experiments [4, 20, 21]. These experiments are typically performed at temperatures in the 90–100 K range, which is conveniently achieved by spinning and cooling with cold nitrogen gas [22–24]. At this temperature the electron relaxation times of the paramagnetic polarizing agent are very short, and high-power (>25 W) THz sources are required to efficiently drive the DNP process. At NMR frequencies below 400 MHz (^1H Larmor), low-power, solid-state sources with several tens of milliwatts of output power can still be used if the sample temperature is lowered below ~30 K (He cooling) [25, 26]. In this work we will focus on high-field DNP-enhanced solid-state NMR spectroscopy using gyrotrons as the THz source.

The first DNP-NMR experiment using a gyrotron was performed in the early 1990s at a magnetic field of 5 T, corresponding to a proton and electron Larmor frequency of 211 MHz and 140 GHz, respectively. Since then, gyrotrons have been used for DNP experiments at frequencies up to 700 MHz [9, 10, 20, 27, 28].

The gyrotron is a “fast-wave” vacuum electronic device (VED) that exploits the relativistic cyclotron resonance maser (CRM) effect to transfer energy between a gyrating electron beam and a transverse electric (TE) mode of a cavity resonator in a strong magnetic field [29]. Gyrotrons are typically used in industrial-heating applications and for plasma heating in nuclear fusion experiments [17]. These applications require several tens of kilowatts (industrial heating) to several tens of megawatts power (plasma heating) and naturally efficient generation and transmission of the power to the fusion reactor is a key requirement; even very small losses result in several kilowatts of lost THz power creating undesired heating effects [30].

Gyrotron technology for DNP-NMR spectroscopy was inspired by the megawatt class fusion gyrotrons and many concepts were directly adopted from high-power gyrotrons. Hence a low-power gyrotron tube (<100 W) for DNP-NMR is often designed and manufactured as a micro-megawatt version by downscaling existing technology; certainly not the optimal way to produce compact and cost-effective devices. Similar concepts have guided the development of transmission line technology for DNP-NMR applications. As such many concepts for building gyrotrons, transmission lines and concepts of coupling the THz power to the sample are inherited from the early days of DNP spectroscopy and nuclear fusion experiments; and such anachronistic approaches often lead to unnecessary increase in cost and complexity.

¹The THz regime is loosely defined as the frequency region between 300 GHz and 3 THz. Today NMR spectroscopy is typically performed at proton frequencies of >400 MHz, corresponding to electron Larmor frequencies of >264 GHz. Therefore, we will use the term THz in the following instead of microwave.

In this work, we present a fresh look at this technology to identify areas of improvements, which will ultimately lead to a new design of THz instrumentation specific for DNP-NMR spectroscopy. The approach described in this work is significantly simpler when compared with contemporary DNP-NMR systems that are used or developed in academia or those that are commercially available [10]. Adaptation of our proposed concepts will lead to more cost-effective instrumentation and therefore a broader availability of the technology.

2 Components of a DNP-NMR System

To identify opportunities for optimization of the current DNP architecture let us first briefly review the state-of-the-art of DNP instrumentation. In Fig. 1 a schematic representation of a DNP system is shown.

Four components are required in addition to the NMR hardware to perform DNP spectroscopy (see Fig. 1):

- a THz source capable of generating sufficient THz power to efficiently drive the EPR transitions. For high-field DNP-NMR experiments at 90 K a gyrotron is typically used.
- A transmission line to deliver the THz power from the source to the sample. Corrugated waveguides are typically used in DNP-NMR systems because of their low transmission losses.
- A DNP probe with the capability to irradiate the (spinning) sample with RF and THz power at low temperatures (<100 K).
- A polarizing agent as the source of the unpaired electrons. Typically a stable, inert mono- or bi-radical is mixed into the sample.

In this work we will not discuss the ongoing effort in creating more efficient polarizing agents and will focus on new concepts of THz technology for DNP-NMR spectroscopy.

3 Transmission Line for DNP-NMR Systems

To deliver the THz radiation from the source to the sample a transmission line is required. In early DNP-NMR systems a fundamental, rectangular waveguide was typically used [31, 32]. However, fundamental waveguides become very inefficient with increasing frequencies, for example at 140 GHz the losses for a WR-08 fundamental, rectangular waveguide are >3 dB/m. To minimize the loss the THz radiation can be delivered using an oversized, rectangular waveguide (e.g. K-band, WR-42, 0.7 dB/m at 140 GHz), which is tapered down to fundamental waveguide (WR-06) to irradiate the sample [33–35]. However, in addition to the substantial losses that occur inside the waveguide, irradiating the sample using a fundamental mode waveguide is very inefficient due to the large diffractive losses that occur once the THz radiation leaves the waveguide.

In contrast, using a Gaussian-like TEM_{00} mode for radiation yields much higher B_{1c} fields at the position of the sample. For example, for 380 MHz DNP-NMR experiments using a 250-GHz gyrotron source an internal quasioptical mode converter was employed to convert the TE_{03} cavity mode into a Gaussian-like TEM_{00} mode [20]. This mode can be injected into a corrugated waveguide (i.d. 22 mm) for transmission in a HE_{11} -like mode. The waveguide was subsequently tapered to 8-mm-diameter waveguide (fabricated with helical corrugations) and the sample was irradiated from the cut end of this waveguide.

Also quasi-optical transmission lines have been used to link the THz source to the sample in DNP-NMR experiments at 600 MHz (395 GHz e^-) and 290 MHz (187 GHz e^-) [36]. This

5-m long, quasi-optical transmission line provides full control over the polarization of the THz radiation and has capabilities to monitor the power level, purity and frequency of the radiation and allows for EPR detection. However, compared with a waveguide-based transmission line this approach is considerably more expensive.

Although the transmission line is only a passive component in the DNP system and is far less complex than the gyrotron, it nevertheless plays a central role in the design of a DNP-NMR system and should have minimal losses. If the THz radiation is transmitted in the HE_{11} mode a corrugated waveguide is required which can be achieved by injecting a TEM_{00} free space Gaussian beam into the corrugated waveguide [37]. However, since the gyrotron cavity typically operates in a high-order mode such as the $TE_{9,3}$ or the TE_{03} mode, this mode cannot be directly used to transmit the THz power. Therefore, the high-order cavity mode is first converted into the TEM_{00} -like mode, which can be injected into the corrugated transmission line [20, 38, 39].

Fabrication of corrugated waveguides is a two-step process: first a short piece of tubing is honed to a precise inner diameter. In a second step the corrugations are machined into the inner wall of the tube. To do this a specific tool is required that needs to be inserted into the tube and therefore only short waveguide pieces can be accurately manufactured, if the inner diameter is of the order of several millimeters as is the case for THz frequency transmission lines used in DNP-NMR systems. These short waveguide pieces are then either soldered together or held in precisely machined sleeves to form a longer section [40]. An alternate method for fabrication of corrugated waveguides by stacking rings has been demonstrated, but in the frequency regime of interest for DNP-NMR, this technique is more expensive than direct machining [41].

Traditionally, corrugated waveguides are preferred in nuclear fusion experiments due to their very small ohmic losses and lower mode conversion losses in corrugated waveguide miterbends provided the HE_{11} mode has very high purity (>99 %) [30, 42]. However, the output mode of gyrotrons used for DNP-NMR does not always meet the same mode-purity standards as gyrotrons used in nuclear fusion experiments resulting in increased losses even if corrugated transmission lines are used. In contrast to nuclear fusion experiments the available power from gyrotron sources used for DNP-NMR is abundant (<100 W) and the transmission line efficiency is not as critical.

Corrugating the inner wall of the waveguide is only required when the THz radiation is transmitted in the HE_{11} mode. In contrast, a smooth-wall waveguide is sufficient for low loss transmission in the circular TE_{01} mode. This significantly simplifies the fabrication of the waveguide and the entire transmission line system since much longer sections of the waveguide can be fabricated at a lower cost.

Power transmission in the TE_{01} mode using an oversized smooth-wall waveguide is comparable in transmission losses to that of corrugated lines supporting the HE_{11} mode [42]. Historically, research on TE_{01} transmission lines was conducted with an interest for using the low-loss properties of such transmission lines and associated components for telecommunication applications [43]. The majority transmission losses occur at the miterbends, regardless if the TE_{01} or HE_{11} mode is used. For example, the attenuation for both corrugated and smooth-wall waveguide is of the order of 0.0025 dB/m [30]. The fractional losses (in dB) due to mode conversion in a 90-miter bend with a flat mirror can be approximated for the HE_{11} and the TE_{01} mode by

$$0.55 \left(\frac{\lambda}{D} \right)^{3/2} \text{ for HE}_{11} \quad (1)$$

$$1.40 \left(\frac{\lambda}{D} \right)^{3/2} \text{ for TE}_{01} \quad (2)$$

with λ the wavelength and D the diameter of the waveguide [42].

Although the theoretical losses are approximately factor 2.55 higher for the TE₀₁ mode compared with the HE₁₁ mode, the absolute values for fractional losses per miterbend increase only from 0.008 dB (HE₁₁) to 0.021 dB (TE₀₁) at a frequency of 395 GHz ($\lambda = 0.7590$ mm) and a waveguide diameter of 12.7 mm.

In addition, ohmic losses of the TE₀₁ and the HE₁₁ mode are comparable and the only disadvantage of the TE₀₁ mode seems to be the slightly elevated diffraction losses in a miterbend when compared with the HE₁₁ mode (compare Eqs. 1, 2). However, the relatively low mode purity (~90 %) of the HE₁₁ mode in a corrugated waveguide for DNP applications suggests that the performance of the HE₁₁ miterbends is unlikely to meet the theoretical expectations and thus may have limited advantage over TE₀₁ miterbends. The exact calculation of the losses in both TE₀₁ and HE₁₁ miterbends depends on the fraction of other modes and most importantly, their relative phases. Such analysis for high mode purity transmission line systems for the ITER fusion experiment has been carried out to some extent by Shapiro et al. [44]. However, these calculations are too complex and therefore impractical to perform for the low-output mode purity of current gyrotrons used in high-field DNP-NMR applications.

4 Coupling of the THz Power to the Sample

The characteristic field profiles of the magnetic field for the HE₁₁, the TE₁₁ and the TE₀₁ modes are shown in Fig. 2. Note that the HE₁₁ is approximated as a linear combination (power) of 85 % TE₁₁ and 15 % TM₁₁ modes and for simplicity we will refer in the following to it as the HE₁₁ mode. The HE₁₁ mode has its peak intensity in the center of the waveguide and negligible fields at the waveguide walls while the TE₀₁ mode has intensity in the form a ring with a peak value at roughly half the radius of the guide.

At present THz no resonators are used in high-field DNP-NMR spectroscopy. The sample is typically illuminated by launching the THz radiation as a free-space Gaussian beam towards the sample, through the turns of the RF coil [23]. This approach is efficient if sufficient THz power is available, because the beam waist of the free Gaussian beam does not increase rapidly if the distance between the waveguide and the sample is within the Rayleigh range of the beam [45]. However, the distance between the open end of the waveguide and the NMR coil needs to be sufficiently large to prevent arcing between them. The identical approach can be used if the THz radiation is delivered in the TE₀₁ mode.

The efficiency of the DNP effect depends on several factors and the intensity of the magnetic field induced by the THz irradiation (B_{1e}) is one of the most important factors. To evaluate the efficiency of illuminating the DNP sample by the HE₁₁, the TE₁₁, or the TE₀₁ mode we performed full 3D HFSS simulations to obtain the precise B_{1e} distribution inside the stator (see “Materials and Methods” for details of the simulation model).

Recently, Nanni et al. [46] reported simulation results for the efficiency of illuminating the NMR sample from an HE₁₁ mode from a corrugated waveguide. In this work our primary

goal is to compare the efficiency of the different modes and thus we chose a simulation model very similar to the one used by Nanni et al. but with a reduced size to limit computation time (e.g. assuming the stator as a perfect conductor and limiting the size of the stator). The geometry used in all simulations is shown in Fig. 3.

For this work all simulations were performed with the THz radiation being launched perpendicular to the rotor axis (see Fig. 3), a concept that is currently employed by many different research groups [10, 23, 47]. However, the sample can also be irradiated along the rotor axis [31, 35]. Originally, rectangular fundamental waveguide was used to deliver the THz power to the sample, but soon this concept was dismissed since the delivered power is very small. The reason for this is because the THz power exiting the waveguide in fundamental mode does not form a focused beam that can be effectively directed towards the sample. This is different when the HE_{11} mode is used in an oversized cylindrical waveguide, in which case the THz radiation can be effectively focused to irradiate the sample [24].

The HFSS simulations provide the electric and magnetic field values for each point of the simulation model and integration of the magnitude of the magnetic field component of the THz radiation over the sample volume, normalized to the sample volume yields the average field values $\overline{B_{1e}}$ across the sample. However, only magnetic field components induced by the THz radiation that are orthogonal to the field direction of the static magnetic field are relevant for DNP and are considered in the calculation of $\overline{B_{1e}}$. Note that all investigated modes have also magnetic field components in the propagation direction of the beam, which also have components orthogonal to the outer static magnetic field and need to be considered when calculating the overall $\overline{B_{1e}}$ value. For the simulations, two different cases can be considered: (1) the THz-induced magnetic field is oriented along the y axis and (2) the magnetic field is parallel to the z axis (see Fig. 3). The effective B_{1e} field responsible for the DNP effect is calculated according to

$$B_{1x'} = B_{1x} \cos \theta_m - B_{1z} \sin \theta_m \quad (3)$$

$$B_{1y'} = B_{1y} \quad (4)$$

$$B_{1e} = \sqrt{B_{1x'}^2 + B_{1y'}^2} \quad (5)$$

The value $\overline{B_{1e}}$ is calculated by averaging the B_{1e} values over the sample volume. The average values for the THz-induced magnetic field strength $\gamma_e \overline{B_{1e}}$ are summarized in Table 1. In our simulations, we obtained values that are approximately factor 4 higher than what was previously reported by Nanni et al. [46]. This increase in the $\overline{B_{1e}}$ value can be attributed to the more proximate location of the face of the radiating waveguide in our simulations; a choice deliberately made to reduce the size of the simulation geometry (without sacrificing other details). However, the goal of our work is to compare the average field values for irradiation of the DNP sample with the HE_{11} , the TE_{11} and the TE_{01} mode and hence, the absolute value of the field strength is not critical assuming other simulation parameters are held identical in all cases.

The simulation results clearly indicate that the average field strength $\overline{B_{1e}}$ is very similar regardless if the HE_{11} , the TE_{11} , or the TE_{01} mode is used to illuminate the sample. In all cases the variation is in the $\pm 2\%$ range.

The magnitude for $\overline{B_{1e}}$ throughout the simulation model for the HE_{11} , the TE_{11} and the TE_{01} mode is shown in Fig. 4. It appears that the B_{1e} field distribution shown for the HE_{11} mode looks different to the results presented by Nanni et al. In our simulations we noticed that the observation of interference patterns strongly depends on the simulation geometry and the frequency at which the simulation is performed. Even small changes of the pitch factor of the RF coil can yield very different B_{1e} intensity patterns throughout the sample. While it is possible to create illustrative interference patterns for certain ratios of frequency and RF coil dimensions, we believe that this is not a general feature and, since no resonance structure (cavity) is present the field intensities are not uniform. While the coil geometry can be accurately controlled in numerical simulations, standard manufacturing tolerances could prohibit the appearance of these standing wave patterns. Therefore, we consider these simulations as an ideal case but the observation or the lack of interference patterns is not crucial for the evaluation of the simulation results. Furthermore, since the sample is spinning during the experiment the fields will be averaged over the sample in the radial direction.

From Fig. 4 it appears that the magnetic field induced by the THz radiation is slightly higher inside the sapphire rotor material for the HE_{11} mode. A possible explanation for this is that the highest field intensity for the HE_{11} mode is in the center while the TE_{01} mode has two maxima located at approximately half the radius of the waveguide.

5 Simplified Design of a Gyrotron for DNP-NMR

The simulation results presented in the previous section show that the $\overline{B_{1e}}$ field generated inside the DNP-NMR sample using the TE_{01} or TE_{11} mode for illumination is comparable to that obtained from illumination from an oversized corrugated waveguide in the HE_{11} mode.

While early gyrotrons for DNP-NMR operated in axisymmetric TE_{0n} modes, later tubes were built to operate in whispering gallery modes (TE_{mn} where $m > n$) to take advantage of the reduced mode competition [48–50]. However, this argument is not generally true and gyrotrons can be designed to work efficiently and stably in axisymmetric TE_{0n} modes. An internal Vlasov type quasioptical mode converter [51] with a dimpled wall launcher for conversion of the operating whispering gallery modes into a TEM_{00} beam is essential in modern high-power gyrotrons, especially for plasma heating applications [52]. The TEM_{00} output permits easy extraction of the microwave power from the gyrotron window and also coupling into the HE_{11} mode of an overmoded corrugated waveguide with high efficiency (~98.6 %).

On the contrary, high-frequency gyrotrons for DNP-NMR operate at low power (10–50 W) in lower-order whispering gallery modes ($TE_{11,2}$ or $TE_{9,3}$, etc.) at hundreds of GHz. At such frequencies it is impractical to design and fabricate a dimpled wall launcher. Hence the output mode purity of the TEM_{00} like beam is below 90 %. In almost all cases, the mode is directly coupled to an oversized corrugated waveguide for excitation of the HE_{11} mode without the use of a matching optics unit (MOU) as it is a common practice in megawatt power level gyrotrons. It is amply clear that the mode purity of the injected mode is poor in the case of DNP gyrotrons and hence it is highly debatable if the corrugated waveguide and the miterbends reliably operate with low ohmic loss and low spurious mode conversion as expected for the case of high mode purity (>99 %) of the HE_{11} mode used in megawatt power level gyrotrons.

5.1 Mode Converter

Our proposed choice of the TE_{01} mode for transmission should not present any additional challenges in the gyrotron design. On the contrary, if the gyrotron is designed to operate in

an axisymmetric TE_{0n} cavity mode [20, 38, 53] then a rippled wall mode converter (see Fig. 5a) can be incorporated either internal or external to the gyrotron tube for converting the operating cavity mode into a TE_{01} mode with high purity [54–56]. When incorporated internally, such a mode converter has several advantages: First, it can be designed to double as a mode converter and collector. Second, it would allow using a narrow-bore magnet, which can lead to substantial cost savings especially at high magnetic fields (>9.4 T). Unlike a quasioptical mode converter (see Fig. 5b), the rippled-wall mode converter is located on-axis, along the propagation direction of the electron beam [48, 53, 57]. This is a clear advantage over a quasioptical mode converter, which is typically located inside the warm bore of the gyrotron magnet and requires a magnet with at least 75 mm warm bore diameter to fit the off-axis quasioptical beam shaping mirrors.

Alternatively, if the gyrotron is designed to operate in a whispering gallery type mode with an output in the TEM_{00} -like Gaussian beam mode the beam can be transformed into a TE_{01} mode in a few steps. For instance, the Gaussian beam can be injected into a corrugated waveguide to excite the HE_{11} mode, which can then be converted into the TE_{11} mode using a surface-impedance mode converter in a corrugated waveguide [58]. Similar to the TE_{01} mode a smooth-wall transmission line can be used to transport the THz power from source to the DNP sample followed by a serpentine converter to transform the TE_{11} mode into TE_{01} mode [54] or the sample can be directly illuminated using the TE_{11} mode.

6 Conclusion

We have presented a new, simplified concept for THz instrumentation specifically designed for the requirements of DNP-NMR spectroscopy. Instead of downscaling gyrotron technology commonly used in megawatt devices to meet the specific requirements of DNP-NMR spectroscopy our proposed concept allowed us to significantly simplify the overall system design. At the heart of our proposed design is the use of the TE_{01} mode as the main mode for transmission of the THz power from the gyrotron source to the sample. The key benefits of the proposed design are

- Simplified transmission line design using a smooth-wall waveguide for transmission of the THz power.
- Simplified gyrotron and mode converter design. Due to the compact design of the mode converter, this will open the possibility to use narrow-bore magnets for gyrotrons.

Using 3D electromagnetic field simulations we have shown that irradiating the DNP sample with the TE_{01} or the TE_{11} mode has no disadvantages over the currently employed HE_{11} mode. In addition, it has been shown that larger enhancement factors can be obtained using a circular polarized mode as shown in recent experiments [26]. A prototype to experimentally study the proposed concepts is currently under fabrication.

7 Materials and Methods

7.1 HFSS Simulations

Electromagnetic field simulations were performed using ANSYS HFSS (ANSYS, Inc., Canonsburg, PA, USA) operating on a dual quad core 2.83 GHz Xeon-based server with 32 GB of RAM and 1.5 TB of hard disk space.

7.2 Simulation Model

The simulation model is very similar to the one described by Nanni et al. [46]. The sample, a frozen solution of glycerol and water ($\epsilon = 3.5$, $\tan\delta = 0.009$ [46]) is contained in a sapphire

rotor ($l = 15$ mm, active sample length) with an outer diameter of 4 mm and a wall thickness of 0.8 mm (sample volume 68 μL). The RF coil (silver) has eight turns with a radius of 2.5 mm and a wire thickness of 0.813 mm. The distance between the input port of the THz irradiation and the rotor axis is 5 mm with a diameter of the input port (waveguide) of 3 mm. The outside of the stator was modeled as a cylinder with perfect conductivity ($r = 6$ mm, $l = 16$ mm).

The simulations were performed for 264 GHz, using a total input power of 1 W and took on average 12 h for each frequency. The HE_{11} mode was modeled as a linear (power) combination of 85 % TE_{11} and 15 % TM_{11} mode.

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Fig. 1.
Schematic representation of components of a DNP-NMR system

Fig. 2. Magnitude and vector plots of the magnetic field components of the THz radiation for the HE_{11} , TE_{01} and TE_{11} modes

Fig. 3.

Geometry used in HFSS simulations. The *bottom* row shows the coordinate systems relevant the simulations (*left*) and the NMR experiment (*right*). The static magnetic field B_0 is aligned along the z' axis and θ_m denotes the magic angle with a value of 54.7° . Note that the y and the y' axis coincide

Fig. 4. HFSS simulations showing the magnetic field values of the THz radiation throughout the simulation model for the HE_{11} , the TE_{11} and the TE_{01} mode at 264 GHz. The RF coil is indicated in *light gray*. The irradiation input port is located at top of the simulation geometry, in the center of the rotor

Fig. 5. Mode converters for gyrotrons. **a** Rippled-wall mode converter to convert the TE_{0n} to TE_{0p} modes. **b** Quasi-optical mode converter with radial output to convert the TE_{mn} ($m \gg n$) to the TEM_{00} -like mode. The propagation direction of the THz beam is indicated by the arrow and the spent electron beam propagates along the axis of the waveguide in (a) and the launcher in (b)

Table 1

HFSS simulation results

Mode	Linear		Circular
	(H y)	(H z)	
HE ₁₁	1.24 (100 %)	1.21 (98 %)	–
TE ₁₁	1.25 (101 %)	1.24 (100 %)	–
TE ₀₁	–	–	1.22 (98 %)

The field strength $\gamma_e \overline{B}_{1e}$ is given in MHz. The percent values given in brackets are the derivation from the value for the HE₁₁ mode (H||y)