Induced Fields in Magnetized Materials: Calculations and the Uses

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Abstract

The induced field distribution in materials, which inherently possess large internal magnetic fields, or in materials which get magnetized when placed in large external Magnetic Fields, is of importance to material scientists to adequately categorize the material for its possible uses. It addresses to the questions pertaining to the structure of the material in the given state of matter by inquiring into the details of the mechanisms by which the materials acquire the property of magnetism. To arrive at the required structural information ultimately, the beginning is made by studying the distribution of the magnetic field distributions within the material (essentially magnetization characteristics) so that the field distribution in the neighborhood of the magnetized (magnetic) material becomes tractable. The consequences external to the material due the internal magnetization is the prime concern in finding the utilization priorities for that material. In the materials known conventionally as the magnetic materials, the internal fields are of large magnitude. To know the magnetic field inducing mechanisms to a greater detail it may be advantageous to study the trends and patterns with a more sensitive situation of the smaller variations in the already small values of induced fields can be studied and the Nuclear Magnetic Resonance Technique turns out to be a technique, which seems suitable for such studies. When the magnetization is homogeneous through out the specimen, it is a simple matter to associate a demagnetization factor for that specimen with a given shape-determining factor. When the magnetized (magnetic) material is in-homogeneously magnetized, then a single demagnetization factor for the entire specimen would not be attributable but only point wise values. Then can an average demagnetization factor be of any avail and how can such average demagnetization factor be defined and calculated .It is a tedious task to evaluate the demagnetization factor for homogeneously magnetized, spherical (ellipsoidal) shapes. An alternative simpler mathematical procedure could be evolved which reproduces the already available tables of values with good accuracy. With this method the questions pertaining to induced field calculations and the inferences become more relevant because of the feasibility of approaches to find answers.

KEY Words: Magnetic materials, Bulk susceptibility, Induced fields, Nuclear shielding, Demagnetization factors

1. Introduction:

The Nuclear Magnetic Resonance Technique can measure the Nuclear Shielding parameters. This Nuclear Shielding, particularly in solid single crystalline samples, arises due to the induced fields at the nuclear site in the molecules when these molecules themselves are placed in the crystal lattice points as determined by the symmetry elements of the Crystallographic Space Groups. As depicted in Fig.1, even though it is the prime concern in NMR experiments to detect the changes in the intra molecular electron-charge circulations by measuring the Nuclear Shielding, in order to obtain this specific molecular contributions, it becomes necessary to estimate the intermolecular [from the near neighbors and the far away bulk] contributions to induced fields at the nuclear site and appropriately take into account quantitatively to retrieve reliably, the intra molecular contributions only(1).

As illustrated in Fig.2, the NMR spectra typically consist of one spectral line from one equivalent set of nuclei. The

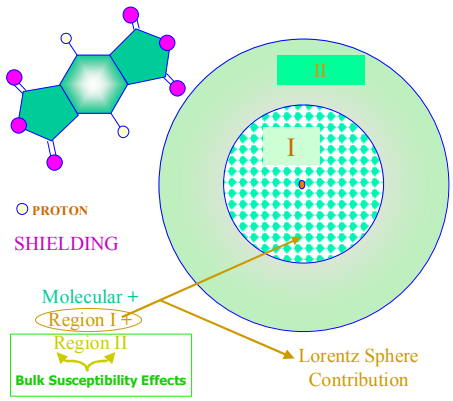
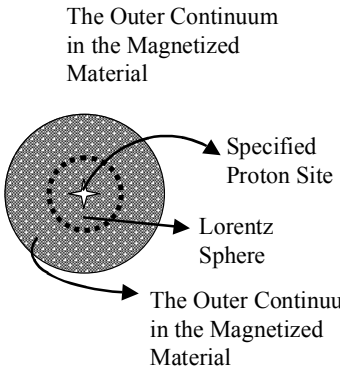


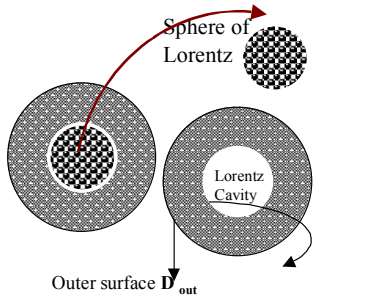
Fig.1 *Induced fields relevant in NMR Measurements*

line positions change when the intra molecular contributions vary from one molecule to another molecule.

If the diamagnetic sample is homogeneously magnetized, then the intermolecular contributions to the induced fields at the nucleus would cause an additional shift of the line. But, if the sample is inhomogeneous magnetized, then the induced field contributions at the nuclear sites over the extent of the sample would very and this can cause a line width and line shape variations. This aspect of the NMR technique is borne out by the considerations in Ref.(2) and the references cited there in.



$$\sigma_i = \Sigma_i \chi_i / R^3_i \, [1-(3.\mathbf{RR_i}/R^5_i)]$$



$$\mathbf{D}_{out} = -\mathbf{D}_{in} \quad \textit{Hence} \quad \mathbf{D}_{out} + \mathbf{D}_{in} = 0$$

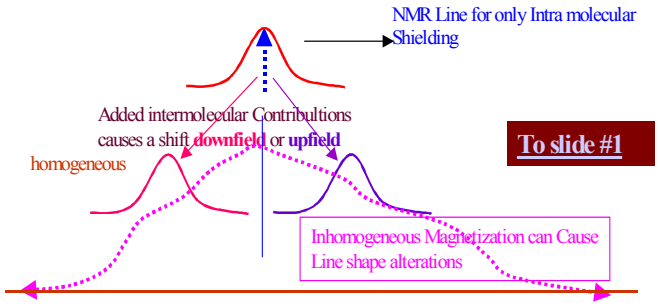


Fig.2 *Defining the terms relevant for induced field calculations in magnetized materials and the possible way line shape and width changes can arise in NMR spectra due to variations in induced field distributions.*

An effort to interpret the results of High Resolution Proton Magnetic Resonance studies in organic molecular single crystals made evident the various contributions to the induced field as described. Further it led to the devising of a simple summation procedure for calculating demagnetization factors for specimens with shapes describable, as the ellipsoids of revolution and this seem to be simplifying the matters with regard to estimating the trends of the induced field contributions in such diamagnetic samples. It is the target set in this paper to bring out this point of view to the material scientists and to make it obvious as to how this can be useful for the understanding of field distribution patterns inside magnetic materials. At this stand point, it would be worthwhile to note also that trying to pin point the origin of the field at a point within a magnetized material raises the issues of whether it has to be a microscopic average or a macroscopic average which is relevant (3).

2. Magnetic Dipole Model for the Calculation of Induced Fields:

Fig.2 illustrates the various demarcations, in a Single Crystalline Spherical specimen, for the calculation of the induced field at the specific site. By definition, the Lorentz Sphere is a semi micro volume element surrounding the specified site. The intermolecular contributions from within this Lorentz Sphere at the central point has to be calculated as a discrete sum over the molecular contributions from every one of the molecules occurring within this spherical volume element. The contribution form the outer region is the macroscopic bulk demagnetization, which depends on the specimen shape factors. The required discrete summation of the contributions from each of the molecule 'i' is accomplished using the Equation 1.

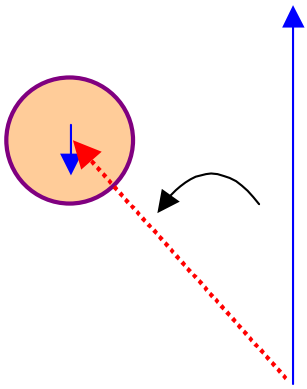
The Fig.3 depicts how at each individual lattice point; a spherical element can be placed with the consequence that due the susceptibility of the material in this spherical volume a magnetic moment is induced which is a dipole originating at the center of the sphere. This magnetic moment results in a Shielding at a distant point as per the Equation 1 and this shielding is proportinal to the induced filed at the distant point. When the radius of this spherical element is very small compared to the distance where its induced field is being calculated, then the point dipole approximation may be a valid approximation for the reliability of the induced filed values thus obtained. Fig.4 gives the equation with all the 3 x 3 matrices are written out in the expanded form so that the required matrix multiplications are obvious. Thus the discrete summation within the sphere appears to be obviously simple to program on the computer.

Even though, in all the efforts to calculate induced fields, ascertaining the magnitude of the induced magnetic dipole moment, which causes the induced field distribution around it, makes the beginning. Since the induced field

distribution around a point magnetic dipole is simpler to envisage and amenable by simpler equations, if one can ensure that the point dipole approximation would be applicable then the corresponding calculation of the induced field would become simpler. The discrete summation within the Lorentz Sphere has this possibility inherently because it is possible to assess the magnetic susceptibility values for the molecules and let this give rise to the magnetic dipole moment at the appropriate central point in the molecule and try to calculate the induced field by Equation 1 at the site of the nucleus. It is usually possible that the distances are much larger than the corresponding molecular dimensions (where the magnetic moment originates) and hence point dipole approximation would be valid and the summation over all the molecular point dipole sources can be computed.

$$\sigma_i = \Sigma_i \chi_i / R^3_i \, [1-(3.\mathbf{RR}_i / R^5_i)]$$

Induced field Calculations using these equations and the magnetic dipole model have been simple enough when the summation procedures were applied as described in the previous presentations and expositions.



Isotropic Susceptibility Tensor

$$\tilde{\chi} = \begin{bmatrix} \chi & 0 & 0 \\ 0 & \chi & 0 \\ 0 & 0 & \chi \end{bmatrix} \qquad |\vec{R}| = r$$

$$\sigma_{zz} = \frac{\chi}{r^3} - \frac{3 \bullet r^2 \bullet \cos^2(\theta) \bullet \chi}{r^5} = \sigma$$

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} = \frac{\begin{bmatrix} \chi_{xx} & \chi_{xy} & \chi_{xz} \\ \chi_{yx} & \chi_{yy} & \chi_{yz} \\ \chi_{zx} & \chi_{zy} & \chi_{zz} \end{bmatrix}}{r^3} - \frac{3 \bullet \begin{bmatrix} xx & xy & xz \\ yx & yy & yz \\ zx & zy & zz \end{bmatrix} \bullet \begin{bmatrix} \chi_{xx} & \chi_{xy} & \chi_{xz} \\ \chi_{yx} & \chi_{yy} & \chi_{yz} \\ \chi_{zx} & \chi_{zy} & \chi_{zz} \end{bmatrix}}{r^5}$$

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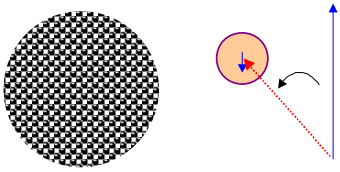


$$\sigma_{zz} = \frac{\chi}{r^3} - \frac{3 \bullet r^2 \bullet \cos^2(\theta) \bullet \chi}{r^5} = \sigma$$

Fig.3. *Equation for calculation of Shielding (induced field) by discrete summation of the contributions from within the Lorentz sphere. Explicit expression in terms of the matrix indicating the required matrix multiplication steps for such calculation.*

While handling a continuum situation, it is necessary to exercise discretion and hypothetically carve out small volume elements and associate the magnetic moment due to that volume susceptibility with that element and place it at the center. This hypothetical division should extend over the entire sample extent and from all these subdivided elements the contribution to induced field at a particular site can be calculated by an appropriate summation. But this concept in the case of a continuum essentially leads to an evaluation of an Integral for the effective summing. And it is well known in this case that the resulting integral thus set up becomes complicated even for the simpler case and evaluating it also is tedious. However for the case of the sample shapes which are regular ellipsoids of revolution evaluations of such integrals have been possible and for the various shape determining factors (the ratio of the polar / axial lengths for the shape) the Demagnetizing factors have been tabulated (4). In spite of this success, at the stages of the evolution the corresponding equations do not any longer retain the conceptualized simple physical picture of the point dipoles and hence at the end when one has a convenient table in the hand to use, this does not provide a convenient physical insight for interpreting the shape dependences for the other variety of shapes of specimen which occur and within which it is required to envisage the induced field distribution. This is more so because, for other shapes than the specific shape referred to above (that of ellipsoids) the materials have inhomogeneous magnetization over the extent of the specimen and it may not be possible to associate a single number as the shape dependent demagnetization factor applicable at any point within the specimen.

3. The Simple Summation Procedure in Place of the Integration Over the Bulk of Sample:

Fig.4 to Fig.6 illustrate in steps the alternative simple summation procedure, which evolved while being concerned with the interpreting the results of HR PMR

studies on organic molecular single crystals for the determination of the shielding tensor of protons in molecules. This procedure seems to be capable of reproducing with good accuracy the tables of Demagnetization factors referred to earlier, which were calculated evaluating the complicated integrals which were set up for the case of shapes attributable with a single demagnetization factor for any point within the specimen. Fig.4 explains the essential principle used for working out such a summation procedure.

At the outset what was sought for, was a possibility to divide the entire continuum bulk part of the specimen (excluding the Lorentz Cavity Fig.2) into small, closely packed elemental spherical volume elements each of which can be assigned a susceptibility value proportional to the volume of that spherical element (to be multiplied with the uniform Volume Susceptibility of the specimen). By the close packing criteria it is to be ensured that the entire volume of the material is considered for the calculation. When placed in a magnetic field, these elemental spherical elements would be considered as giving rise to a magnetic moment due to its inherent susceptibility assigned as above and thus induced Magnetic Dipole Moment is placed at the center of that sphere for its origin.

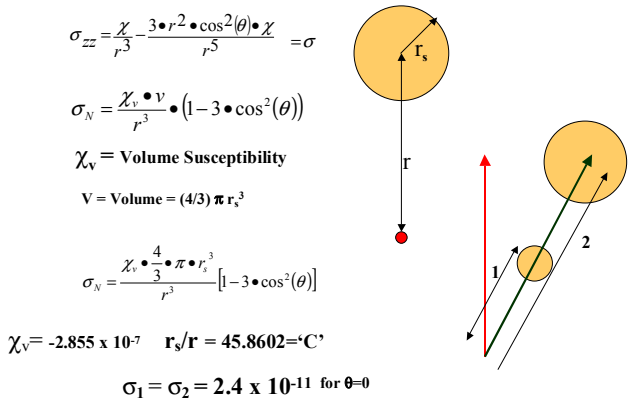


Fig.4. *The basic principle of the summation procedure illustrated.*

Thus this subdivision ensures that the total magnetic susceptibility of the entire specimen has been localized into closely packed elements with proportionate susceptibility values and the sum of all the elemental susceptibility values would yield the total susceptibility of the entire specimen. The main purpose of this subdivision is to ensure that, when, at any given point the induced field contribution is to be calculated, the distance from the center of the respective small volume element to that point would be much larger than the radius of the spherical element and hence the point dipole approximation would be valid. Setting up such an inherent criterion for the subdivision was the key to open up the possibility of this simple summation procedure, so that the resulting radius to distance ratio is small enough for all spherical elements when a particular point is specified where the induced field is to be calculated and for this particular case the point dipole approximation becomes automatically the valid approximation. As can be seen in Fig.4, this first step for the basic criterion is to ensure not only that the point dipole approximation is inherently valid but also that from every one of the elemental spheres along the length of a vector the subdivision ensures the contribution is the same. Which means if one knows the number of subdivided elements along the line, it is only required to know the number of such spheres to multiply with the contribution form any one spherical element. Fig.5 explains the equation used for evaluating the number 'n' of such point dipoles along the length of the vector. And the equation for 'n' was the result of a simple derivation. The Fig.6 illustrates the comprehensive situation for a macroscopic spherical sample, which will have to be considered with the subdivision criteria as above for arriving at the

For the Point Dipole Approximation to be valid practical criteria had been that the ratio $r : r_S = 10:1$

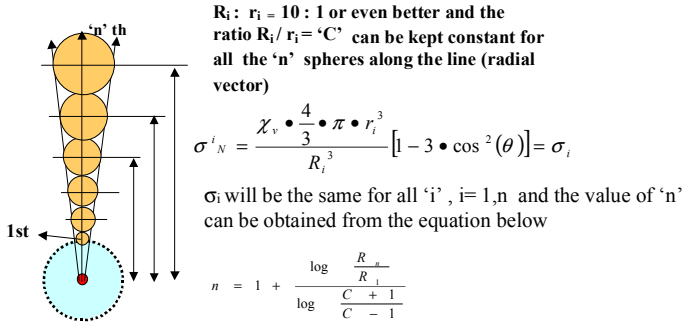


Fig.5. *An illustration of the equation required for the calculation of the number of close-packed spheres and the simultaneous criterion for the validity of point dipole approximation*

Demagnetization factor and induced fields at a central point in the sphere. This approach for evaluating the induced fields retained the simple physical basis of a dipole field distribution all through and at every stage and made it possible to think out such unconventional combination of outer specimen shapes with the inner Lorentz cavity shapes and deduce also the induced field variation trends by simple arguments. as depicted in Fig.7. In Fig.7 there is also a part, which explains the trends of discrete summations within the Lorentz Sphere.

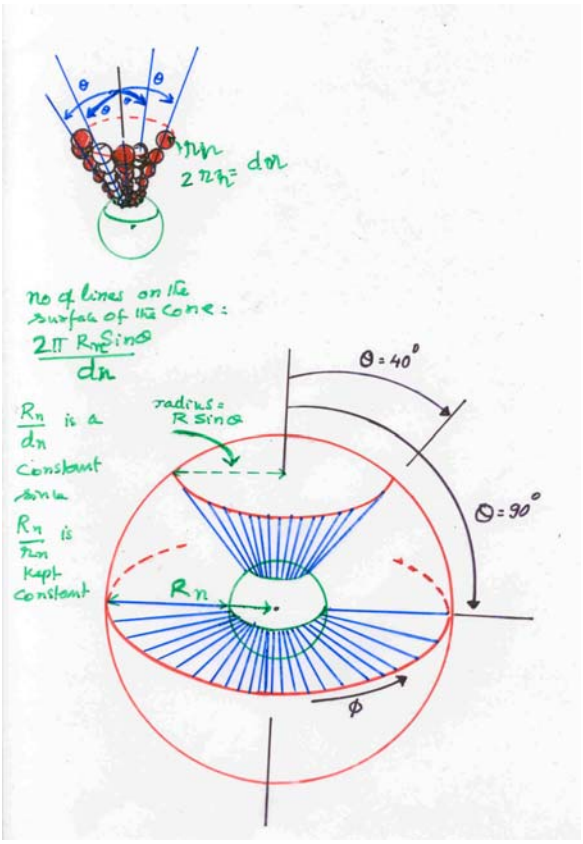
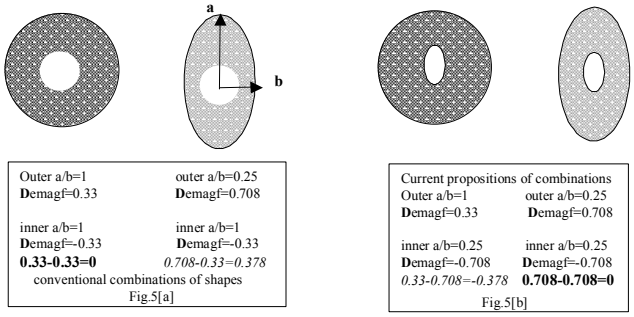


Fig.6. *A figure indicating the summation required over all the radial vectors with different pola and azimuthal angular coordinates.*



Conventional cases

Fig.7. *The summation procedure in the case of homogeneously magnetized sample;leading to the consideration of the unconventional combination of outer and inner shapes and the simplicity of handling such combinations to infer on the induced fields within the sample*

4. The Case of Homogeneous Magnetization and Inhomogeneous Magnetization:

Fig.8 illustrates the advantages of this summation procedure, which is the direct consequence of the possibility to retain the physical picture in view at every stage during the calculation. Besides this qualitative advantage which is to be emphasized as the most important achievement now, quantitative aspects also stand to gain for the possibility of handling a spindle like shape or a cylindrical shape and use these basic criterion for subdividing the magnetized sample to arrive at the induced filed values at any point and at every point even if the induced filed values would not be the same at all points as ensured for the special shapes of the regular ellipsoids of revolution. It is no consolation for such shapes that the sample is made up of the same material with the same susceptibility value uniformly through out the spindle-shaped specimen. The magnetization attributable to the susceptibility of a small volume element would be proportional to its volume. But, due to these induced magnetic moments the induced fields at various points within the specimen would sum up to the same value because of the resulting geometrical considerations for that shape. Thus if one can account for the fact that the ellipsoids result in the same value for the demagnetizing factor at every point within the specimen, then an account can be made also for the fact that for a spindle shaped specimen of the same material, the point by point values for the demagnetization factor within the specimen are not the same. In fact, by tabulating the values of the induced fields as a function of the spatial coordinate within the specimen for a given shape it is possible to compare the trends of the contributions as specific sums for comparable polar coordinates for different shapes and gain much greater insights than what was possible with the earlier method. These details would not be part of this paper since it would add to the length of this publication to such an extent as to become a distraction from the understanding of essential principles.

5. Further Advantages and the NMR as a Sensitive Tool:

1. First and Foremost, it was a very simple effort to reproduce the demagnetization factor values, which were obtained and tabulated in very early works on magnetic materials. Those Calculations which could yield such Tables of demagnetization factor values were rather complicated and required setting up elliptic integrals which had to be evaluated.
2. Secondly, the principle involved is simply the convenient point dipole approximation of the magnetic dipole. And, the method requires hypothetically dividing the sample to be consisting of closely spaced spheres and the radii of these magnetized spheres are made to hold a

convenient fixed ratio with their respective distances from the specified site at which point the induced fields are calculated. This fixed ratio is chosen such that for all the spheres the point dipole approximation would be valid while calculating the magnetic dipole field distribution.

3. The demagnetization factors have been tabulated only for such shapes and shape factors for which the magnetization of the sample in the external magnetic field is uniform when the magnetic susceptibility of the material is the same homogeneously through out the sample. This restricts the tabulation to only to the shapes, which are ellipsoids of rotation. Where as, if the magnetization is not homogeneous through out the sample, then, there were no such methods possible for getting the induced field values at a point or the field distribution pattern over the entire specimen. The present method provides a greatly simplified approach to obtain such distributions.
4. It seems it is also a simple matter, because of the present method, to calculate the contributions at a given site only from a part of the sample and account for this portion as an independent part from the remaining part without having to physically cause any such demarcations. This also makes it possible to calculate the field contribution from one part of the sample, which is within itself a part with homogeneously, magnetized part and the remaining part being another homogeneously magnetized part with different magnetization values. Hence a single specimen which is inherently in two distinguishable part can each be considered independently and their independent contribution can be added.

For the point 1 mentioned above view the web page URL:
http://saravamudhan.tripod.com/

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