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Stripline probes for nuclear magnetic resonance

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Abstract

A novel route towards chip integrated NMR analysis is evaluated. The basic element in the design is a stripline RF 'coil' which can be defined in a single layer lithographic process and which is fully scalable to smaller dimensions. The sensitivity of such a planar structure can be superior to that of a conventional 3D helix. The basic properties, such as RF field strength, homogeneity and susceptibility broadening are discussed in detail. Secondary effects related to the thermal characteristics are discussed in simplified models. Preliminary NMR tests of basic solid and liquid samples measured at 600 MHz confirm the central findings of the design study. It is concluded that the stripline structure can be a valuable addition to the NMR toolbox; it combines high sensitivity with low susceptibility broadening and high power handling capabilities in a simple scalable design.

Keywords: NMR; Microcoils; Stripline; Microfluidics; High resolution NMR; Thin films; Wide-line NMR; RF coil design

1. Introduction

Nuclear magnetic resonance (NMR) has become the analytical method of choice in many areas of research. The main bottleneck that impedes certain advancements in the field of NMR spectroscopy is the relatively low sensitivity of the NMR detection method. The Boltzmann factors that determine the thermodynamic population difference between nuclear spin levels lead to very low signal intensities. For routine NMR analysis one typically requires several cubic millimeters of sample with at least 10^{16} nuclear spins present. There are many potential applications where the NMR technique could provide invaluable information on local structure and dynamics but where sample volumes are prohibitively small. For example in the case of small (bio) crystals, oriented fibrils, membranes or thin epitaxial layers, traditional NMR probes are not well matched to the sample dimensions and the less than optimal filling factor of the RF detection coil leads to reduced signal to noise performance. It was suggested more than a decade ago that microcoil probes can achieve a much better filling factor and thus the limit of detection can be reduced to less than 10^{15} nuclear spins [1,2]. This represents about a factor 10 improvement in signal to noise for small mass-limited samples when compared to the common macroscopic NMR probes. Capillary microcoil probes with sample volumes of around 1 μl are now available commercially and have become competitive for a number of analytical applications [3]. Nevertheless, it is desirable to be able to work with even smaller sample volumes, as e.g. encountered in microfluidic devices. The present detection limit for NMR is at the nanomole level, while for example mass spectroscopy detection limits are many orders of magnitude lower and fluorescence techniques approach the single molecule level. Commercial microcoil probes are based on capillary sample chambers with a tightly wound helical RF coil wrapped around this capillary. The coil itself is immersed in a cylindrical chamber filled with susceptibility matching fluid to avoid the static field distortions by the copper helix [4,5]. Without the

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susceptibility matching, the spectroscopic resolution is seriously compromised. With the method of handmade discrete element assembly it is not easy to scale this design down in size.

Several groups have explored lithographic methods for microcoil production [6–10]. In a typical example, the RF coil is a planar helix and the sample chamber is incorporated in a microfluidic chip to achieve a versatile 'lab on a chip' with in-situ NMR analysis of reaction products and process dynamics. Despite many efforts, these approaches have not yet penetrated mainstream NMR spectroscopy. To a large extend this is due to some practical and some more fundamental limitations of these planar microcoil designs. In general, the B_1 field homogeneity for these planar helices is less than ideal and multidimensional NMR methods are more difficult to implement. Also, it is not easy to achieve a low loss connection to the inner electrode of the helix. RF shielding currents increase the effective resistance and this leads to higher noise factors. The most important problem is the fact that the nearby windings of the microcoil tend to induce static field distortions that limit both the resolution and the signal to noise performance. In order to realize the potential sensitivity gain in microcoil NMR these problems must be solved, preferably in an affordable way that allows for automated mass production. Recently we introduced a novel type of NMR 'coil', the stripline, that departs from the idea of a helical structure to generate RF B_1 fields and detect NMR signals [11]. The microslot design by Maguire and coworkers [12] is another appealing alternative to helical NMR coils. The basic philosophy behind the microslot approach is comparable to the present stripline approach. In both cases the rf current is carried by a thin strip of metal in close contact with the sample. The main difference is that in the stripline geometry there is a symmetric ground plane that confines the rf radiation. The boundary conditions impose a homogeneous current distribution and thus a homogeneous B_1 field. In the microslot case, discrete elements are used to create to form the resonator. The stripline concept presented here is based on quarter or half wavelength resonators that can in principle be constructed on chip with no discrete soldered elements in the resonating circuit. The prototype stripline probe presented here is a double tuned H/X. In the present contribution we concentrate on the basic principles of the stripline design, aiming to overcome the problems encountered with planar helix coils. Proof of principle will be given in the form of preliminary results with a prototype double resonant stripline probe. It is well known that stripline technology provides a versatile method to route high frequency signals with low losses and well-defined delay times on printed circuit boards and semiconductor chips. Basically, planar stripline technology is the two-dimensional analog of the coaxial cable that is common in high frequency instrumentation. The sensitivity of the stripline configuration will be described in comparison to the more common 3D and planar helix coils, emphasizing in particular on the potential for further miniaturization. Furthermore the thermal characteristics that determine the limits in excitation bandwidth will be discussed. Next the issue of susceptibility broadening will be analyzed as this determines the ultimate resolution that can be achieved. Finally, a preliminary implementation and experimental verification of the stripline configuration will be presented.

2. Stripline modeling

Following Maxwell's equations, the only requirement to achieve a strong RF B_1 field is to create a high RF current density close to the sample volume. A helix is a convenient configuration, but by far not the only one. For example in a saddle coil, the relevant RF fields are generated by straight parallel wire sections. In a stripline the current is fed through a thin metal strip which is placed at some distance above a metal ground plane. A non-radiative closed configuration is realized by placing ground planes both above and below the strip. The magnetic field lines encircle the central strip, so the B_1 field points in opposite directions above and below the stripline. The boundary conditions at the metal surface dictate that the field lines run parallel to this surface and as a result the B_1 field homogeneity is quite good. A secondary consequence is that the current distribution in the strip is nearly homogeneous and the power dissipation is minimized. In Fig. 1 the B_1 field distribution for a micro stripline cross section is shown. In the following this geometry will be analyzed in more detail. It will be shown that for typical sample volumes the sensitivity is comparable or better than that of an optimized helix. The most important advantage, however, is the fact that the stripline design is fully scalable, so that the probe can be adjusted to the specific sample geometry. Since the structures are all single layer lithographically defined, it is straightforward to produce multiple probes on a single semiconductor wafer.

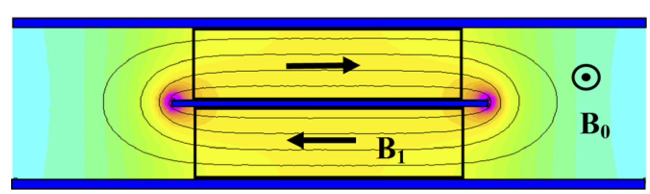

Fig. 1. Schematic cross-section of the stripline design. The RF field B_1 circulates the strip as is indicated by the field lines. The local RF field strength is indicated by the color map (blue corresponds to low B_1 field and red to high B_1 field). Because of the boundary conditions imposed by the metallic planes above and beneath the strip, the magnetic field lines are forced parallel to the surface. The result is a large volume with a homogeneous B_1 field. Suitable sample chambers are indicated by the two black rectangles where the B_1 field is homogeneous within about 10%. Also, the current distribution in the strip is homogeneous thus minimizing electrical losses. For NMR applications one can use the stripline geometry both for excitation and detection by insertion of this structure inside an external field. The static field B_0 can be oriented perpendicular to the cross section shown in the figure (along the stripline axis). The RF current that runs through the central copper strip flows parallel to the static field.