Effect of Inhomogeneous Disorder on the Superheating Field of SRF Cavities

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Northwestern and Fermilab established the Center for Applied Physics and Superconducting Technologies (CAPST) with a focus on superconductivity at the forefronts of accelerator physics, quantum simulation and computing, and discovery of superconducting materials for next generation quantum devices [Press Release].

Superconducting RF Cavities

Superconducting Niobium RF cavities for particle acceleration operate near the limit of their electrical current carrying capacity. A goal of CAPST research is to determine the factors limiting their performance and to provide ideas and criteria for next generation superconducting RF cavities for particle acceleration. CAPST research is a multi-disciplinary approach to achieve a fundamental understanding of the physical, chemical and structural mechanisms responsible for dissipation of electrical currents in SRF cavities.

CAPST Research
Superconducting Materials

CAPST researchers grow high-quality single crystals and thin film superconductors for basic and applied research. Single crystals of high temperature cuprate superconductors, heavy fermion superconductors and multi-band superconductors are grown and studied by NMR, SANS and transport studies. Superconducting compounds of NbSn3 and MgB2 are investigated for use in SRF technology for particle acceleration.

Superconducting Devices

CAPST researchers are fabricating and characterizing hybrid superconducting, magnetic, and strong spin-orbit materials as for electronic and spintronic devices. Josephson Junctions fabricated with Ferromagnetic tunnel barriers (SFS devices) provide a route for generating voltage-controlled superconducting spin currents that can interact and control nano-scale magnetic elements (magnetic quantum dots).
Electrodynamics of Superconductor-Vacuum Interfaces

Program: First-Principles + Materials Inputs:
Current Response & Local EM Fields for Superconducting-Vacuum Interfaces

\[ \mathbf{J}(q, \omega) = -\frac{1}{c} \mathcal{K}(q, \omega; \mathbf{A}) \cdot \mathbf{A}(q, \omega) \]
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Material Inputs:
- Fermi Surfaces - DFT & dHvA
- Pairing/Decoherence via Electron-Phonon Coupling

\[ \vec{J}(q, \omega) = -\frac{1}{c} \leftrightarrow R \left( \frac{q}{\omega; \vec{A}} \right) \cdot \vec{A}(q, \omega) \]
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Material Inputs:

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- Impurity & Structural Disorder
- Surface Scattering: \(S_{\text{surf}}(\mathbf{p}, \mathbf{p}')\)

- surface structure factor
- mesoscopic roughness
- backscattering
- Andreev scattering
- sub-gap dissipation

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Theoretical & Analytical Tools
- Migdal-Eliashberg: electron-phonon
- Asymptotic Expansions:
  \[ \frac{k_B T_c}{E_f}, \frac{\hbar}{\tau E_f}, \frac{\hbar}{p_f \xi}, \frac{\hbar \omega}{E_f} \ldots \]

- Selection Rules & Scattering Theory
- Keldysh Transport Equations

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Developing Methods & Codes to Compute the Nonlinear A.C. Surface Impedance
- Nonequilibrium Quasiparticle, Cooper Pair & Vortex Dynamics

Electronic band structure of Niobium

DFT Calculation of the Electronic Band Structure

\[ \text{Ef} = 18.1 \text{ eV} \]

\[ \text{Nb} = \text{[Kr]} 4d^4 5s^1 \]

24 bands

Fermi Energy = 18.1 eV

2 bands cross the Fermi energy

\[ \text{P. Giannozzi et al., J. Phys. Cond. Mat. 29 465901 (2017)} \]
Phonons in Niobium

Theory - Phonon dispersion
Inelastic Neutron Scattering

- DFT Perturbation Theory
  - Baroni, S., de Gironcoli, S., Dal Corso, A. & Giannozzi, P., Rev. Mod. Phys. 73, 515562 (2001),
  Phonons and related crystal properties from density-functional perturbation theory
Electron-Phonon Spectral Function $\alpha^2 F(\omega)$

- Maxium Phonon Frequency: $\hbar \omega_{\text{max}} = 27.0 \text{ meV}$
- $\lambda = 2 \int_{0}^{\infty} d\omega \frac{\alpha^2 F(\omega)}{\omega} = 1.18$
- Electron-Electron Repulsion: $\mu^* = 0.30$
- Eliashberg Theory: $T_c = 9.47 K$
- Tunneling Inversion
  G. Arnold et al., JLTP 40, 225 (1980).

- DFT Perturbation theory fails for Nb?
- Inversion of $dI/dV$ from PETS does not yield bulk $\alpha^2 F(\omega)$?
- Nb surface has defects that suppress the high-$\omega$ spectrum?
Eliashberg Equations

\[ \hat{\Sigma}_{npa} (i\omega_j) = g_{nm,\nu}(k', k) \hat{G}_{mk'} (i\omega_{j'}) g_{mn,\nu}(k, k') + V_{k-k'} (i\omega_j - i\omega_{j'}) \hat{G}_{mk'} (i\omega_{j'}) \]

\[ Z_{nk} (i\omega_j) = 1 + \frac{\pi T}{N(\varepsilon_F) \omega_j} \sum_{mk' j'} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta_{mk'}^2 (i\omega_{j'})}} \lambda (nk, mk', \omega_j - \omega_{j'}) \delta (\varepsilon_{mk'} - \varepsilon_f) \]

\[ Z_{nk} (i\omega_j) \Delta_{nk} (i\omega_j) = \frac{\pi T}{N(\varepsilon_F)} \sum_{mk' j'} \frac{\Delta_{mk'} (i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{mk'}^2 (i\omega_{j'})}} [\lambda (nk, mk', \omega_j - \omega_{j'}) - \mu_c^*] \delta (\varepsilon_{mk'} - \varepsilon_f) \]
Strong coupling superconducting gap

\[ \Delta_0 = 1.56 \text{ meV} \]

\[ T_c = 9.45 \text{ K} \]
Anisotropy of the Gap and Fermi Velocity

- **Gap Anisotropy:**
  \[ \Delta_{\text{max}} = 2.54 \, \text{meV} \quad \Delta_{\text{min}} = 1.38 \, \text{meV} \quad \Delta_{\text{av}} = 1.56 \, \text{meV} \]

- **Velocity Anisotropy:**
  \[ v_f^{\text{max}} = 1.3 \times 10^6 \, \text{m/s} \quad v_f^{\text{min}} = 0.2 \times 10^6 \, \text{m/s} \]

- **Strong Anisotropy of the Fermi Velocity - Impact on Critical Currents?**
Theoretical Program

- Develop Computational Code & Tools for Electronic Structure of Nb
  - Phonon Spectra & Density of States - DFT Perturbation Theory
  - Electron-Phonon Coupling - Eliashberg Theory
  - Strong-Coupling Superconducting Gap on the Fermi Surface

- Incorporate Disorder and Surface Scattering
  - Constraints from Surface and Materials characterization

- Develop computational transport theory - charge and heat response under strong EM field conditions at the superconductor-vacuum interface
SRF Performance Goals - What Can Theory Provide?

- Push to high Q-factor & Reduce a.c. dissipation up to high $E_{\text{acc}}$

- Understand physics of current response at $f \gtrsim \text{GHz}$ at high $B_s$

- Push $E_{\text{acc}}^{\text{max}}$ - processes determining Meissner stability/breakdown

$\Downarrow$

Materials based theory of Non-Equilibrium Superconductivity under Strong Nonlinear A.C. Conditions
Meissner state is metastable up to the superheating field.

Superheating field (Max Field Gradient)
Superheating field is determined from local critical current

- We solve *simultaneously*
  1. Eilenberger equation
     - for quasiparticle spectrum
  2. Gap equation
     - for excitation gap
  3. Impurity T-matrix equation
     - for the effect of disorder
  4. Maxwell’s equation
     - for $B$-field and current profiles

- To obtain *superheating field*, increase surface field until current reaches critical value
Nonlinear D.C. Current Response

\[ \vec{j}_s(x) = -eN_f \int d\varepsilon \tanh \frac{\varepsilon}{2T} \langle \mathbf{v}_f \mathscr{A}(\hat{\mathbf{p}}, \varepsilon, x) \rangle_{\hat{\mathbf{p}}} \]

- Spectral Function: \( \mathscr{A}(\hat{\mathbf{p}}, \varepsilon; x) \equiv \frac{-1}{\pi} \text{Im} \mathcal{G}(\hat{\mathbf{p}}, \varepsilon; x) \)
- Local impurity self-energies, \( \hat{\Sigma}_{\text{imp}}(x) = \gamma(x) \langle \hat{\mathcal{G}} \rangle \)
- Local superconducting order parameter: \( \Delta(x) \)
- Local condensate momentum, \( \mathbf{p}_s = \frac{\hbar}{2} \nabla \vartheta - \frac{e}{c} \mathbf{A} \)
- Perturbation expansion in \( \varepsilon \in \{ \xi/\lambda_L, \xi/\zeta \} \)

Propagator for Quasiparticles and Cooper Pairs:

\[ \frac{-1}{\pi} \hat{\mathcal{G}}(\hat{\mathbf{p}}, \varepsilon, x) = \frac{[\tilde{\varepsilon}(\varepsilon, x) - \mathbf{v}_f \cdot \mathbf{p}_s(x)] \hat{\tau}_3 - \tilde{\Delta}(\varepsilon, x) (i \sigma_y \hat{\tau}_1)}{\sqrt{|\tilde{\Delta}(\varepsilon, x)|^2 - [\tilde{\varepsilon}(\varepsilon, x) - \mathbf{v}_f \cdot \mathbf{p}_s(x)]^2}} \equiv \left[ \mathcal{G} \hat{\tau}_3 - \mathcal{F} (i \sigma_y \hat{\tau}_1) \right] \]

\[ \tilde{\varepsilon}(\varepsilon, x) = \varepsilon + \gamma(x) \langle \mathcal{G}(\hat{\mathbf{p}}, \varepsilon, x) \rangle_{\hat{\mathbf{p}}} \quad \tilde{\Delta}(\varepsilon, x) = \Delta(x) + \gamma(x) \langle \mathcal{F}(\hat{\mathbf{p}}, \varepsilon, x) \rangle_{\hat{\mathbf{p}}} \]

\[ \Delta(x) = \frac{g}{2} \int d\varepsilon \tanh \frac{\varepsilon}{2T} \text{Im} \langle f(\hat{\mathbf{p}}, \varepsilon, x) \rangle_{\hat{\mathbf{p}}} , \]

\[ \partial_x^2 \mathbf{p}_s(x) - \frac{4\pi e}{c^2} \vec{j}_s[\mathbf{p}_s(x), \gamma(x)] = 0 \]
Disorder Suppresses Supercurrents

$B_{sh}$ is affected via 2 mechanisms

- **✓** Longer penetration depth
  - $more$ screening current

- **✗** Lower critical supercurrent
  - $less$ screening current

\[
\lambda_{eff} = B_{sh}^{-1} \int_0^\infty dx B(x)
\]

For uniform disorder

\[
\frac{B_{sh}}{B_0}
\]

Penetration depth dominates

Current suppression dominates

\[
\begin{align*}
\text{Effective penetration depth} & \\
\text{Impurity scattering rate, } \gamma & \end{align*}
\]

\[
\begin{align*}
\text{Critical current density} & \\
\text{Impurity scattering rate, } \gamma & \end{align*}
\]

Enhanced Superheating Fields in Multi-Layer Systems

Maximum Gradient increased with N infusion into Nb

Disorder heterogeneity can enhance $B_{sh}$

- $Y$: Impurity scattering rate
- $j_s$: Screening current density
- $B_{sh}$: Magnetic field
- $B$: Magnetic field

Referenced literature:
Disorder heterogeneity can enhance $B_{sh}$

- Longer effective penetration depth due to dirty layer
  - Slowly varying B-field requires less screening current density
Disorder heterogeneity can enhance $B_{sh}$

- Longer effective penetration depth due to dirty layer
  - Slowly varying $B$-field requires less screening current density
- Most screening current is in the clean region and is not suppressed by disorder
Superheating Field with an Impurity Diffusion Region

Superheating Field at $T = 0$

$B_{sh}/B_0$ (mT)

- 0.8 (160)
- 1.0 (200)
- 1.2 (240)

$\gamma_0/\Delta_{00}$

- 0.5
- 1.0
- 3.0
- $\infty$

$\zeta/\lambda_0$

- 0.3
- 0.5
- 1.0

Impurity Diffusion Profile

$\gamma(x) = n_{imp}(x) \frac{2\pi}{\hbar} \langle |T|^2 \rangle_{FS}$

$\gamma(x) = \gamma_0 e^{-x/\zeta}$

- 0.5
- 1.0
- 3.0
- $\infty$

Clean Limit Critical Field: $B_0 = \sqrt{4\pi N_f \Delta_{00}^2}$

Clean Limit London Penetration Length: $\lambda_{L0} = 1/(8\pi e^2 v_f^2 N_f / 3c^2)^{1/2}$

The Effect of Inhomogeneous Surface Disorder on the Superheating Field of Superconducting RF Cavities, V. Ngampruetikorn & JAS, arXiv:1809.04057
Summary plus Comments

► Ongoing development of computational transport theory for Superconductors under strong EM field conditions directed at understanding of physics of SRF cavities

► Nonlinear Current Response for Impurity Diffusion into Nb
  - Increase the Superheating Field with Impurity Disorder
  - Balance between increased $\lambda_{\text{eff}}$ & decreased $J_c$

► Instabilities before the Superheating Field:
  - Dangerous local regions of high current density
  - For $J_s \to J_c$, $\Delta(J_s) \to 0 \implies$ Nonequilibrium QP generation @ 1 GHz