SRF THEORY DEVELOPMENTS FROM THE CENTER FOR BRIGHT BEAMS*

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Abstract

We present theoretical studies of SRF materials from the Center for Bright Beams. First, we discuss the effects of disorder, inhomogeneities, and materials anisotropy on the maximum parallel surface field that a superconductor can sustain in an SRF cavity, using linear stability in conjunction with Ginzburg-Landau and Eilenberger theory. We connect our disorder mediated vortex nucleation model to current experimental developments of Nb3Sn and other cavity materials. Second, we use time-dependent Ginzburg-Landau simulations to explore the role of inhomogeneities in nucleating vortices, and discuss the effects of trapped magnetic flux on the residual resistance of weakly-pinned Nb3Sn cavities. Third, we present first-principles density-functional theory (DFT) calculations to uncover and characterize the key fundamental materials processes underlying the growth of Nb3Sn. Our calculations give us key information about how, where, and when the observed tin-depleted regions form. Based on this we plan to develop new coating protocols to mitigate the formation of tin depleted regions.

INTRODUCTION

The fundamental limit to the accelerating $E$-field in an SRF cavity is the ability of the superconductor to resist penetration of the associated magnetic field $H$ (or equivalently $B$). SRF cavities are routinely run at peak magnetic fields above the maximum field $H_{c,1}$ sustainable in equilibrium; there is a metastable regime at higher fields due to an energy barrier at the surface \cite{12}. $H_{th}$ marks the stability threshold of the Meissner state. In Fig. 1 we show results from linear stability analysis \cite{14}, valid near $T_c$, for $H_{th}$ as a function of the Ginzburg-Landau parameter $\kappa$, the ratio $\lambda/\xi$ of the London penetration depth $\lambda$ to the coherence length $\xi$. Niobium has $\kappa \approx 1.5$, most of the promising new materials have large $\kappa$. At lower temperatures, one must move to more sophisticated Eliashberg theories \cite{4}, for which $H_{th}$ is known analytically for large $\kappa$; numerical studies at lower $\kappa$ are in progress \cite{3}. Broadly speaking, the results so far for isotropic materials appear similar to those of Ginzburg-Landau.

This manuscript will briefly summarize theoretical work on $H_{th}$ (the threshold of vortex penetration and hence the quench field). First, we discuss the effect of materials anisotropy on $H_{th}$ \cite{12}. Second, we discuss theoretical estimates of the effect of disorder \cite{13}, and preliminary unpublished simulations of the effects of surface roughness and materials inhomogeneity. Third, we discuss key practical implications of theoretically calculated point defect energies, interactions, relaxation times, and mobilities in the promising new cavity material Nb3Sn. Finally, some magnetic flux is trapped in cavities during the cooldown phase, and the response of these flux lines to the oscillating external fields appears to be the dominant source of dissipation in modern cavities. We model potentially important effects of multiple weak-pinning centers on this dissipation due to trapped flux.

THE EFFECT OF MATERIALS ANISOTROPY ON THE MAXIMUM FIELD

Some of the promising new materials are layered, with strongly anisotropic superconducting properties (MgB$_2$ and the pnictides, for example, but not Nb$_3$Sn or NbN). Fig. 2 illustrates an anisotropic vortex (magnetized region blue, vortex core red) penetrating into the surface of a superconductor (grey). The anisotropy here is characteristic of MgB$_2$ at low temperatures, except that the vortex core is expanded by a factor of 30 to make it visible.

Near $T_c$, we find in ref. \cite{12} that a simple coordinate change and rescaling maps the anisotropic system onto the isotropic case (Fig. 1 above, as studied in ref. \cite{14}). We find, near $T_c$ where Ginzburg-Landau theory is valid, that $H_{th}$ is nearly isotropic for large $\kappa$ materials (Fig. 3). At lower temperatures, different heuristic estimates of the effects of anisotropy on $H_{th}$ yield conflicting results. Further work at lower temperatures could provide valuable insight into the

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Figure 2: From ref. [13], showing vortex (blue disk) and vortex core (red disk) of zero-temperature MgB$_2$ in the $ac$ plane, with the external magnetic field parallel to the normal of the plane of the figure. We have drawn the core region about 30 times larger with respect to the penetration depth, so that the core becomes discernible.

**Possible role of controlled surface orientation for cavities grown from these new materials.**

Figure 3: From ref. [12], showing the phase diagram of anisotropic superconductors in terms of mass anisotropy and GL parameters. The shaded blue and orange regions correspond to regions where the superheating field anisotropy can be approximated by $\gamma^{1/2}$ and 1, respectively, within 10% of accuracy. Note that the superheating field of MgB$_2$ is nearly isotropic near $T = T_c$.

**DISORDER-MEDIATED FLUX ENTRY AND MATERIALS ANISOTROPY**

Defect regions and inhomogeneity of superconductor properties can weaken the performance of SRF cavities. In ref. [12] we used simple estimates based on Bean and Livingston’s energy barrier arguments [2], to estimate the effects of disorder in lowering $H_{sh}$ by providing flaws that lower the barrier to vortex penetration. Here we use these calculations to shed light about the relationship between tin depleted regions, low critical temperature profiles, defect sizes and quench fields.

Consider an external magnetic field $B$, parallel to the surface of a semi-infinite superconductor occupying the half-space $x > 0$. If $B$ is larger than the lower critical field $B_{c1}$ (and smaller than $B_{c2}$), the vortex lattice phase is thermodynamically favored. However, if the field is not large enough, a newborn vortex line near the superconductor surface will have to surpass an energy barrier to penetrate the superconductor towards the bulk of the material. This instability typically is surmounted by the simultaneous entry of an entire array of vortices, whose interactions lower one another’s barriers. Disorder, in contrast, will lead to a localized region allowing one vortex entry at a time. Bean and Livingston provided simple analytical calculations for the energy barrier felt by one vortex line; we extended their calculation to estimate the dirt needed to reduce this barrier to zero at a quench field $H_q < H_{sh}$.

The new materials have larger $\kappa$, and in particular smaller vortex core sizes $\xi$; naively one would expect vortex penetration when flaws of size $\xi$ arise. Are these new materials far more sensitive to dirt than niobium? Reassuringly, Fig. 4 shows that the low values of the coherence length do not make these new materials substantially more susceptible to disorder-induced vortex penetration [13].

**Figure 4: From ref. [13], showing the reliability of vortex nucleation, in a simple model of Gaussian random disorder, for three candidate superconductors. Solid curves are for a 3D semicircular vortex barrier model; dashed curves are for 2D pancake vortex nucleation in a 2D superconducting layer.**

We can use our model to estimate the suppressed superconducting transition temperature $T_{cmin}$ and the flaw depth $D_c$ needed to allow vortex penetration, as a function of $H_{q}$ (or, in Tesla, $B_q$) (Fig. 5). For Nb$_3$Sn we find a flaw size of $D_c \sim 100$nm and $T_{cmin} \sim 12$K can allow vortex penetration and quenches at fields of $\sim 77$mT (Fig. 5), consistent with experimental results [8].

**TIME-DEPENDENT GINZBURG-LANDAU SIMULATIONS OF ROUGH SURFACES AND DISORDER**

To quantify the dependence of $H_{sh}$ on surface roughness and disorder, we have developed a time-dependent Ginzburg-Landau simulation. Fig. 6 shows the density $|\psi|^2$ of superconducting electrons at a field just above $H_{sh}$ (top left), showing the entry of several vortices for a 2D system with an irregular surface. On the bottom left, we show the corresponding...
Figure 5: (a) Critical temperature profile that allow nucleation of vortices in Nb$_3$Sn cavities at a field of $\sim 77$ mT. (b) Suppressed superconducting transition temperature $T_{c_{\text{min}}}$ (black), and flaw depth $D_c$ (red), as a function of the quench field.

supercurrent $j$; on the top right we show the magnetic field $H$ (perpendicular to the plane of the simulation), and on the bottom right we show the effect of surface roughness on $|\psi(\theta)|^2$ around the perimeter. Our initial results quantify how inward-curving regions in the plane perpendicular to the applied field on the perimeter can act as vortex nucleation sites in this geometry. An open question remains what the effect of curvature and surface roughness have when oriented parallel to the applied field.

The effect of roughness in Fig. 6 is to lower $H_{sh}$ by a few percent. By systematically varying the details of the roughness parameters, we can use this tool to identify at what scale roughness will have significant impact on vortex nucleation. SRF cavity roughness can be smoothed to varying degrees. Our TDGL environment can be used to find dangerous regimes or configurations that can have serious consequences for cavity performance.

We can also use this tool as a way to explore vortex dynamics and the effects of pinning sites on trapped residual magnetic flux. Pinning sites originate from inhomogeneities in the material, such as grain boundaries or spatial inhomogeneities in the alloy stoichiometry. By incorporating this information into our TDGL environment we can try to better understand the mechanisms driving residual resistance for typical cavities.

Figure 6: Spatial dependence of the density of superconducting electrons (top left), supercurrent (bottom left), and the induced magnetic field (top right). On the bottom right, we show the variation of the order parameter around the perimeter of the superconductor.

Figure 7: Illustration of antisite disorder. We estimate that on the order of 1% of lattice sites are affected by antisite defects “frozen in” from the high coating temperature. This would make them by far the most common point defect in Nb$_3$Sn layers.

Our initial work uses in-house DFT software to calculate defect formation and interaction energies, impurity energies, and energy barriers in Nb$_3$Sn. We have found that antisite disorder (Figure 7), rather than impurities or vacancies, likely sets the electron mean free path in Nb$_3$Sn and may

DFT CALCULATIONS

Nb$_3$Sn cavities are created by depositing tin vapor on the surface of a niobium cavity, which reacts with the niobium to form an irregular surface layer of the compound. Of interest are regions of “tin depleted” Nb$_3$Sn, known to have a lower superconducting transition temperature than the surrounding Nb$_3$Sn. These regions may be the nucleation centers responsible for quenches observed well below $H_{sh}$ expected for perfect Nb$_3$Sn [8].

Density functional theory (DFT) can be used to study layer growth, tin depletion, and other features of Nb$_3$Sn layers at the single-particle level. This information, combined with experimental data and accounting for the effects of grain boundaries and strain, makes it possible to build a multiscale model of layer growth.
also be responsible for collective weak pinning. We have also found that under certain conditions during growth, it is energetically favorable for Nb$_3$Sn to form at tin-depleted stoichiometry, while during annealing existing Nb$_3$Sn near the surface or grain boundaries can become tin-depleted by diffusion (Figure 8). Either or both of these tin depletion mechanisms may result in quench nucleation centers; by understanding them we can for the first time make informed modifications to the coating process in an attempt to limit tin depletion and produce better cavities.

![Figure 8: Experimental data showing tin depletion.](image)

DYNAMICS OF TRAPPED VORTICES; POTENTIAL ROLE OF WEAK PINNING

When the field is high enough for penetration of new vortices, one expects a cascade of vortices leading to a quench. Vortices trapped during the cooling process, while not immediately fatal, do act as sources of residual resistance. Experiments show that the non-BCS surface resistance is proportional to the trapped flux, both for nitrogen-doped Nb cavities [6] and for Nb$_3$Sn [9]. This suggests that trapped vortices may be a dominant contribution to the quality factor of the cavity.

Previous studies of the residual resistance due to a trapped flux line [7] focused on the Bardeen-Stephen viscous dissipation [1] of a free line pinned a distance below the surface, as the external field drags the line through a otherwise uniform superconducting medium. Experimental measurements in nitrogen-doped Nb cavities showed good agreement to this theory, except that the distance to the pinning center was presumed to change linearly with the mean-free path [6] as it changes due to nitrogen doping. Since nitrogen (or other contaminant gases [10][11]) should act as weak pinning centers (with many impurities per coherence length cubed), we have been modeling the role of weak pinning in vortex dissipation.
calculations suggest that incorporating both can provide a reasonable explanation of the experimental data, but we still do not obtain quantitative agreement.

![Figure 11](image.png)

Figure 11: From ref. [9], showing the sensitivity of residual resistance to trapped magnetic flux, as a function of the peak rf field.

**CONCLUSION**

The collaboration between scientists inside and outside traditional accelerator physicists made possible by the Center for Bright Beams has been immensely fruitful. This proceedings illustrates the richness of the science at the intersection of accelerator experimentalists working on SRF cavities with condensed-matter physicists with interests in continuum field theories and *ab-initio* electronic structure calculations of materials properties. (One must also note the important contributions of experimental condensed matter physicists in the collaboration.) Current SRF cavities are pushing fundamental limits of superconductors, and are a source of fascinating challenges for theoretical condensed-matter physics. Conversely, we find that theoretical calculations are remarkably fruitful in guiding and interpreting experimental findings.

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