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1991 J. Phys.: Condens. Matter 3 9811

(http://iopscience.iop.org/0953-8984/3/48/022)

J. Phys.: Condens. Matter 3 (1991) 9811–9816. Printed in the UK

COMMENT

Influence of diffused impurities on radiofrequency penetration

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Received 27 August 1991

Abstract. The low-temperature RF penetration profile is obtained for the particular case of impurity NMR probes diffused into the surface of a metallic host specimen. Conditions under which an exponential RF profile description remains appropriate are presented and the significance of the results for a previous analysis of single-passage NMRON data for ^{125}SbFe is assessed.

1. Introduction

In a recent article published in this journal (Yazidjoglou *et al* 1991), single-passage NMR on oriented nuclei (NMRON) results for single-crystal ^{125}SbFe were analysed in terms of an absolute theory without recourse to arbitrary scaling factors. Central to the analysis was the assumption that a radiofrequency (RF) field decays exponentially as it penetrates a metallic specimen. To this end, a weighted average (according to ^{125}Sb probe concentration) of single-passage curves computed for different RF strengths was performed. Further, a simple 'enhancement-like' model for the permeability was introduced to account for the dependence of the RF penetration on an additional DC polarizing field.

However, the situation is potentially more complicated because of the influence of impurities on the local electrical resistivity. This is particularly so at the low temperatures ($\leqslant$ 10 mK) employed for NMRON experiments where the residual resistivity is significantly dependent on impurity concentration. It has been suggested that a non-uniform impurity probe concentration will then lead to a non-exponential RF profile. The purpose of this brief article is to determine the form of the low-temperature RF profile for an impurity concentration which decreases exponentially with depth and, more specifically, to assess the significance of this postulated effect for the previous ^{125}SbFe analysis.

2. Theory

In the case of an RF field applied parallel to the infinite surface of a thick, planar specimen (which is a reasonable representation of the experimental situation so long as the probe nuclei are diffused into a small central region of the specimen's surface), the attenuation of the local RF field, $B_{\rm RF}$, as it penetrates the conducting medium is described by

$$\frac{\mathrm{d}B_{\rm RF}}{B_{\rm RF}} = -\frac{\mathrm{d}x}{\delta} \tag{1}$$

where x is the penetration depth and δ is the local RF skin depth given by

$$\delta = \left(\frac{2\rho}{\omega\mu}\right)^{1/2}. \tag{2}$$

ρ is the electrical resistivity, μ is the permeability and ω is the RF angular frequency. It is usual to assume that the concentration of thermally diffused probes decreases exponentially with depth according to

$$c(x) = c(0)\exp\left(\frac{-x\sqrt{2}}{x_{\rm RMS}}\right) \tag{3}$$

where $x_{\rm RMS}$ is the root mean square diffusion depth and $c(0)$ is the concentration at the surface ($x = 0$).

For probes which are chemically indistinguishable from the host atoms, the resistivity ρ is independent of the probe concentration and equal to that of the host material. Following Isbister and Chaplin (1990), the dimensionless parameter, w, is defined as

$$w = \frac{x_{\rm RMS}}{\delta_{\rm host}} \tag{4}$$

where $\delta_{\rm host}$ is the depth-independent RF skin depth, given by equation (2) for $\rho = \rho_{\rm host}$. The solution to equation (1) is then the familiar exponential decay,

$$\frac{B_{\rm RF}(x)}{B_{\rm RF}(0)} = \exp(-x/\delta_{\rm host}) = \exp(-wx/x_{\rm RMS}) \tag{5}$$

which was assumed for the recent analysis of ^{125}SbFe single-passage NMRON data.

However, for probes which are chemically distinguishable from the host atoms (i.e. for impurity probes), the low-temperature residual resistivity typically increases linearly with the local impurity concentration (Schröder 1983, pp 15–18) according to

$$\rho(x) = \rho_{\rm host} + Kc(x) = \rho_{\rm host} + \Delta\rho(x). \tag{6}$$

If it is assumed that the permeability, μ, remains unaffected by the impurities, then equations (2), (3) and (6) lead to a depth-dependent RF skin depth, $\delta(x)$, where

$$\frac{\delta(x)}{\delta_{\rm host}} = \left\{1 + \frac{\Delta\rho(0)}{\rho_{\rm host}}\exp\left(-\frac{x\sqrt{2}}{x_{\rm RMS}}\right)\right\}^{1/2} \tag{7}$$

and $\Delta\rho(0)$ is the impurity-induced increment in residual resistivity at the specimen's surface. Substitution of equation (7) into equation (1), followed by integration leads to

$$\frac{B_{\rm RF}(x)}{B_{\rm RF}(0)} = \left\{\frac{[1-(\delta(x)/\delta_{\rm host})]}{[1+(\delta(x)/\delta_{\rm host})]}\frac{[1+(\delta(0)/\delta_{\rm host})]}{[1-(\delta(0)/\delta_{\rm host})]}\right\}^{w/\sqrt{2}} \tag{8}$$

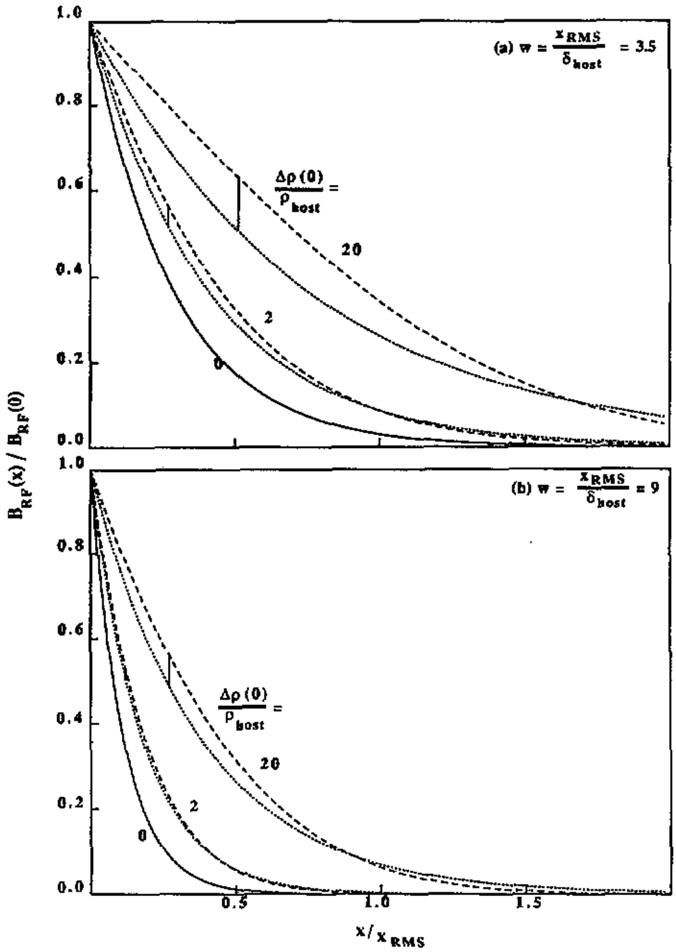

Figure 1. Low-temperature RF profiles computed for $\Delta\rho(0)/\rho_{\text{host}} = 0$ (full curves) and $\Delta\rho(0)/\rho_{\text{host}} = 2, 20$ (broken curves) with (*a*) $w = 3.5$ and (*b*) $w = 9$. The maximum deviations, D, of exponential curves (dotted curves) least squares fitted to the RF profiles are represented by full vertical lines.

where $\delta(0)$ is the local RF skin depth at the surface ($x = 0$). The dependence of $B_{\text{RF}}(x)/B_{\text{RF}}(0)$ on x/x_{RMS} (via equations (7) and (8)) is thus determined by the two parameters, w and $\Delta\rho(0)/\rho_{\text{host}}$. By comparison, the more familiar case for chemically indistinguishable probes (equation (5)) is determined by w alone.

RF profiles computed using equation (8) are shown in figure 1(*a*) ($w = 3.5$) and figure 1(*b*) ($w = 9$) for selected values of $\Delta\rho(0)/\rho_{\text{host}}$. The RF profile for $\Delta\rho(0)/\rho_{\text{host}} = 0$ corresponds to the pure host case (equation (5)). As expected, the RF penetrates further into the specimen as the impurity concentration, and hence $\Delta\rho(0)/\rho_{\text{host}}$, is increased. However, the transformation from an exponential RF profile into one which is significantly non-exponential is gradual. This means that, for sufficiently small impurity concentrations, it should be possible to treat the RF profile as an exponential of the form of equation (5) but with an effective parameter, w_{eff}, which will be larger than the w defined in equation (4). This work has employed standard linear regression procedure to analyse the semi-log plots of RF profiles computed in the range $0 \leqslant$

$x/x_{RMS} \leqslant 3$, subject to the condition that $B_{RF}(x)/B_{RF}(0) > 0.03$. Exponential curves so derived are shown as dotted curves in figure 1. One measure of the quality of the exponential approximation for any particular combination of w and $\Delta\rho(0)/\rho_{host}$ is the maximum deviation, D, of the computed RF profile from its fitted exponential. These maximum deviations are included in figure 1 as full vertical bars.

Figure 2 presents the full dependence of w_{eff} on $\Delta\rho(0)/\rho_{host}$ for selected values of w. In order to depict the variation in the quality of the exponential approximation to the RF profiles, the field has been divided arbitrarily into three regions; full curves have been used where $D \leqslant 0.03$, broken curves where $0.03 < D < 0.06$, and dotted curves where $D \geqslant 0.06$.

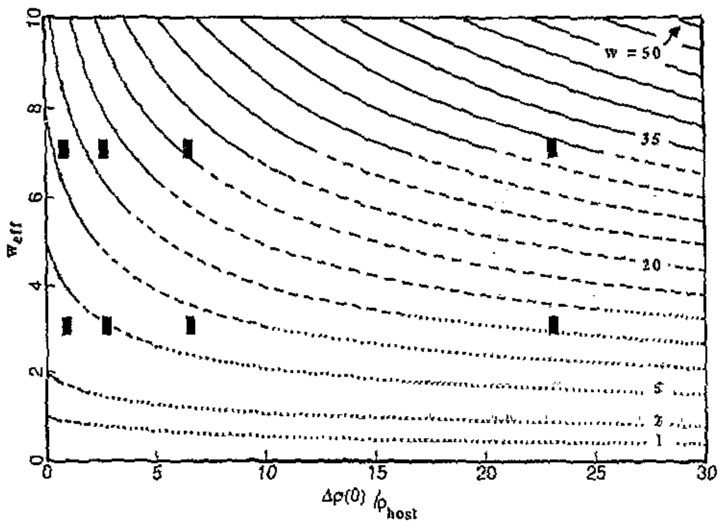

Figure 2. w_{eff} as a function of $\Delta\rho(0)/\rho_{host}$ for selected values of w. The full curves indicate regions where $D \leqslant 0.03$, the broken curves indicate regions where $0.03 < D < 0.06$, and the dotted curves regions where $D \geqslant 0.06$. The shaded regions refer to the possible interpretations of an earlier ^{125}SbFe analysis (see text).

3. Discussion and conclusions

The recent analysis of ^{125}SbFe single-passage NMRON data (Yazidjoglou *et al* 1991) ignored the influence of the diffused Sb impurities on electrical resistivity and assumed an exponential RF profile. Hence the analysis should be interpreted as having yielded the effective parameter, w_{eff}. In principle, w can be obtained from figure 2 if $\Delta\rho(0)/\rho_{host}$ is known. Furthermore, the reliability of the exponential approximation will, itself, depend on the value of $\Delta\rho(0)/\rho_{host}$.

However, in practice it is just as difficult to estimate $\Delta\rho(0)/\rho_{host}$ as it is to estimate w itself. Equation (6) relates $\Delta\rho(0)$ to the impurity concentration at the specimen's surface which, in turn, is determined by x_{RMS}. Estimation of $\Delta\rho(0)/\rho_{host}$ therefore requires values for the two parameters x_{RMS} and ρ_{host}. If the permeability model introduced by Yazidjoglou *et al* (1991) is employed, then estimation of a theoretical w requires values for these same two parameters. Table 1 demonstrates that estimates of $\Delta\rho(0)/\rho_{host}$ (column 3) and w (columns 4 and 6), for the investigated ^{125}SbFe

Table 1. Comparison of w estimates for ^{125}SbFe for both zero and saturating ($B_{app} = 0.6$ T) DC applied fields.

ρ_{Fe} $(\Omega$ m$) \times 10^{-9}$	x_{RMS} (μm)	$\Delta\rho(0)^e/\rho_{Fe}$	$B_{app} = 0$ T		$B_{app} = 0.6$ T	
			w^f_{theory}	$w(w_{eff} = 7)^g$	w^f_{theory}	$w(w_{eff} = 3)^g$
3.3[a]	5.3[c]	0.7	13	9	5	3.5
	1.4[d]	2.7	3.5	12.5	1.3	4.5
0.374[b]	5.3[c]	6.2	38	16.5	13	6
	1.4[d]	23	10	30	3.5	11

[a,b] Based on conductivity values of $\sigma = 3.3 \times 10^8 (\Omega\ \mathrm{m})^{-1}$ (White 1968) and $\sigma = 26.7 \times 10^8 (\Omega\ \mathrm{m})^{-1}$ (Fulkerson *et al* 1966) respectively.
[c,d] x_{RMS} estimates using diffusion constants of $D_0 = 0.11$ m^2 s^{-1} (Bruggeman and Roberts 1968) and $D_0 = 0.008$ m^2 s^{-1} (Myers and Rack 1978) respectively.
[e] $\Delta\rho(0) = Kc(0)$ where K(SbFe) $= 7 \times 10^{-8}$ Ω m/(at.% Sb) (Schröder 1983, p 253).
[f] Via equation (2) employing resonance frequencies and modelled $\mu_r^{\perp}$ values from Yazidjoglou *et al* (1991).
[g] According to figure 2 for given w_{eff} and $\Delta\rho(0)/\rho_{host}$ values.

specimen, depend very much on which combination of published diffusion constants and electrical resistivities is adopted.

Assuming that the single-passage NMRON data analysis yielded valid effective parameter values of $w_{eff} = 7$ (for $B_{app} = 0$ T) and $w_{eff} = 3$ (for $B_{app} = 0.6$ T), then the $\Delta\rho(0)/\rho_{host}$ estimates can be used in conjunction with figure 2 (shaded regions) to obtain the w values given in columns 5 and 7, respectively, of table 1. From table 1 it is seen that the best agreement between w so derived and the theoretical w, is achieved for $\Delta\rho(0)/\rho_{host} = 0.7$. This is the smallest of the $\Delta\rho(0)/\rho_{host}$ estimates which suggests that the exponential RF profile assumption was probably a good one. It is the authors' opinion that $D \leqslant 0.03$ is sufficient for the exponential approximation to be valid. In this regard, note that all $w_{eff} = 7$ shaded areas in figure 2 fall where $D \leqslant 0.03$, irrespective of the value of $\Delta\rho(0)/\rho_{host}$.

In conclusion, the influence of diffused impurities is to increase the overall RF penetration and, ultimately, to significantly distort the exponential RF profile. However, for the recent single-passage NMRON investigation of ^{125}SbFe, the assumption of an exponential RF profile most likely remains a valid approximation.

Acknowledgments

The authors thank Associate Professor D H Chaplin for his thorough reading of the manuscript. This work was supported by a grant from the Australian Research Council.

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