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A Theoretical Design Approach for Passive Shimming of a Magic-Angle-Spinning NMR Magnet

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Abstract

This paper presents a passive shimming design approach for a magic-angle-spinning (MAS) NMR magnet. In order to achieve a 1.5-T magic-angle field in NMR samples, we created two independent orthogonal magnetic vector fields by two separate coils: the dipole and solenoid. These two coils create a combined 1.5-T magnetic field vector directed at the magic angle (54.74° from the spinning axis). Additionally, the stringent magnetic field homogeneity requirement of the MAS magnet is the same as that of a solenoidal NMR magnet. The challenge for the magic-angle passive shimming design is to correct both the dipole and solenoid magnetic field spherical harmonics with one set of iron pieces, the so-called ferromagnetic shimming. Furthermore, the magnetization of the iron pieces is produced by both the dipole and solenoid coils. In our design approach, a matrix of 2 mm by 5 mm iron pieces with different thicknesses was attached to a thin-

walled tube, 90-mm diameter and 40-mm high. Two sets of spherical harmonic coefficients were calculated for both the dipole and solenoid coil windings. By using the multiple-objective linear programming optimization technique and coordinate transformations, we have designed a passive shimming set that can theoretically reduce 22 lower-order spherical harmonics and improve the homogeneity of our MAS NMR magnet.

Keywords

Ferromagnetic; linear programming; magic-angle-spinning NMR magnet; NMR; shimming

I. INTRODUCTION

A 1.5-tesla magic-angle-spinning (MAS) magnet was designed and built at the MIT Francis Bitter Magnet Laboratory [1]-[3]. The magnet assembly consists of one solenoid coil winding (z -axis) and one dipole coil winding (y -axis), as illustrated in Fig. 1. The combined magnetic field is at the 54.74° magic angle. Magnetic field mapping was performed with Hall probes when the MAS magnet was fully energized; the measured field homogeneity is around 200 part per million (ppm) in a 35 mm DSV (diameter spherical vume). Therefore, a shimming mechanism is required to improve the homogeneity to an NMR quality.

The basic principle of the MAS magnet is to minimize the dipole interaction in a nuclear magnetic resonance imaging process. The spinning feature is important, because some samples, if they were to be spun, are not able to survive spinning in the commercially available non-spinning magic-angle magnet [4]-[6].

A classic shimming approach is to use ferromagnetic pieces to decrease unwanted spherical harmonics. Much research has been conducted in ferromagnetic and active shimming of a solenoidal (z -axis) NMR magnet [7]-[11]. Additionally, previous research has shown ferromagnetic shimming algorithms for the magic-angle magnet [12]-[14].

For the passive shimming of a solenoidal NMR magnet, the magnetization direction and strength of the iron pieces are assumed to be the same; our design approach for a 700-MHz NMR magnet, we applied a harmonic coefficient reduction method to significantly improve the magnet homogeneity [15]. The difficulty for passive shimming of the magic-angle magnet is that the magnetizations of individual iron pieces are different from each other depending on their respective locations. In this paper we propose the following steps for passive shimming of a magic-angle magnet:

- Map the magnetic field with a high-resolution NMR probe following a helical path on a 10 mm radius and 40 mm long cylindrical surface along z -axis
- Derive 22 low-order spherical harmonic coefficients from the magnetic field measurement data for the z -axis only.
- Map the magnetic field with a high-resolution NMR probe following a helical path on a 10 mm radius and 40 mm long cylindrical surface along y -axis.

- Derive 22 low-order spherical harmonic coefficients from the magnetic field measurement data for the y -axis only.
- Calculate two sets of spherical harmonic coefficients for all iron pieces, each 25.4- μm thick.
- Develop a multi-objective linear programming model to increase the homogeneity of the magic-angle magnet in both z - and y -axes simultaneously.

II. COMPUTER MODELING AND SIMULATION OF MAGNETIC FIELD FOR A MAGICAL ANGLE MAGNET

Due to the complexity of the magic-angle magnet, magnetic field analysis is necessary to better understand the field distribution inside the magnet. A 3D finite element model was created using COMSOL Multi-physics software. The dimension and operating conditions are shown in Table 1. For simplicity, the solenoid coil (divided into top, middle, and bottom coils) and the dipole coil were treated as ring cylinders. The operating currents for the solenoid coils were modeled as multi-turn coils. However, it is very difficult for the software simulation engine to comprehend the dipole coil as a multi-turn coil; hence, two separate external current sources were created to simulate the dipole operating current.

Other components in the model include the iron yoke and the air cylinder (for empty spaces). The iron yoke was modeled as a hollow cylinder, 150-mm i.d., 275-mm o.d., and 600-mm high. The iron yoke in the simulation is low-carbon steel 1008 and the non-linear permeability of the steel 1008 was taken into considerations. The boundary condition of the magic-angle magnet model was created by a 0.3-m radius, and 1.0-m high air cylinder. The size of the air cylinder was big enough to get consistent simulation results without necessitating a large size file. Both the iron yoke and air cylinder are modeled with the Free Tetrahedral element mesh. The software is designed for a maximum mesh element size of 8 cm, and the minimum mesh size of 1 cm with a maximum element growth rate of 1.45.

The simulation result is shown in Fig. 2 (a). With both solenoid and dipole coils energized to generate a 1.5-T magic-angle field. The red arrows are normalized arrow volumes, which indicate the magnetic field has a direction at approximately 54° off the z -axis. The magnified 2-D plot of the y - z plane along x -axis are shown in Fig. 2 (b), which shows that the magnetic field in the center of the magic-angle magnet is uniform with several hot spots (or higher magnetic field strength regions) close to the inside diameter of the solenoid coil windings.

In a typical solenoid NMR magnet, the passive shimming iron pieces can be located on any part of the shimming tube, because the iron pieces are all assumed to have the same amount of magnetization. To understand the magnetization of iron pieces in the magic-angle magnet, four quadrants were created for the magnet by crossing x - z and z - y planes, and the magnetic field distributions are theoretically identical to each quadrant on the x - y plane. A line graph was created along a 45-mm radius circle on the x - y plane with the origin point located at (0, 0, 0), as shown in Fig. 3. Assuming the iron pieces have a 2-T saturation field, the magnetic field is saturated approximately between 0° and 35° . In other words, the iron pieces could

have uniform magnetization only in small regions within a 45-mm radius and 40-mm high shimming tube.

We examine two possible iron piece locations for our magic-angle NMR magnet, as shown in Fig. 4. If iron piece location #1 were chosen, the magnetization of the iron pieces would not be uniform. In our approach, the location option #2 is selected with two 40 mm by 50 mm possible shimming areas. The dimensions for a single iron piece are 5-mm wide, 2-mm high, and $1 \times 20 \times 25.4$ - μm thick. If the two shimming areas were covered fully with iron pieces, the number of iron pieces would be 400 total.

The next step is to determine locations and thicknesses of iron pieces to improve homogeneity. Although the finite element model is able to provide graphical illustrations of the magnetic field distribution, the resolution of the simulation result is very poor due to the mesh size limitations. Therefore, a mathematical model is developed in the next section.

III. DERIVE SPHERICAL HARMONIC COEFFICIENTS FOR A MAGNETIZED IRON PIECE

The ferromagnetic shimming principle is to select correct locations and thickness of the iron pieces such that the superposition magnetic fields created by the magnetized iron pieces can improve field homogeneity. A typical NMR magnet has a single solenoidal axis, and only spherical harmonic coefficients in one axis are considered. The magic-angle magnet field can be divided into two orthogonal fields, dipole and solenoid. Therefore, the magnetized iron piece also generates two separate fields, the z -axis and y -axis fields. Each magnetized iron piece acts as a small magnetic dipole and the corresponding magnetic field can be expressed as a finite series of low-order spherical harmonic terms. The iron piece in an arbitration point Q posses two separate magnetic dipole moments: $\mathbf{m}_z$, and $\mathbf{m}_y$.

For $\mathbf{m}_z$, polar coordinate is shown in Fig. 5 (a). Similar to a single-axis NMR magnet, for $r < r_q$ the magnetic field at point P can be expressed as a infinite series of expansions [16],

$$\mathbf{B}_{mz} = \mu_0 \frac{\chi \cdot dV \cdot H_z}{4\pi \cdot r_q^2} \sum_{n=1}^{\infty} \sum_{m=0}^{n-1} \epsilon_m \frac{1}{r_q^n} \frac{(n-m+1)!}{(n+m)!} P_{n+1}^m(\cos\alpha) r^{n-1} (n+m) P_{n-1}^m(\cos\theta) \cos m(\phi - \psi) \mathbf{z} \quad (1)$$

where $\mathbf{B}_{mz}$ is the magnetic field at point P generated by the magnetic dipole moment at point Q , n and m are positive integers, r_q is the distance between point Q and origin, χ is the susceptibility, dV is the differential volume of the iron piece, and r, θ are the polar coordinates for the point P .

By using a similar approach, the magnetic field at point P generated by the magnetic dipole moment $\mathbf{m}_y$ can be calculated using equation (1) with the coordinate system transformations, as shown in Fig. 5 (b). There are two independent spherical harmonic coefficient sets--one is for $\mathbf{m}_z$ denoted by $SH_{z_{\text{Iron } n}}^m$ and the other one is for $\mathbf{m}_y$ denoted by $SH_{y_{\text{Iron } n}}^m$

IV. THEORETICAL FERROMAGNETIC SHIMMING DESIGN FOR MAGICAL ANGLE MAGNET

Two separate magnetic field mapping runs will be performed, one along the z -axis and the other one is along the y -axis (or z' -axis). The spherical harmonic coefficients for z -axis ($SHz_{-mapping_n}^m$) and y -axis ($SHy_{-mapping_n}^m$) can be derived from the filed mapping data.

Since each iron piece in the shimming set is magnetized in both z - and y -axes, the overall spherical harmonic coefficients after the iron pieces are in place may be calculated as follows:

$$SHz_n^m = SHz_{-mapping_n}^m + SHz_{iron_n}^m \quad (2)$$

$$SHy_n^m = SHy_{-mapping_n}^m + SHy_{iron_n}^m \quad (3)$$

where SHz_n^m and SHy_n^m are the overall spherical harmonic coefficients for z -axis and y -axis respectively.

The objective of the passive shimming is to minimize the overall spherical harmonic coefficients for both the z - and y -axes. The magic angle magnet shimming involves solving the following minimization problem:

$$\min \left\{ \alpha_1 \sum_{n=0}^{\infty} SHz_n^m + \alpha_2 \sum_{n=0}^{\infty} SHy_n^m \right\} \quad (4)$$

where a_1 and a_2 are weight factors. Assuming the limit of n is 7 and limit of m is 6, there are 22 harmonic coefficients for the z -axis and another different 22 harmonic coefficients for the y -axis. Equation (4) can be rewritten as forty-four separate minimization objective equations. Therefore, the passive shimming problem can be solved by multiple-objective linear programming techniques with the following constraints:

$$0 \leq t_l \leq 20 \quad (5)$$

where t_l is the thickness of number l iron piece, $1 \leq l \leq 400$, and l is identified by the unique location of the iron piece. If the thickness t_l is zero, there is no iron piece at location l .

V. CONCLUSION AND FUTURE PLANS

A theoretical passive ferromagnetic shimming design approach for a magic-angle magnet is presented. By using the multi-objective linear programming technique, we may determine the thickness and locations of the iron pieces to minimize the unwanted spherical harmonics.

The future plan is to design and build ferromagnetic shimming for our 1.5-T MAS magnet. A special NMR magnetic probe apparatus will be designed and built to map the magnetic

fields along z-axis and y-axis. The measured magic-angle fields will be utilized to determine the spherical harmonic coefficients before and after the ferromagnetic shimming. We expect the ferromagnetic shimming will experimentally verify our design approach presented in this paper

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Fig. 1.
3D rendering of a simplified magical-angle-spinning NMR magnet.

(a)

(b)

Fig. 2.

(a) 3D simulation results with magnetic flux density plot of in the y-z plane slice, (b) zoomed in detail magnet flux density distribution near the magnet center.

Fig. 3. Magnetic flux density vs. arc angle plot along a quarter of circle with 45-mm radius on the x - y plane.

Fig. 4.
Illustrations of two possible passive shimming iron piece locations

Fig. 5.
 (a) Polar coordinate system for z -axis dipole moment, (b) Polar coordinate for y -axis dipole moment.

Table 1

COIL PARAMETERS FOR SPHERICAL HARMONIC ANALYSIS AND MAGNETIC FIELD SIMULATIONS

	Top Coil	Middle Coil	Bottom Coil	Dipole Coil
Inside Radius [mm]	52.5	52.5	52.5	62.5
Outside Radius [mm]	56.5	55.5	56.5	68.7
Length [mm]	57.0	49.0	57.0	486.0
Number of Turns	228	147	228	320
Max. mesh size [mm]	0.05	0.05	0.05	0.1
Min. mesh size [mm]	0.001	0.001	0.001	0.01
Operating current [A]	250	250	250	370