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THEORETICAL ANALYSIS OF QUASIPARTICLE OVERHEATING, POSITIVE Q-SLOPE, AND VORTEX LOSSES IN SRF CAVITIES*

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Abstract

The surface resistance of an SRF cavity is an important measure of its performance and utility: lower resistance leads directly to lower cryogenic losses and power consumption. This surface resistance comprises two components, namely the "BCS resistance", which depends strongly on the quasiparticle temperature, and a temperature-independent "residual resistance", which is often dominated by losses due to trapped magnetic vortices. Both components are generally dependent on the RF field strength. Here we present a summary of recent theoretical advances in understanding the microscopic mechanisms of the surface resistance, in particular addressing niobium hydride formation and quasiparticle overheating (using the tools of density functional theory) and discussing issues with existing models of the positive Q-slope, a field-dependent decrease in the BCS resistance, and possible paths for improvement of these models. We also discuss trapped flux losses using ideas from collective weak pinning theory.

INTRODUCTION

In SRF (superconducting radio-frequency) accelerators, the chief intrinsic loss mechanism is the surface resistance R_s of the superconducting cavities. In general R_s can be considered as the sum of a temperature-dependent "BCS resistance" and a temperature-independent "residual resistance":

$$R_s = R_{BCS}(T) + R_0. \qquad (1)$$

These surface resistances are generally dependent on the RF field strength; much of modern SRF research is dedicated to understanding and reducing the loss mechanisms quantified by R_s.

In the CBB (Center for Bright Beams), an NSF Science and Technology Center, we have been studying and developing theoretical models of the BCS and residual components of the surface resistance. This work can be grouped into three areas: studies and assessment of existing models of the positive Q-slope observed in nitrogen-doped and high-frequency cavities; studies using DFT (Density Functional Theory) to explore the effects of microscopic impurities and impurity structures; and modeling of vortex-oscillation losses.

THEORIES OF POSITIVE Q-SLOPE

Nitrogen-doped niobium SRF cavities have been demonstrated to have intrinsic quality factor Q_0 that is greater than that of clean niobium at low fields and that *increases* as the RF field strength increases, contrasting the traditionally observed "Q-slope" where Q_0 decreases with increasing B_{RF} [1, 2]. The magnitude of this "anti-Q-slope" or "positive Q-slope" has been demonstrated empirically to depend on the doping level, quantified by the electron mean free path, as well as the cavity frequency [3, 4]. A few models have been proposed to explain this remarkable phenomenon; here we discuss some of these models and possible issues therein.

In general, a model of the temperature-dependent superconducting surface resistance (the "BCS resistance") can be calculated from the net transition rate between energy levels ϵ and $\epsilon + \hbar\omega$, where $\omega = 2\pi$ times the RF frequency. The resistance is proportional to a convolution integral of the density of states weighted by the difference of the distribution $f(\epsilon)$ of quasiparticles (broken Cooper pairs) at these energy levels, as in the Mattis-Bardeen theory [5, 6]:

$$R_{BCS} \propto \int_{\Delta}^{\infty} N(\epsilon)N(\epsilon + \hbar\omega)\,[f(\epsilon) - f(\epsilon + \hbar\omega)]\,d\epsilon. \qquad (2)$$

The above relation suggests that field-dependent reduction in R_{BCS} can be achieved by smearing the density of states N near the singularity at $\epsilon = \Delta$ or by populating levels of high ϵ, thereby reducing $f(\epsilon) - f(\epsilon + \hbar\omega)$.

A 2012 theory developed by Goldie and Withington assumes the standard BCS form of the quasiparticle density of states and then uses kinetic methods to calculate a stationary *non-thermal* distribution function due to photon emission or absorption, increasing $f(\epsilon)$ at high energy levels [7]. The proposed population of high-energy quasiparticles is consistent with the reduction in the microwave surface resistance observed by de Visser *et al.* [8]. However, the reduction in this experiment occurs at temperatures and field strengths much lower than those typically encountered in SRF cavities and in particular those where the positive Q-slope has been observed in nitrogen-doped niobium cavities. It remains unclear whether this model is valid for the material parameters and environments pertinent to SRF applications.

A 2014 theory developed by Gurevich uses the Keldish technique of non-equilibrium Green's functions to rederive the nonlinear quasiparticle conductivity, which is used to

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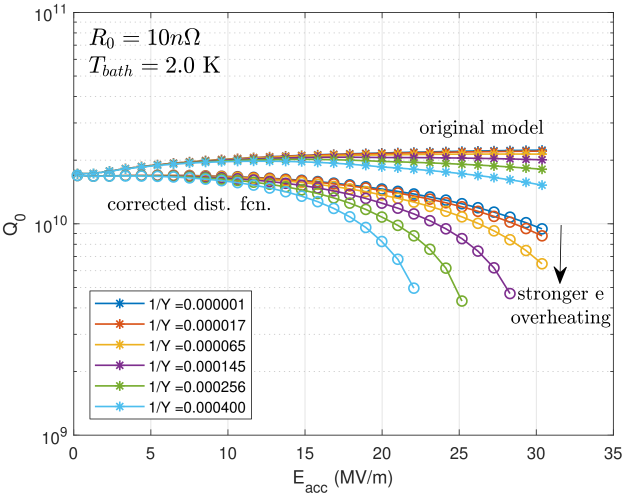

Figure 1: Theoretical calculations of the field-dependent quality factor of a 1.3 GHz cavity using the as-written Gurevich model and our corrected distribution function, shown for a range of magnitude of quasiparticle overheating (quantified by $1/Y$). In the corrected calculation the positive Q-slope becomes negligible.

compute the surface resistance [9]. The model is presented in two regimes, one "weak RF" case where a relatively strong DC magnetic field is applied to a superconducting surface superimposed over a low-amplitude RF field $B_{\text{RF}} \ll B_{\text{DC}}$ and one "strong RF" case where there is only an RF field applied. A further consideration given is the effect of quasiparticle overheating due to thermal effects. The "strong RF" regime is claimed to be directly applicable to dirty-limit niobium SRF cavities operating near 1 GHz and 2 K. We have found success fitting this model to experiment at 1.3 GHz, both for cavities doped at high temperature (traditional nitrogen doping) as well as for "nitrogen-infused" cavities [3, 10, 11]. On the other hand, the model's predictions for the strong RF case at other frequencies are not in good agreement with experiment (measured at 650 MHz to 3.9 GHz) [4, 12].

Our deeper consideration of the theory finds two areas of concern for its applicability. First, the model assumes that the distribution of quasiparticles $f(\epsilon)$ at arbitrary time t is equal to the *zero-field* distribution; this assumption is not properly justified and leads to considerable enhancement of the positive Q-slope by mitigating the losses due to the smaller gap at high fields. After correcting this assumption and replacing the zero-field distribution function by a stationary field-averaged distribution, we find that the positive Q-slope becomes negligible at strong fields. Figure 1 demonstrates the results of the corrected calculation compared to the as-written model. In our understanding, this correction does not affect the "weak RF" case or the conclusions about quasiparticle overheating, which do not rely on the non-equilibrium distribution function.

Second, and more generally, it is our belief that the appropriate basis of eigenstates for periodically-driven quantum systems is the Floquet basis, with energy levels generalized to Floquet quasi-energies (see for example [13]). We are currently investigating simple models and plan to use Density Functional Theory to explain the role played by Floquet states in microwave suppression, which will ultimately lead to a theory of the positive Q-slope.

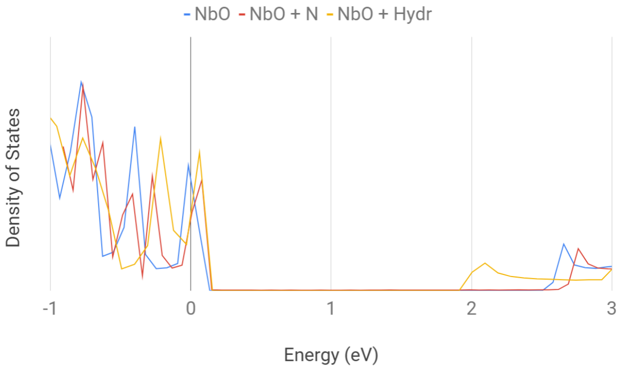

Figure 2: DFT calculation of the bandgap in the electron density of states at a niobium surface with native oxide. Lines indicate pure niobium and niobium with nitrogen and hydrogen sub-surface structures; nitrogen impurities increase the bandgap while hydrides reduce it.

PROGRESS WITH DFT STUDIES

Recent work in the CBB has used Density Functional Theory [14] to investigate the effects of impurities in niobium SRF cavities; in particular these studies have focused on hydride formation and the effect of interstitial C, N, O, and H impurities on the electron mean free path and on quasiparticle overheating.

Niobium hydrides are known to contribute to R_0 losses, and have been empirically reduced by high-temperature degassing of affected cavities [15]. Our calculations show that interstitial hydrogen in a niobium lattice preferentially forms surface hydrides in the form of platelets, consistent with previous experimental observations (*e.g.* [16]) as well as recent CBB studies with STM (scanning tunneling microscopy); publication of the CBB results is forthcoming. Further, we have calculated how sub-surface structures such as hydrides or interstitial impurities might affect the surface bandgap; since STM normally only probes the first atomic layer, this sub-surface information will be useful for STM studies of impurity-doped niobium surfaces investigating the hydride-suppressing effect of nitrogen and other impurities [17, 18]. Figure 2 demonstrates how the bandgap changes for different sub-surface structures.

Using DFT we have also estimated the effect of the most common impurities (H, C, N, O) on the electron mean free path ℓ, finding for a 1/128 atomic concentration $\ell \approx 50$ nm for H and $\ell \approx 10$ nm for C, N, and O, scaling inversely with changing concentration. This is consistent with experimental observations [19, 20] and is an important step in understanding quasiparticle overheating in SRF cavities, particularly those with positive Q-slope [3, 9]. Building on this success,

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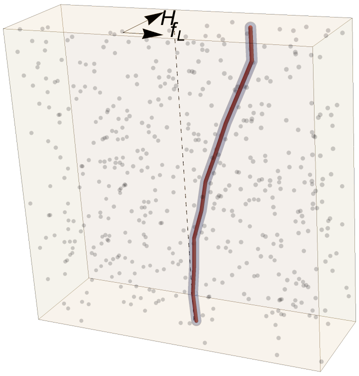

Figure 3: Illustration of a superconducting vortex line subject to a surface Lorentz force and the collective action of random pinning forces.

we are in the process of studying the effect of interstitial impurities on quasiparticle-phonon heat transfer efficiency; we expect results of these calculations to be published soon.

VORTEX LOSSES IN SRF CAVITIES

A major component of the microwave surface resistance in SRF cavities is the residual resistance due to trapped magnetic flux. Magnetic flux is trapped as the cavity is cooled through its critical temperature T_c: while steep temperature gradients make for a well-defined superconducting phase front that can fully expel magnetic flux (*i.e.* the Meissner effect), if a cool-down is performed without a sufficiently large temperature gradient, magnetic flux can become trapped in defect areas with reduced superconducting properties such as T_c, H_c, or Δ. This flux forms quantized vortices of flux Φ_0 as the surrounding material transitions to the superconducting state. Figure 3 illustrates such a vortex. Under excitation by the RF field in an accelerator cavity, these vortices can oscillate and dissipate power, decreasing the intrinsic quality factor Q_0 of the cavity and manifesting as a temperature-independent residual resistance $R_0 = \alpha B_{\text{trapped}} + \beta B_{\text{trapped}} B_{\text{RF}}$ with linear "sensitivity" to the strengths of the trapped field and the RF field (given here by α and β) [21].

Recent work in the CBB has resulted in the development of a model of these losses in dirty-limit superconducting cavities based on vortex dynamics and collective-weak-pinning theory [22]. Using simple estimates, approximate analytical calculations, and numerical simulations, Liarte *et al.* make predictions and comparisons with experiments performed at CERN and Cornell on Nb-Cu, doped Nb, and Nb_3Sn SRF cavities. The model considers the effect of a rugged pinning potential landscape, finding hysteretic losses that result in the observed linear dependence of the sensitivity of $R_0(B_{\text{trapped}})$ to the trapped flux as a function of the amplitude of the RF field. There are two distinct regimes of vortex dissipation; at low field, losses due to trapped flux are dominated by hysteretic losses due to pinning and increase linearly with the strength of the RF field, while at high field, the losses are dominated by viscous forces and approach a constant value with respect to the RF field strength. The transition between these regimes is predicted by the model for various material parameters; Fig. 4 illustrates this sensitivity to trapped magnetic flux.

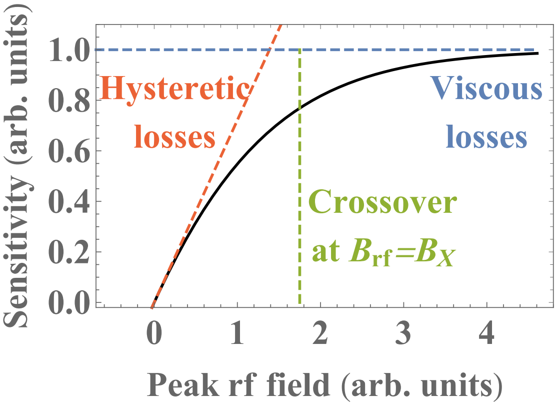

Figure 4: Illustration of the sensitivity of the residual resistance due to trapped magnetic flux as a function of the RF field strength, with crossover between the low-field linear regime and the high-field constant regime. Originally published in [22].

The model yields a set of formulas describing the sensitivity of R_0 to trapped flux, finding for the *low-field* hysteretic losses

$$\beta = \frac{R_0}{B_{\text{trapped}} B_{\text{RF}}} = \frac{16\pi}{3\Phi_0} \frac{f\lambda^2}{c(\kappa) j_{\text{d}}}, \tag{3}$$

where Φ_0 is the flux quantum, f, λ, and κ are the resonant frequency, penetration depth, and Ginzburg-Landau parameter of the superconductor, $c(\kappa)$ gives a correction to the line tension of the vortices, and j_{d} is the depinning current. The transition to the viscous-force-dominated constant loss regime is given by

$$B_{\text{X}} = \sqrt{\frac{2}{3\sqrt{3}\pi} \frac{\mu_0 \rho_{\text{n}} c(\kappa) j_{\text{d}}^2}{\kappa^2 f}}, \tag{4}$$

where ρ_{n} is the normal-conducting resistivity of the material.

CONCLUSIONS

We summarize recent work in the Center for Bright Beams towards improving our theoretical understanding of SRF cavity efficiency. We have assessed existing models of the positive Q-slope, finding them in need of improvement and proposing Floquet theory as a possible tool for understanding the SRF surface resistance; we have used Density Functional Theory to study the effects of impurities on hydride growth, the electron mean free path, and quasiparticle overheating; and we have modeled vortex-oscillation losses in several relevant SRF material regimes.

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