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Effect of Inhomogeneous Disorder on the Superheating Field of SRF Cavities

James A. Sauls

Department of Physics
Center for Applied Physics & Superconducting Technologies
Northwestern University & Fermilab

• Wave Ngampruetikorn • Mehdi Zarea

• Fermilab Collaborators:
Anna Grassellino, Mattia Checchin, Martina Martinello, Sam Posen, Alex Romanenko

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Center for Applied Physics and Superconducting Technologies

Northwestern University and Fermi National Acclerator 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

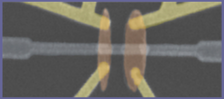
Superconducting RF Cavities

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.

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

Superconducting Devices

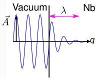


CAPST researchers are fabricating and characterizing hybrid superconducting, magnetic, and strong spin-orbit materials as for electronic and spintronic devices. Josephson Junctions fabricated with Ferromagnetic tunnel barriers (SFS devices) provide a route for generating voltage-controlled superconducting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

V. Chandrasekhar W. Halperin J. Ketterson J. Koch D. Seidman N. Stern
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



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

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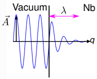

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  - Fermi Surfaces - DFT & dHvA
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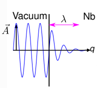

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  - Impurity & Structural Disorder
  - Surface Scattering: $S_{\text{surf}}(\mathbf{p},\mathbf{p}')$

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

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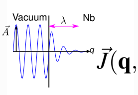

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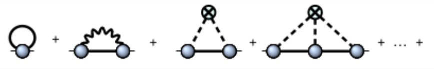
▶ Theoretical & Analytical Tools

- Migdal-Eliashberg: electron-phonon
- Asymptotic Expansions: $k_B T_c/E_f,\ \hbar/\tau E_f,\ \hbar/p_f\xi,\ \hbar\omega/E_f\ \ldots$



- Selection Rules & Scattering Theory
- Keldysh Transport Equations

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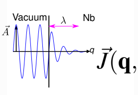

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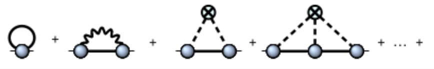

- Selection Rules & Scattering Theory
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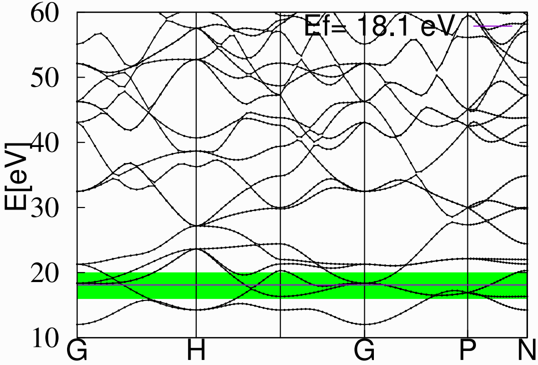
▶ Developing Methods & Codes to Compute the Nonlinear A.C. Surface Impedance
▶ Nonequilibrium Quasiparticle, Cooper Pair & Vortex Dynamics

D. Rainer & J. A. Sauls, Strong-Coupling Theory of Superconductivity, World Scientific (1995); arXiv:1809.05264

Electronic band structure of Niobium

DFT Calculation of the Electronic Band Strucuture



Nb=[Kr]$4d^4 5s^1$

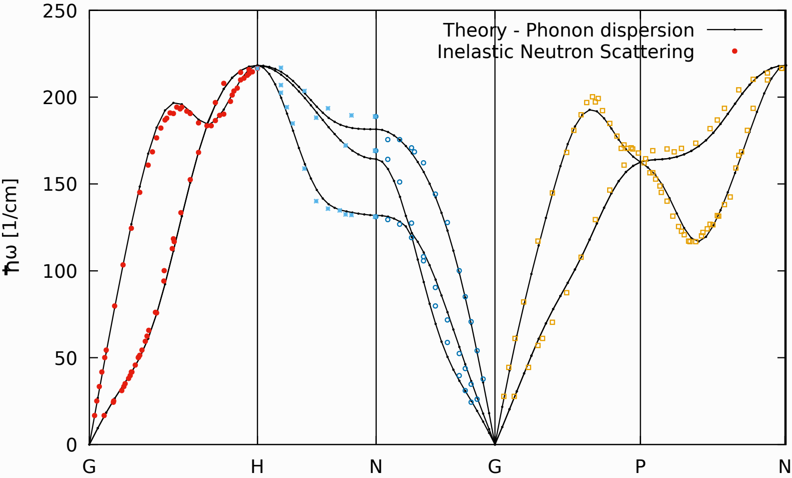
24 bands

Fermi Energy = 18.1 eV

2 bands cross the Fermi energy

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

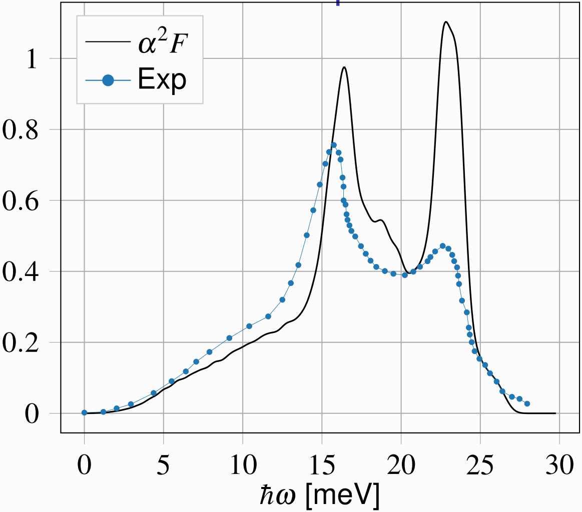
Phonons in Niobium



– 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 $\alpha^2 F(\omega)$



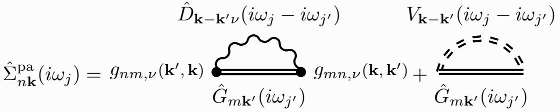
- Maxium Phonon Frequency: $\hbar\omega_{\text{max}} = 27.0\, meV$
- $\lambda = 2\int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega} = 1.18$
- Electron-Electron Repulsion: $\mu^* = 0.30$
- Eliashberg Theory: $T_c = 9.47\, K$
- Tunneling Inversion

  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-ω spectrum ?

  G. Schierning et al., Phys. Stat. Solidi RRL 9, 431 (2015)

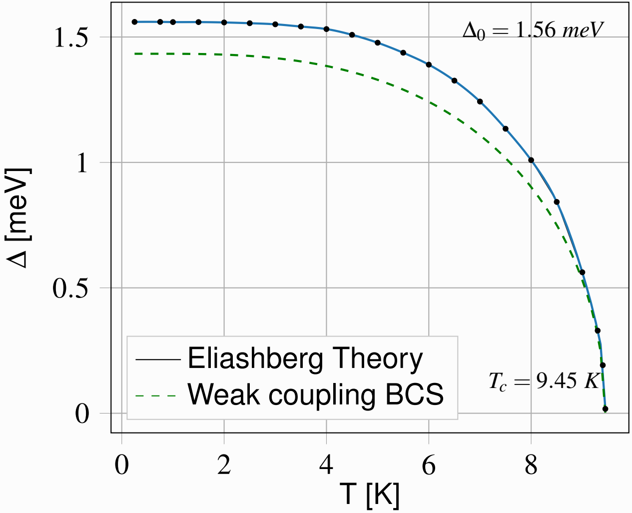
Eliashberg Equations



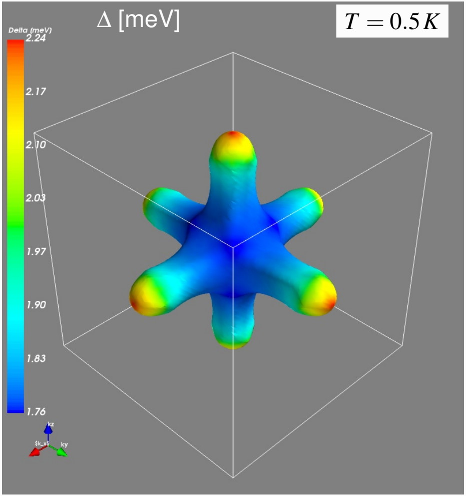
$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{N(\varepsilon_{\mathrm{F}})\omega_j} \sum_{m\mathbf{k}'j'} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}'}^2(i\omega_{j'})}} \lambda(n\mathbf{k}, m\mathbf{k}', \omega_j - \omega_{j'})\delta(\varepsilon_{m\mathbf{k}'} - \varepsilon_{\mathrm{f}})$$

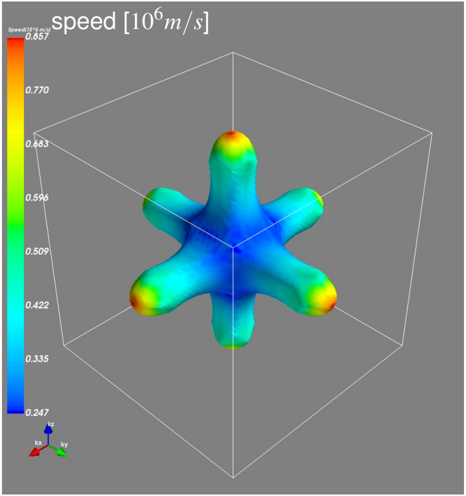
$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{N(\varepsilon_{\mathrm{F}})} \sum_{m\mathbf{k}'j'} \frac{\Delta_{m\mathbf{k}'}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}'}^2(i\omega_{j'})}} [\lambda(n\mathbf{k}, m\mathbf{k}', \omega_j - \omega_{j'}) - \mu_{\mathrm{c}}^*]\delta(\varepsilon_{m\mathbf{k}'} - \varepsilon_{\mathrm{f}})$$

Strong coupling superconducting gap



Anisotropy of the Gap and Fermi Velocity





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

$$\Downarrow$$

- Develop computational transport theory - charge and heat response under strong EM field conditions at the superconductor-vacuum interface

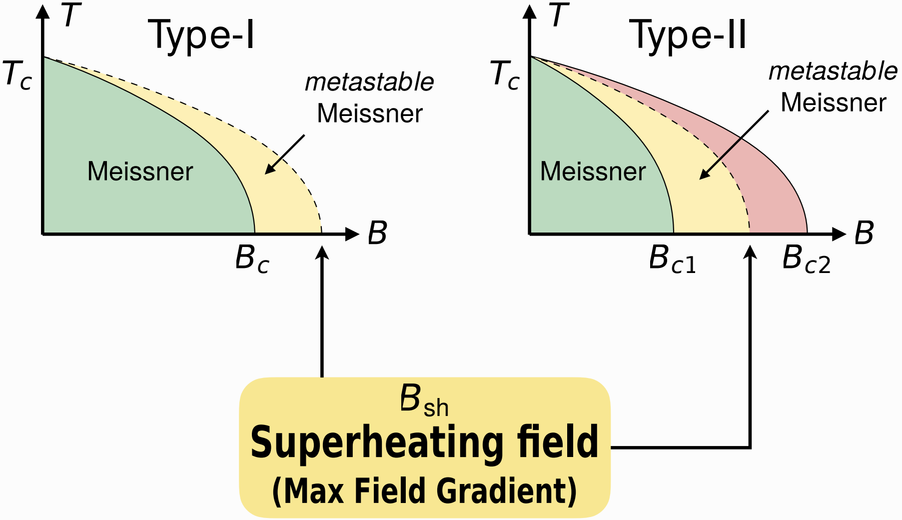
SRF Performance Goals - What Can Theory Provide?

- 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

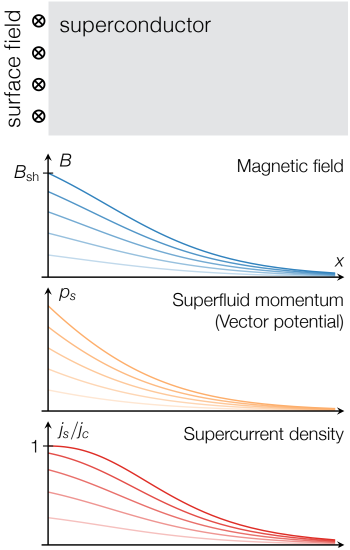
$\Downarrow$

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

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



Superheating field 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

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

- Spectral Function: $\mathscr{A}(\hat{\mathbf{p}},\varepsilon;x) \equiv \frac{-1}{\pi} \mathrm{Im}\, \mathfrak{G}(\hat{\mathbf{p}},\varepsilon;x)$
- local impurity self-energies, $\widehat{\Sigma}_{\mathrm{imp}}(x) = \gamma(x)\langle\widehat{\mathfrak{G}}\rangle$
- 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:

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

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

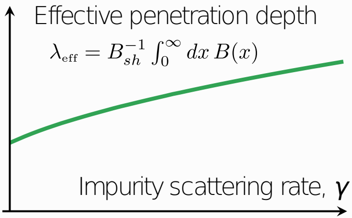
$$\Delta(x) = \frac{g}{2}\int d\varepsilon \tanh\frac{\varepsilon}{2T}\,\mathrm{Im}\left\langle f(\hat{\mathbf{p}},\varepsilon,x)\right\rangle_{\hat{\mathbf{p}}},$$

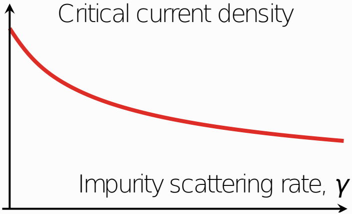
$$\partial_x^2\mathbf{p}_s(x) - \frac{4\pi e}{c^2}\vec{j}_s[\mathbf{p}_s(x),\gamma(x)] = 0$$

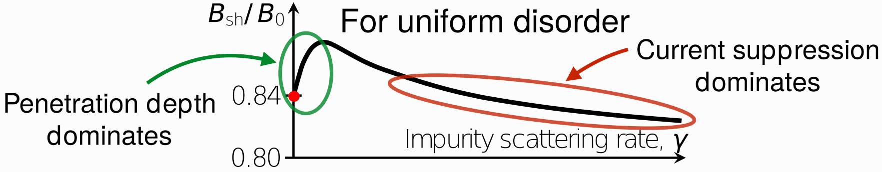
Disorder Suppresses Supercurrents
B_{sh} is affected via 2 mechanisms

✓ Longer penetration depth
➤ *more* screening current

✗ Lower critical supercurrent
➤ *less* screening current

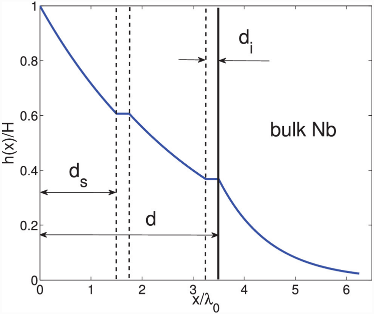


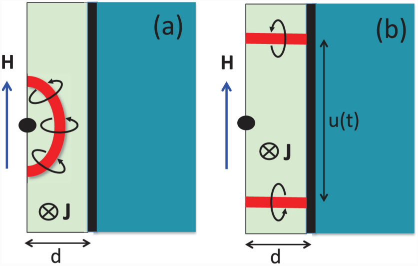




► F. P.-J. Lin and A. Gurevich, Effect of impurities on the superheating field of type-II superconductors, PRB 85, 054513 (2012).
● G. Catelani and J. P. Sethna, The superheating field for superconductors in the high-κ London limit, PRB 78, 224509 (2008).

Enhanced Superheating Fields in Multi-Layer Systems





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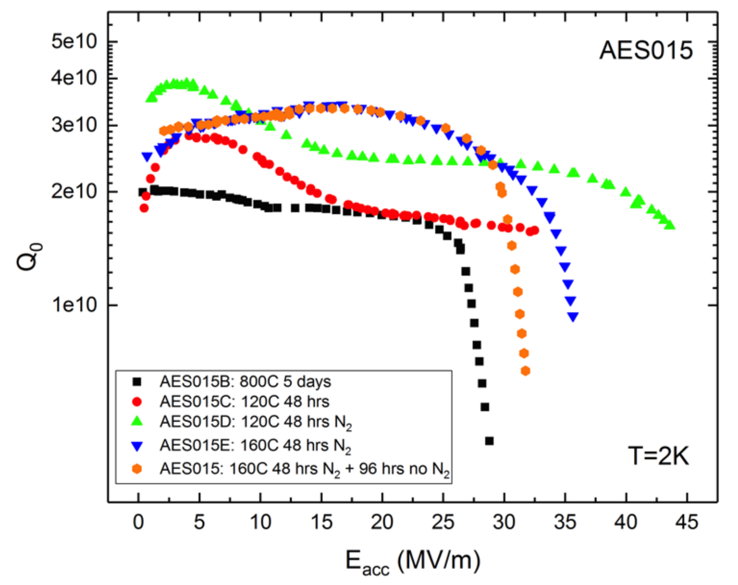
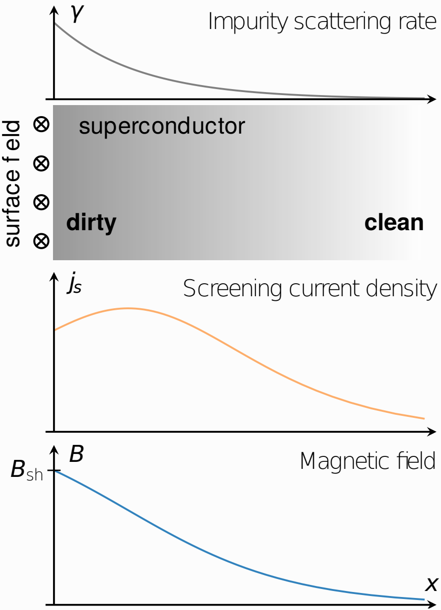
- S. Posen, M. K. Transtrum, G. Catelani, M. U. Liepe, and J. P. Sethna, Shielding Superconductors with Thin Films as Applied to RF Cavities for Particle Accelerators, Phys. Rev. Applied 4, 044019 (2015).
- A. Gurevich, Maximum screening fields of superconducting multilayer structures, AIP Adv. 5, 017112 (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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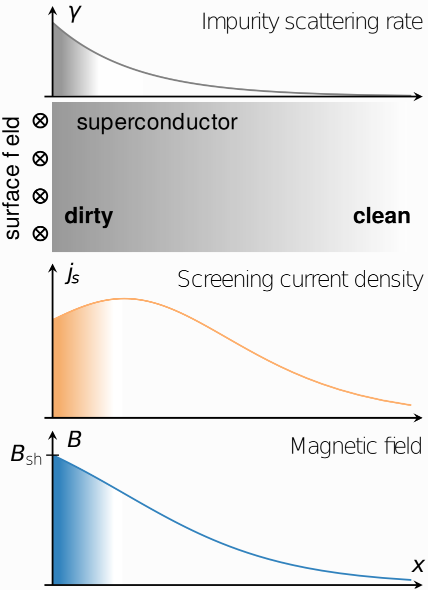
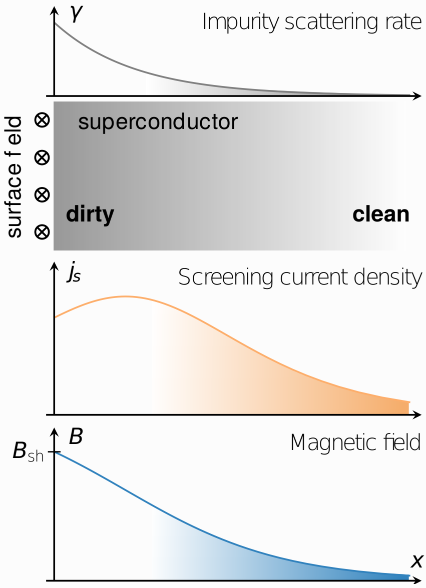


✓ Longer effective penetration depth due to dirty layer

- Slowly varying B-f eld requires less screening current density

Disorder heterogeneity can enhance B_{sh}



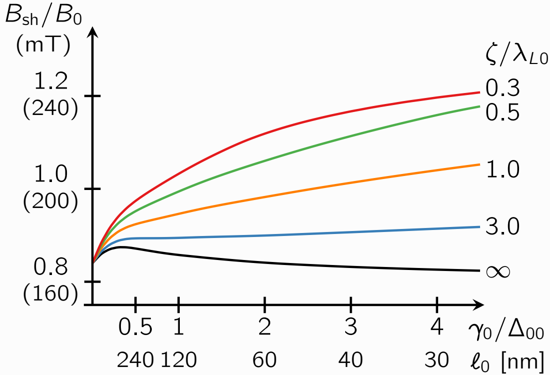
✓ Longer effective penetration depth due to dirty layer

- Slowly varying B-f eld requires less screening current density

✓ Most screening current is in the clean region and is not suppressed by disorder

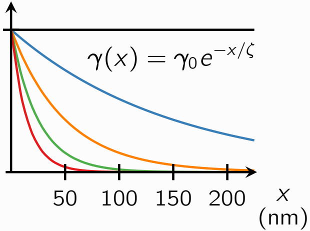
Superheating Field with an Impurity Diffusion Region

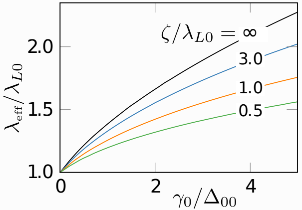
Superheating Field at $T = 0$



Impurity Diffusion Profile

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





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

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

- *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 $J_s \to J_c$, $\Delta(J_s) \to 0 \rightsquigarrow$ Nonequilibrium QP generation @ 1 GHz