Quantitative Predictions of Dead Layers Induced by Surface Roughness in Isotropic Type II Superconductors

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July 17, 2015

Abstract

In type II superconductors where the coherence length $\xi$ is small compared to the London penetration depth $\lambda$, the London equation is valid and it predicts that magnetic fields decay exponentially in magnitude with the depth into the superconductor with a length scale $\lambda$, provided the interface is flat. Various direct measurements of $\lambda$ using low energy $\mu$SR on superconductors such as Yttrium-Barium-Copper-Oxide measure field profiles that differ from the anticipated exponential decay. There seems to be a dead layer, a distance $\delta$ over which the magnetic field magnitude does not decay, and some speculation has been made that this dead layer may be due to a suppression of the order parameter that causes the decay of a magnetic field, or surface roughness. A model of surface roughness has been studied for the case of a sinusoidally modulated surface roughness on an isotropic superconductor showing that in some cases the profiles resulting from surface roughness may be qualitatively similar to the dead layer phenomena in that the field magnitude decay rate may be slowed near the surface relative to a flat interface but that for modest roughness, the quantitative value of the dead layer is much smaller than the experiments measure. In this paper we extend this work in two directions: firstly, by using Atomic Force Microscopy data of Yttrium-Barium-Copper-Oxide crystals, we predict the field profiles the crystals could produce within the context of the isotropic London model of superconductivity given their actual surface geometry; and secondly, we consider how surface roughness could affect experimental values for $\lambda$ and $\delta$. Our work suggests that roughness within an isotropic model cannot produce the dead layers found in experiments on YBCO and that perhaps roughness must be combined with an anisotropy to yield the experimental dead layers; that the measurement of $\lambda$ may be influenced by the presence of roughness; and that the local field orientation does change slightly with respect to the direction of the applied field.

1 Introduction

A superconductor is a metal or alloy that undergoes a phase transition at a critical temperature, below which its resistance drops to zero. In this superconducting state, a superconductor will also expel externally applied magnetic fields. This phenomena of expelling a magnetic field is known as the Meissner effect. The superconducting state is maintained provided the external magnetic field is smaller than the critical applied field and the temperature is below the critical temperature, where this critical temperature decreases with the external magnetic field strength [5]. One of the early explanations for superconductivity is based on the London equation. This equation models the expulsion of the magnetic field.

The London equation of superconductivity governs how the magnetic field $B$ varies spatially inside a superconductor [5]. In an isotropic superconductor, as a partial differential equation it states

$$\nabla \times \nabla \times B = -B/\lambda^2$$

which when coupled with the divergence-free condition of magnetic fields as given by Maxwell’s equations

$$\nabla \cdot B = 0$$

gives

$$\nabla^2 B = B/\lambda^2.$$  

The length scale $\lambda$ is called the London penetration depth. If a superconductor takes up the region in the $(x,y,z)$—coordinate space $z > 0$ and the applied magnetic field at the interface pointing in the $\hat{x}$ direction is $B\hat{x}$ for some $B > 0$ then the magnetic field everywhere within the superconductor is given by

$$B = Be^{-z/\lambda}\hat{x}.$$  

Thus, as a function of depth $z$ into a flat superconductor, the magnetic field magnitude decays exponentially with a length scale of $\lambda$. A more detailed theory of superconductivity uses the Ginzburg-Landau equations, which include a parameter $\xi$ known as the coherence length. The coherence length is the length scale over which the value of $\lambda$ changes and reaches its bulk value. The London model is recovered for superconductors in which $\xi \ll \lambda$.  


There are notably two types of superconductors, type I and type II. Above the critical field, a type I superconductor immediately allows for magnetic field penetration, whereas a type II superconductor still partially expels the magnetic field until the field is large enough for all superconducting effects to be extinguished. Yttrium-Barium-Copper-Oxide (YBCO) is a type II superconductor with a planar crystal structure with highly anisotropic superconducting properties. In experiments, typically the orientation is chosen so that \( \lambda = \lambda_{a,b} \approx 110 - 130 \text{ nm} \). Given another orientation, \( \lambda = \lambda_c \gg \lambda_{a,b} \) [3]. The London penetration depth is a fundamental quantity to identify in a superconductor because the order parameter, the density of superconducting electrons \( n \), is directly related to \( \lambda \) with \( \lambda \propto 1/\sqrt{n} \). Understanding superconductivity and the effects of doping relies heavily upon accurate measurements of \( \lambda \). In our modelling work here, we will adopt an isotropic model, with \( \lambda = \lambda_{a,b} \) in order to study the effects of roughness alone.

Recently low energy \( \mu \)SR techniques have allowed for a direct measurement of \( \lambda \) by measuring the profile of magnetic field penetration in YBCO. These results have shown that near the interface, the magnetic field profile differs from a pure exponential decay predicted by the London equation with a flat interface [6]. There appears to be a dead layer of size roughly 10 nm - some distance over which the field decay is slowed. The work suggested that for modest roughness amplitudes \( A \) and spatial frequencies \( \omega_x \) and \( \omega_y \), the roughness effects were not quantitatively consistent with experimental data. However, without knowing the value of \( A \), the spatial frequencies present in the surface, or localized behaviours of the magnetic field near surface anomalies, the work cannot provide conclusive evidence one way or the other for surface roughness being the cause of the altered decay rates. In this paper, by using data collected through AFM measurements of YBCO crystals, we provide quantitative estimates of the values of \( \lambda \) and \( \delta \) that could be obtained in the presence of roughness where we assume an isotropic value of \( \lambda = 110 \text{ nm} \). The surface data we consider are given in figure 2.

Fig. 1: This diagram illustrates the geometry that we model. The superconductor can be thought to take up the region in space \( z \geq f(x, y) \), with the region \( z < f(x, y) \) being a vacuum. A magnetic field \( \mathbf{B}_{\text{applied}} = B\hat{x} \) is applied far away from the superconductor in the vacuum \( (z \to -\infty) \). Deep within the superconductor \( (z \to \infty) \), the London equation gives us that the field decays to zero.

The paper is organized as follows: section 2 provides a high-level overview of the numerical method we use to conduct our study and how it is validated; section 3 outlines our key results for the effects of surface roughness; finally, we conclude our paper and discuss future work in section 4.

2 Method of Study

The work here extends the numerical framework previously done in [9] to surfaces of arbitrary periodic shape. We refer the interested reader to this paper for a full discussion of the numerical formulation. This section explains briefly how the code has been extended and validated. A reader primarily interested in the results of
2.1 About the Numerical Framework

After nondimensionalizing and recasting the equations describing magnetic fields in free space and those describing magnetic fields in superconductors into an analytically equivalent form suitable for finite difference techniques, a new coordinate system is introduced, one in which the rough interface is made flat. Under such a transformation, the spatial derivatives in $x$, $y$, and $z$ are rewritten in the new coordinate system which involves derivatives of $\epsilon \cos(\omega_x x) \cos(\omega_y y)$. In this case, the surface shape is given analytically and the $x-$ and $y-$derivatives could be computed as such. If the surface is only known experimentally at a discrete set of points $z_{ij} = z(x_i, y_j)$ where $i$ and $j$ are discrete indices on some finite range, the exact value of the derivatives may be unknown, but it is possible to compute the derivatives to an arbitrary order of accuracy with respect to spatial mesh size. To ensure agreement between the two codes (the code of [9] that we refer to as the analytic approach and this extension that we refer to as the discrete approach) to second-order accuracy, it is necessary to compute the derivatives of the surface to at least third-order accuracy. The entire framework for the analytic code was based on second-order finite differences and thus the discrete code is second-order accurate.

We also take a further precaution in dealing with the surface numerically in ensuring the surface is reasonably smooth. Because the London equation and the numerical formulation require two derivatives to be taken, having regions of discontinuity could pose problems to the numerics. The numerical method works for surfaces that are periodic in $x$ and $y$. To deal with this in the case of the subsets we analyze in section 3.1, we take each subset and produce a periodic surface through reflections, essentially repeating the surface 4 times in different orientations as in figure 3. This ensures periodicity and continuity. Differentiability is not necessarily preserved but we do not notice behaviour in the numerical simulations indicative of problems due to lack of differentiability. Upon studying figure 2, we see that most surface variations vary slowly with a mean amplitude (average absolute deviation from the mean height) of around 4.6 nm. Relative to a length scale of $\lambda = 110$ nm, the surface amplitudes are small with a slow spatial modulation and we would expect the roughness to have a small effect. There are, however, very localized regions where the surface height changes rapidly and it is unclear if these regions could cause the non-exponential field profiles found in experiment.

Due to the discrete nature of the surface data in section 3.1, it is not possible to refine the finite difference mesh arbitrarily. We choose to take small subsets of the surface where the mesh size can be as small as the AFM data allow.

2.2 Validation of Numerical Results

The previous framework was rigorously verified to be second-order convergent and to be consistent with a three-term asymptotic expansion (in roughness amplitude) for the magnetic field everywhere in space when provided with a sinusoidal surface roughness. In order to validate the modified numerical work, we can compare...
the results of the analytic approach with the discrete approach in the average field profiles they predict. The analytic approach was second order accurate, and the discrete approach has been designed as such, by ensuring the discrete computation of the solution has an error, relative to the analytic code, that is smaller than second order for all surfaces of the form $z = \epsilon \cos(\omega_x x) \cos(\omega_y y)$. We verify that the maximum difference is indeed smaller than second-order, and that the discrete approach results converge to the analytic approach results. See table

<table>
<thead>
<tr>
<th>Discretization $N$</th>
<th>Max difference in profiles</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$2.2 \times 10^{-2}$</td>
</tr>
<tr>
<td>7</td>
<td>$2.4 \times 10^{-3}$</td>
</tr>
<tr>
<td>15</td>
<td>$3.0 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Table 1: Verification that the discretely extended code converges to the sinusoidal code with $z = 0.05 \cos(2\pi x) \cos(2\pi y)$. We compute the average field profiles in both versions of the code and calculate the maximum pointwise difference between the two predictions at different values of the mesh size which is $h = O(1/N)$. We validate that solutions of the two codes converge to each other at a rate of $O(h^{2.7})$ (through finding the slope of a log-log plot of the difference versus $h$), and given the sinusoidal code converged to the true analytic approach was second order accurate, and the discrete approach has been designed as such, by ensuring the discrete computation of the solution has an error, relative to the analytic code, that is smaller than second order for all surfaces of the form $z = \epsilon \cos(\omega_x x) \cos(\omega_y y)$. We verify that the maximum difference is indeed smaller than second-order, and that the discrete approach results converge to the analytic approach results. See table

2.3 Finding a Best Fit for the Penetration Depth and Dead Layer

In our numerical simulations, we assume the London penetration depth is precisely $\lambda_{\text{true}} = 110$ nm, but in the fitting, we seek to find values for $\lambda$ and $\delta$, the dead layer, so as to minimize the sum of the residuals squared between the data set $(z_i, B_i)$ and $(z_i, f_i)$ where

$$f_i = \begin{cases} B & z_i < \delta \\ B e^{-(z_i-\delta)/\lambda} & z_i \geq \delta, \end{cases}$$

$1 \leq i \leq N$. Deviations in the best fit $\lambda$ from $\lambda_{\text{true}}$ illustrate how the true $\lambda$ may be distorted due to surface roughness; positive values for the dead layer $\delta$ show that the roughness can produce a dead layer effect. We observe that most best-fitting dead layers are negative. For full clarity, we define the dead layer and penetration depth with the pseudocode given below:

- We begin with a set of numerically computed values for the average magnetic field $B_i$ at depth $z_i$, all in dimensionless units so that a scaled field strength of $|B_{\text{applied}}|$ has a value of 1 and a scaled distance of $\lambda_{\text{true}}$ has a value of 1. We then choose a value of $\lambda$.
  - For $1 \leq j \leq N - 1$ we define
    $$\delta_j = \min\{z_{j+1} - z_j, \max\{0, \log(\frac{\sum_{k=j+1}^{N} B_k e^{-z_k/\lambda}}{\sum_{k=j+1}^{N} e^{-2z_k/\lambda}})\}\}$$
    to be the value of $\delta \in [z_j, z_{j+1}]$ that minimizes the sum of squares of the residuals. If the minimizer lies to the left of the interval, the left endpoint is chosen, similarly with the right.
  - For $1 \leq j \leq N - 1$, we compute the sum of squares error with $\delta = \delta_j$ giving us $S_j = \sum_{k=1}^{j} (1 - B_k)^2 + \sum_{k=j+1}^{N} (e^{-z_k-\delta_j} - B_k)^2$.
  - Compute $j^* = \arg \min_j S_j$ and define the dead layer for this $\lambda$ to be $\delta^*_\lambda = \delta_{j^*}$.
  - Iterate this procedure over different $\lambda$ and determine the $(\lambda, \delta^*_\lambda)$ pairing that has the minimum sum of squares of all the cases.
- The dimensional quantities are then the above values multiplied by $\lambda_{\text{true}}$.

By giving the algorithm an input of a profile that is constant with value 1 up to a depth $\delta$ and which subsequently decays exponentially with dimensionless length scale $\lambda$, we find that the algorithm correctly calculates $\delta$ and $\lambda$.

3 Results

We compute the field profiles for different localized surface geometries and observe the field orientation. In all cases, we assume the underlying London penetration depth is $\lambda_{\text{true}} = 110$ nm. Through the simulations, we consider the average field magnitude as a function of depth (denoted by $s$). Note that $s$ is not the $z$–position, but the $z$–displacement with respect to the superconductor surface with $s < 0$ for vacuum and $s > 0$ for superconductor. Precisely, $s = z - f(x, y)$. The profiles are averaged over $x$ and $y$. Through the average field magnitude profiles, we estimate the best fitting dead layer $\delta$ and London penetration depth $\lambda$ as described above in section 2.3. By a dead layer, we refer to a depth $\delta$ so that if $s < \delta$ then the average field magnitude is constant and equal to its applied value and if $s > \delta$ then the average field magnitude decays exponentially from its applied value with length scale $\lambda$. This analysis gives insight into
Table 2: Best fit parameters for subsets of YBCO sample surface. All parameters are scaled relative to $\lambda_{\text{true}}$.

<table>
<thead>
<tr>
<th>Subset</th>
<th>London Depth $[\lambda_{\text{true}}]$</th>
<th>Dead Layer $[\delta_{\text{true}}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td>1.000</td>
<td>0.000</td>
</tr>
<tr>
<td>S2</td>
<td>0.987</td>
<td>0.001</td>
</tr>
<tr>
<td>S3</td>
<td>0.956</td>
<td>0.015</td>
</tr>
<tr>
<td>S4</td>
<td>0.951</td>
<td>-0.016</td>
</tr>
<tr>
<td>S5</td>
<td>0.960</td>
<td>-0.012</td>
</tr>
<tr>
<td>S6</td>
<td>0.956</td>
<td>0.016</td>
</tr>
<tr>
<td>S7</td>
<td>0.951</td>
<td>-0.016</td>
</tr>
<tr>
<td>S8</td>
<td>0.960</td>
<td>-0.009</td>
</tr>
</tbody>
</table>

how much the measured value of $\lambda$ differs from the true value when surface roughness is considered. We remark, however, that in the actual experiments, the field is not measured in the vacuum $s < 0$, however the numerical simulations do give this flexibility. As has been found in [9], the magnetic field magnitude in general decreases before reaching the superconductor surface and as a result many best-fitting dead layers appear to be slightly negative. Other experiments in the future could entail coating the superconductor with silver, which would allow for a measurement of the field in the $s < 0$ region.

3.1 YBCO Field Profiles

The full surface is depicted in figure 5, but we only analyze small subsets. We take eight subsets of the surface shown in figure 4. In some cases, we consider different orientations of the subset as explained in the figure. Through analyzing these subsets, we can assess how the actual surface of YBCO could affect the field profile and experimentally measured dead layers and penetration depths.

The dead layers and penetration depths predicted for subsets 1-8 are given in table 2. As we can observe, the dead layers are much smaller than the 10 nm measured in experiments [6], and are in fact mostly negative. This is a result of the fact that the magnetic field in general decays slightly in magnitude before reaching the interface and a negative dead layer captures this phenomena better. We also observe that in general, the best fitting penetration depth is smaller than $\lambda_{\text{true}}$ by roughly 5%. It is interesting to remark that the roughness orientation is important: subsets 3 and 4 are transposes of each other, as are subsets 6 and 7. In both cases, while the $\lambda$ values are similar, the values of $\delta$ change sign. Furthermore, subsets 3 and 6 are reflections of each other (with respect to depth), just as 4 and 7 are, and both fit parameters of $\lambda$ and $\delta$ are quite similar in value.

We provide plots of the average field magnitude and standard deviation in field magnitude of the two cases.
Figure 5: This is what the full YBCO surface looks like after it has been converted to a surface. Only every sixteenth point was plotted.

Figure 6: For subset S4, we plot the profiles of the average field magnitude ($|B_{\text{avg}}|$), the standard deviation in the average field ($|B_{\text{std}}|$), the average field profile for a flat superconductor with $\lambda = \lambda_{\text{true}}$ (“Flat”), and the fitted field profile with best fitting $\lambda$ and $\delta$ (“Fitted”).

Figure 7: For subset S6, we plot the profiles of the average field magnitude ($|B_{\text{avg}}|$), the standard deviation in the average field ($|B_{\text{std}}|$), the average field profile for a flat superconductor with $\lambda = \lambda_{\text{true}}$ (“Flat”), and the fitted field profile with best fitting $\lambda$ and $\delta$ (“Fitted”).

3.2 Field Orientation

One of the most interesting results from [9] was that due to roughness, the field orientation is perturbed. The field does not remain parallel to its applied direction throughout the superconductor. We remark that this is a key assumption in the interpretation of experimental results.
data: the magnetic field is assumed always to point in the same direction with fluctuations in magnitude at a given depth following Gaussian distributions \[2\].

Based on the numerical simulations, we plot the probability density functions for various parameters of interest for the magnetic field at various depths for subset 6. These probability density plots are generated with a Matlab routine for kernel density estimation \( \text{kde} \); this technique allows for an estimation of a probability density function (pdf) without making any assumptions about the underlying distribution.

The pdfs are both interesting and intuitive. If \( \theta \) denotes the angle between the applied field direction and the magnetic field direction at a given depth, then from the pdf of \( \cos^2 \theta \), we observe that the angle is heavily peaked near \( \theta = 0 \) and that the spread decreases with depth. Our choice of \( \cos^2 \theta \) as a parameter of interest instead of simply the angle \( \theta \) is due to the \( \cos^2 \theta \) reflecting the signal strength due to the muons in experiments precessing about an axis orthogonal to their polarization direction; the bigger this value, the more that a signal in the experiments can be attributed to the size of the magnetic field magnitude in the direction of the applied field. We affirm that the assumption that the magnetic field remains parallel to the applied field is quite accurate. Also, given that experiments cannot measure local magnetic properties right at the surface of a superconductor but rather at some finite depth inside, the assumption of the field remaining parallel to its applied direction appears to be even more valid in experimental interpretation.

The plots of the pdfs for the field magnitude and components are not Gaussian. With increasing depth, the average field values decrease in magnitude, consistent with a decay in field magnitude. It is interesting that the spreads in magnetic field \( y \)- and \( z \)-component values decrease but the spread for the \( x \)-component value increases with depth.

4 Conclusions

Based on experimental data of YBCO surface roughness, we have studied and made predictions about the effects roughness induces upon an isotropic type II superconductor.

The surface roughness causes an effect that is often not considered experimentally - that of a changing field orientation. Our results suggest, however, that despite the changing field orientation, for the roughnesses characteristic of YBCO, the effects would be negligible and therefore for the purposes of analysis of data, the field profiles can be assumed to have a local field that is parallel to the applied field.

Figure 8: The probability density function (pdf) of \( \cos^2 \theta \) describes the pdf of the value of \( \cos^2 \theta \) where \( \theta \) is the angle between the local magnetic field and the applied field direction. The pdfs for the field magnitude, and individual \( x \)-, \( y \)-, and \( z \)-components are also displayed. We considered three depths: \( s = 0\lambda_{\text{true}}, s = 0.1\lambda_{\text{true}}, \) and \( s = 0.4\lambda_{\text{true}} \).
Figure 9: Shielding supercurrents should flow parallel to the superconducting interface.

Through experimental measurements, the dead layer for YBCO appears to be on the order of 10 nm [6], which is much bigger than the dead layers that could be attributed to the surface roughness given by the AFM measurements of YBCO within the isotropic London model. On average we anticipate the figures provided in table 2 to be accurate predictors of how actual surface roughness could affect the fit values of $\lambda$ and $\delta$. It is very interesting that while the dead layers are effectively negligible for the AFM field profile predictions, the best fitting value of $\lambda$ is smaller than its true value, and it may be possible that experimentally fitted values of $\lambda$ are smaller than the true value of $\lambda$. We also note, however, that experimental fits have a non-negligible dead layer, which we do not obtain in our fitting. It is not necessarily true that if our model yielded a larger dead layer that $\lambda$ would be underestimated.

To explain a true dead layer phenomena in YBCO, it may be necessary to analyze the fully anisotropic model. In order to flow parallel to the interface, supercurrents would need to have a non-negligible component in the $c-$axis direction. With a strong anisotropy such that currents are heavily impeded in the $c-$direction, we anticipate the shielding would be much less effective and the field should not decay until after the roughness. See figure 9. Given that the surface roughness is on the order of 10 nm, it seems possible the roughness in combination with the anisotropy causes the dead layers. Such an analysis could in principle be done by further extending the numerical framework developed in this study.

It may also seem appropriate to consider the effects of the coherence length $\xi$ in YBCO on the field profile with the Ginzburg-Landau equations. The Ginzburg-Landau equations include the effects of the coherence length which describes how the magnetic field decay rate changes [8]. If it is comparable to $\lambda$, a non-exponential decay of field strength is noticed near the interface [12]. Although we have not considered such equations here, given the coherence length for YBCO is approximately 1.6 nm [10], it would be surprising for such a small length scale to give rise to an effect as large as the dead layers measured in experiments. Another potential explanation for the dead layer could be the suppression of the order parameter near the interface, possibly due oxidation effects [14], to a layering effect in chemical composition near the interface as studied in [13] for different conductors, or some other means.

We finally comment that this isotropic analysis could be appropriate in understanding measurements of more isotropic type II superconductors such as Rb$_3$C$_{60}$. The superconductor Rb$_3$C$_{60}$ has a cubic structure such that isotropy can be assumed with $\lambda \approx 247$ nm and a small coherence length $\xi \approx 2$ nm [15] [16] [17]. The isotropic London model should apply very well in this situation and we would not expect a dead layer if $\mu$SR were used to measure the field profile.

5 Acknowledgments

We would like to thank Rob Kiefl for his insightful comments in preparing this manuscript.

References

[1] Data provided by Rob Kiefl.


