

Effect of Inhomogeneous Disorder on the Superheating Field of SRF Cavities

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Center for Applied Physics and Superconducting Technologies

Northwestern University and Fermi National Accelerator Laboratory



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 [\[Press Release\]](#).

CAPST Research Superconducting Materials

Superconducting RF Cavities

Superconducting Devices



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.

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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 NbSn_3 and MgB_2 are investigated for use in SRF technology for particle acceleration.

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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).

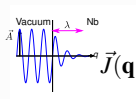
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Anna Grassellino Mattia Checchin Martina Martinello Sam Posen Alex Romanenko

Electrodynamics of Superconductor-Vacuum Interfaces

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

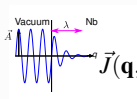


$$\vec{J}(\mathbf{q}, \omega) = -\frac{1}{c} \overset{\leftrightarrow R}{K}(\mathbf{q}, \omega; \vec{A}) \cdot \vec{A}(\mathbf{q}, \omega)$$

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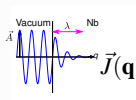
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- Pairing/Decoherence via
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▶ Material Inputs:

- ▶ Fermi Surfaces - DFT & dHvA
- ▶ Pairing/Decoherence via Electron-Phonon Coupling
- ▶ 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:
 - $k_B T_c / E_f$, $\hbar / \tau E_f$, $\hbar / p_f \xi$, $\hbar \omega / E_f \dots$



- ▶ Selection Rules & Scattering Theory
- ▶ Keldysh Transport Equations

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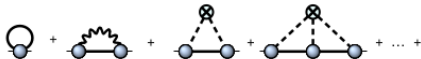
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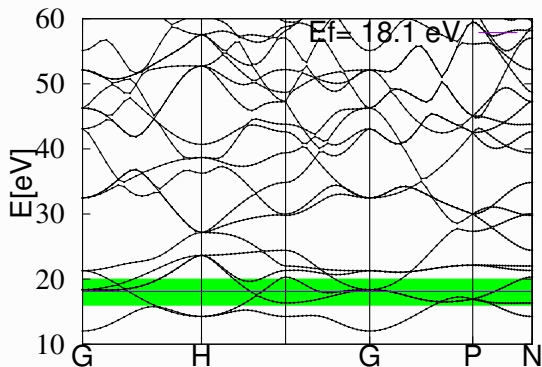


- ▶ Selection Rules & Scattering Theory
- ▶ Keldysh Transport Equations

- ▶ 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



$\text{Nb}=[\text{Kr}]4d^45s^1$

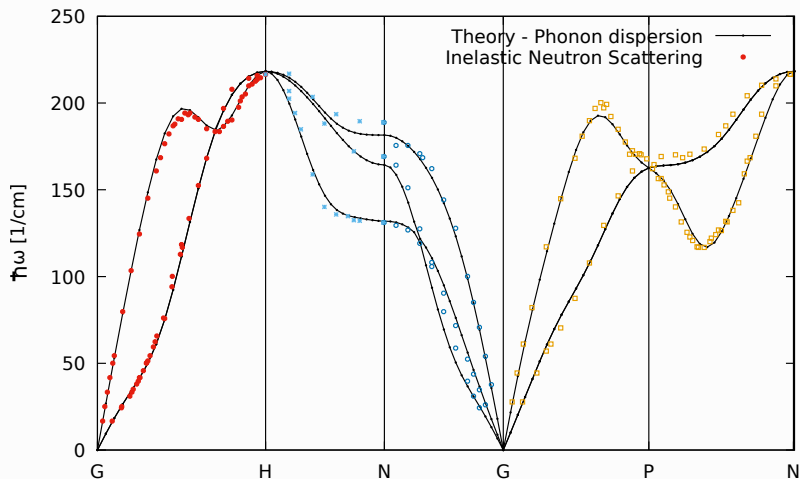
24 bands

Fermi Energy = 18.1 eV

2 bands cross the Fermi energy

► P. Giannozzi et al., J. Phys. Cond. Mat. 29 465901 (2017)

Phonons in Niobium



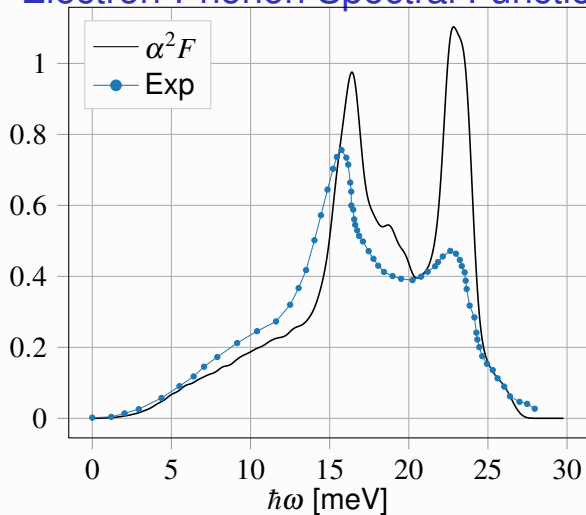
— DFT Perturbation Theory ● Inelastic Neutron Scattering;

▶ 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

▶ B.M. Powell, et al., Phonon properties of niobium ..., Can. J. Phys. 55, 1601 (1977)

Electron-Phonon Spectral Function $\alpha^2F(\omega)$



- ▶ Maximum Phonon Frequency:
 $\hbar\omega_{\max} = 27.0 \text{ meV}$
- ▶ $\lambda = 2 \int_0^\infty d\omega \frac{\alpha^2F(\omega)}{\omega} = 1.18$
- ▶ Electron-Electron Repulsion:
 $\mu^* = 0.30$
- ▶ Eliashberg Theory:
 $T_c = 9.47 \text{ K}$
- ▶ Tunneling Inversion
G. Arnold et al., JLTTP 40,
225 (1980).

- ▶ DFT Perturbation theory fails for Nb ?
- ▶ Inversion of dI/dV from PETS does not yield bulk $\alpha^2F(\omega)$?
- ▶ Nb surface has defects that suppress the high- ω spectrum ?
G. Schierning et al., Phys. Stat. Solidi RRL 9, 431 (2015)

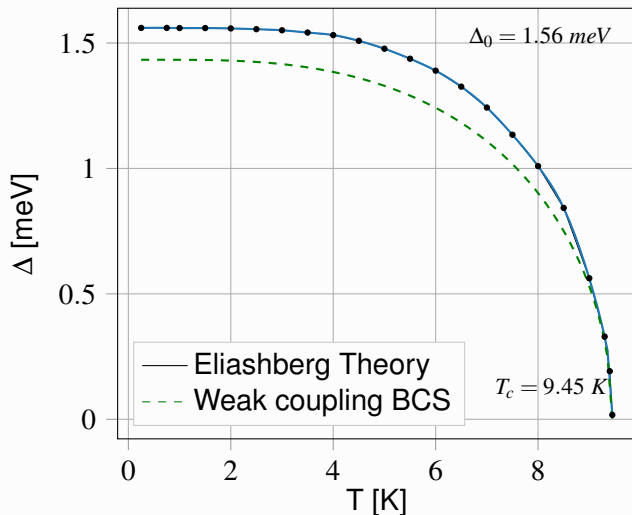
Eliashberg Equations

$$\hat{\Sigma}_{n\mathbf{k}}^{\text{pa}}(i\omega_j) = g_{nm,\nu}(\mathbf{k}', \mathbf{k}) \hat{D}_{\mathbf{k}-\mathbf{k}'\nu}(i\omega_j - i\omega_{j'}) \hat{G}_{m\mathbf{k}'}(i\omega_{j'}) + V_{\mathbf{k}-\mathbf{k}'}(i\omega_j - i\omega_{j'}) \hat{G}_{m\mathbf{k}'}(i\omega_{j'})$$

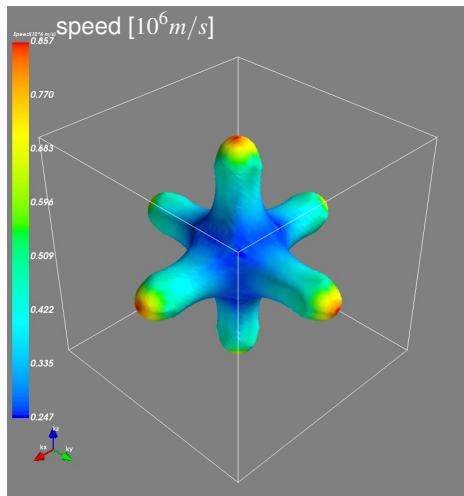
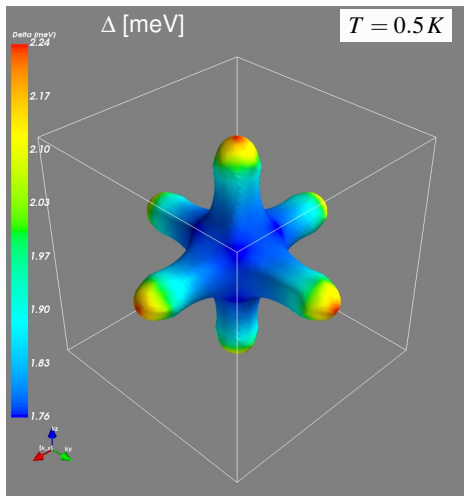
$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{N(\epsilon_F) \omega_j} \sum_{m\mathbf{k}'j'} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}'}^2(i\omega_{j'})}} \lambda(n\mathbf{k}, m\mathbf{k}', \omega_j - \omega_{j'}) \delta(\epsilon_{m\mathbf{k}'} - \epsilon_f)$$

$$Z_{n\mathbf{k}}(i\omega_j) \Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{N(\epsilon_F)} \sum_{m\mathbf{k}'j'} \frac{\Delta_{m\mathbf{k}'}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}'}^2(i\omega_{j'})}} [\lambda(n\mathbf{k}, m\mathbf{k}', \omega_j - \omega_{j'}) - \mu_c^*] \delta(\epsilon_{m\mathbf{k}'} - \epsilon_f)$$

Strong coupling superconducting gap



Anisotropy of the Gap and Fermi Velocity



- ▶ Gap Anisotropy: $\Delta_{\max} = 2.54 \text{ meV}$ $\Delta_{\min} = 1.38 \text{ meV}$ $\Delta_{\text{av}} = 1.56 \text{ meV}$
- ▶ Velocity Anisotropy: $v_f^{\max} = 1.3 \times 10^6 \text{ m/s}$ $v_f^{\min} = 0.2 \times 10^6 \text{ m/s}$
- ▶ 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

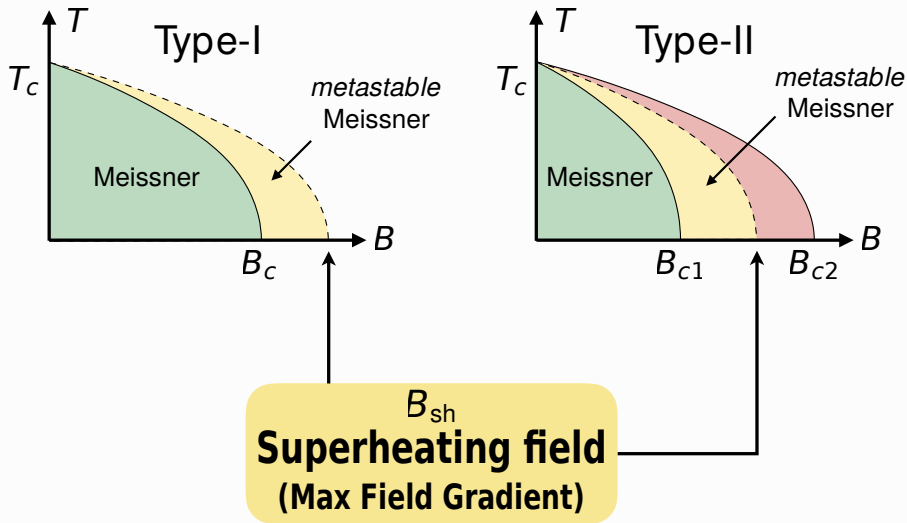
SRF Performance Goals - What Can Theory Provide?

- ▶ Push to high Q-factor & Reduce a.c. dissipation up to high E_{acc}
- ▶ Understand physics of current response at $f \gtrsim$ GHz at high B_s
- ▶ Push E_{acc}^{max} - processes determining Meissner stability/breakdown

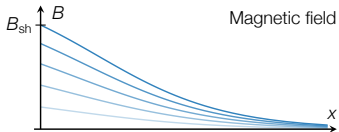
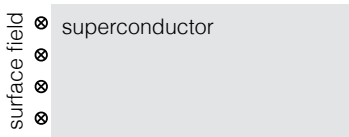


Materials based theory of Non-Equilibrium Superconductivity under Strong Nonlinear A.C. Conditions

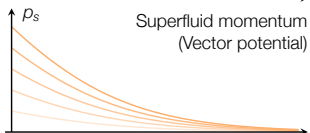
Meissner state is *metastable* up to the *superheating field*



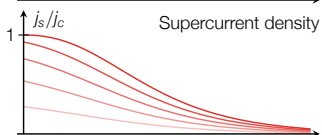
Superheating field is determined from local critical current



Magnetic field



Superfluid momentum
(Vector potential)



Supercurrent density

- 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

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

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

Propagator for Quasiparticles and Cooper Pairs:

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

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

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

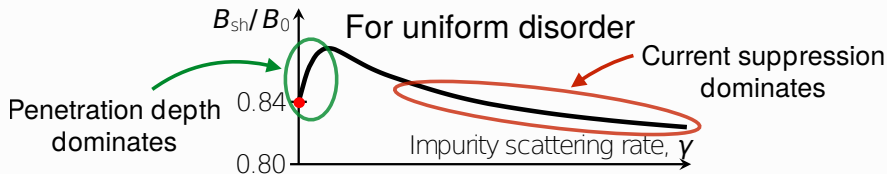
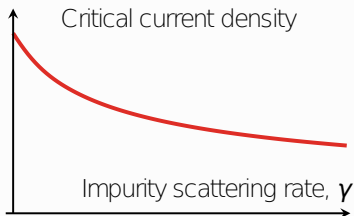
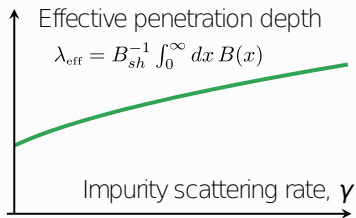
$$\partial_x^2 \mathbf{p}_s(x) - \frac{4\pi e}{c^2} \vec{j}_s[\mathbf{p}_s(x), \gamma(x)] = 0$$

Disorder Suppresses Supercurrents

B_{sh} is affected via 2 mechanisms

✓ Longer penetration depth
➤ more screening current

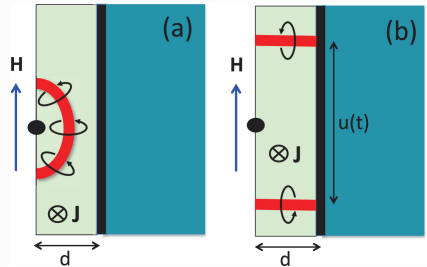
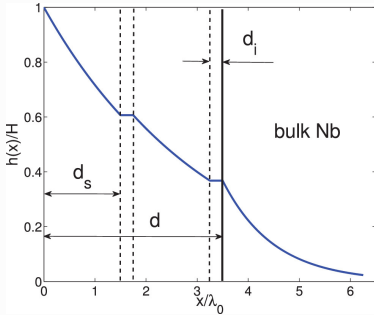
✗ Lower critical supercurrent
➤ less screening current



► F. P.-J. Lin and A. Gurevich, Effect of impurities on the superheating field of type-II superconductors, PRB 85, 054513 (2012).

• G. Catelani and J. P. Sethna, The superheating field for superconductors in the high- κ London limit, PRB 78, 224509 (2008).

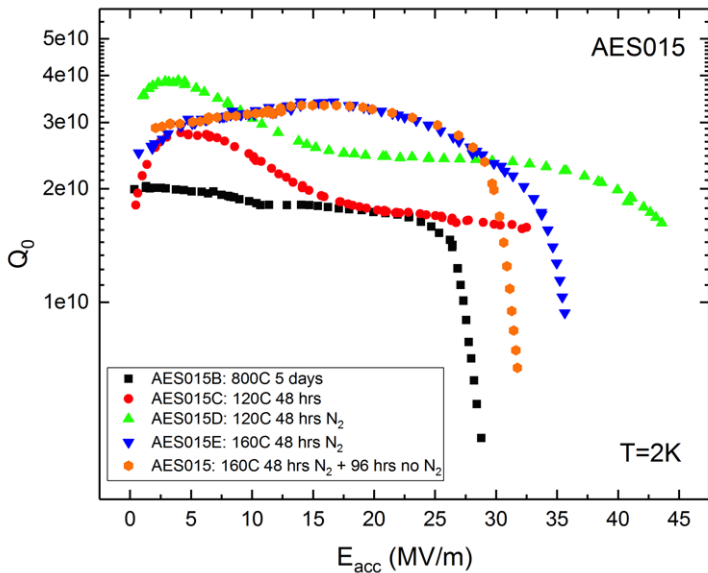
Enhanced Superheating Fields in Multi-Layer Systems



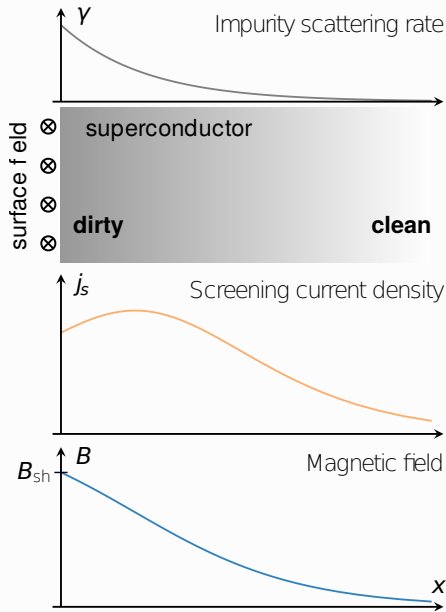
- ▶ T. Kubo, Y. Iwashita, and T. Saeki, R.F. electromagnetic field and vortex penetration in multi-layered superconductors, *Appl. Phys. Lett.* 104, 032603 (2014).
- ▶ S. Posen, M. K. Transtrum, G. Catelani, M. U. Liepe, and J. P. Sethna, Shielding Superconductors with Thin Films as Applied to RF Cavities for Particle Accelerators, *Phys. Rev. Applied* 4, 044019 (2015).
- ▶ A. Gurevich, Maximum screening fields of superconducting multilayer structures, *AIP Adv.* 5, 017112 (2015).
- ▶ D. B. Liarte, M. K. Transtrum, and J. P. Sethna, Ginzburg-Landau theory of the superheating field anisotropy of layered superconductors, *Phys. Rev. B* 94, 144504 (2016).
- ▶ D. B. Liarte, S. Posen, M. K. Transtrum, G. Catelani, M. Liepe, and J. P. Sethna, Theoretical estimates of maximum fields in superconducting resonant radio frequency cavities: stability theory, disorder, and laminates, *Supercond. Sci. Tech.* 30, 033002 (2017).
- ▶ T. Kubo, Multilayer coating for higher accelerating fields in superconducting radio-frequency cavities: a review of theoretical aspects, *Supercond. Sci. Tech.* 30, 023001 (2017).

Maximum Gradient increased with N infusion into Nb

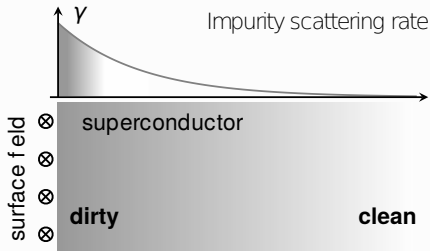
A. Grassellino, et al. arXiv:1701.06077



Disorder heterogeneity can enhance B_{sh}

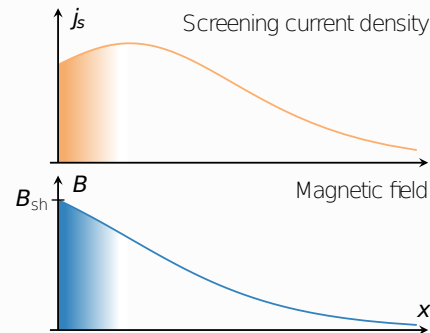


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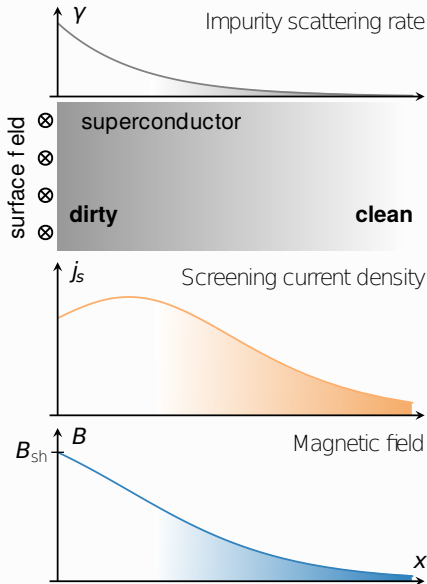


✓ Longer effective penetration depth due to dirty layer

- Slowly varying B-field requires less screening current density



Disorder heterogeneity can enhance B_{sh}



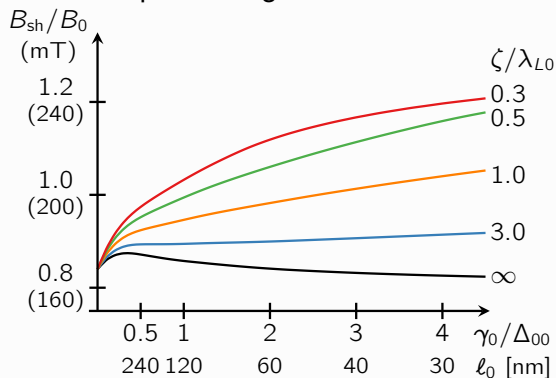
✓ Longer effective penetration depth due to dirty layer

- 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

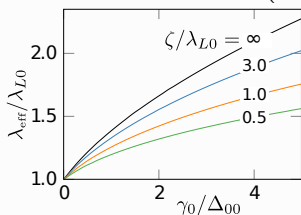
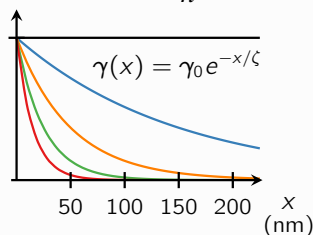
Superheating Field at $T = 0$



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

Impurity Diffusion Profile

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



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 λ_{eff} & decreased J_c
- ▶ Instabilities before the Superheating Field:
 - Dangerous local regions of high current density
 - For $J_s \rightarrow J_c$, $\Delta(J_s) \rightarrow 0 \rightsquigarrow$ Nonequilibrium QP generation @ 1 GHz