First Principles Study of Impurity and Vacancy Structures in Niobium

Accelerator Physics and Technology Seminar
Fermilab, December 16, 2014

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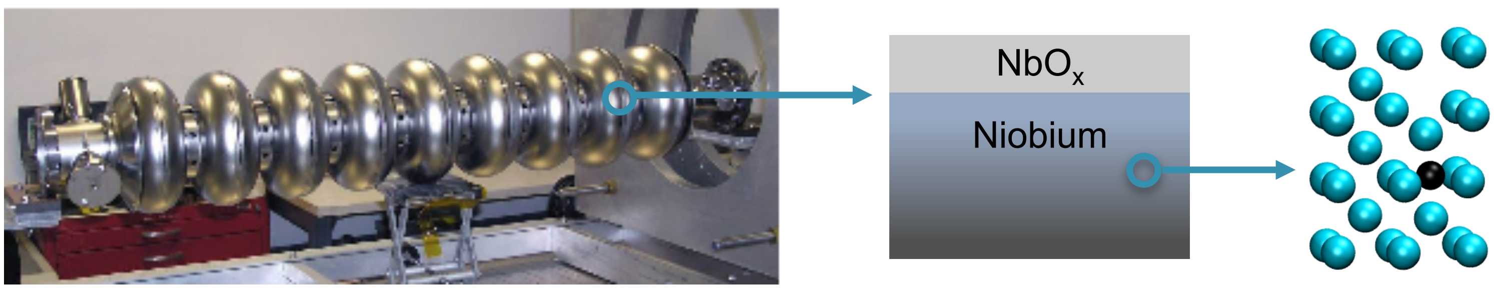

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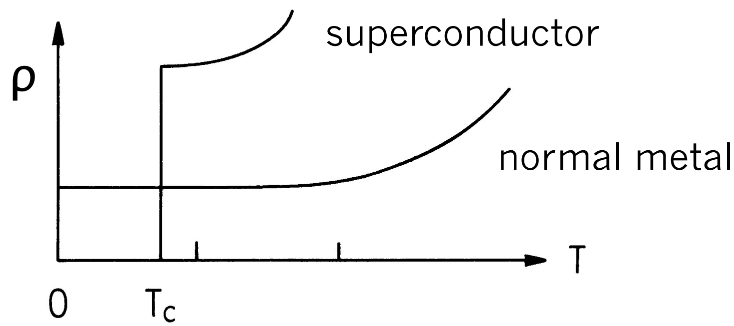
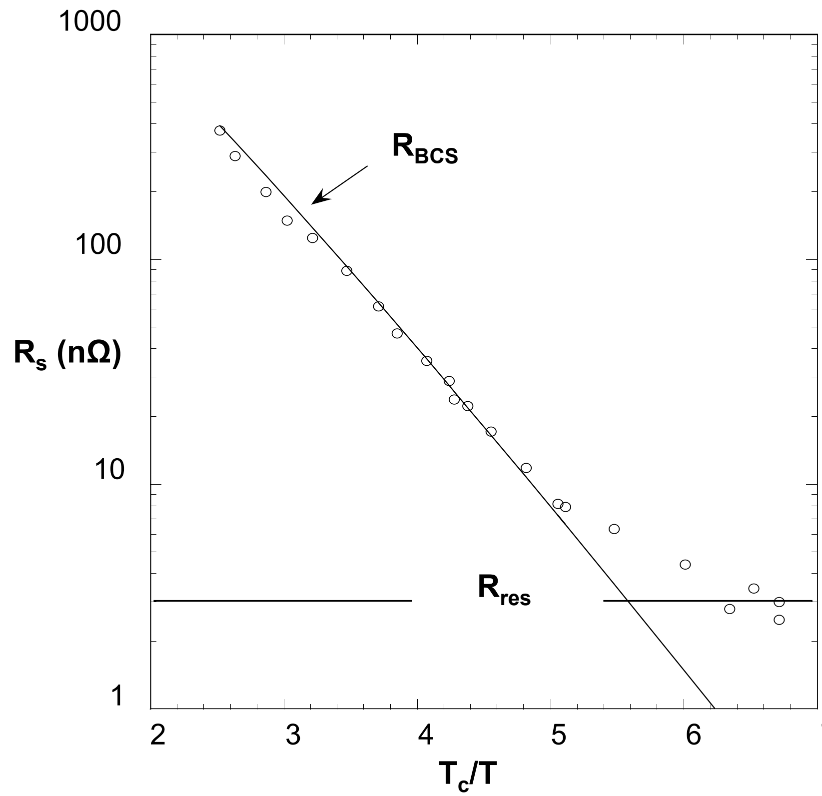
Motivation: Superconducting RF Cavities

- Provide accelerating gradient for high-performance linear particle accelerators
  - Applications include the International Linear Collider, Project X, nuclear energy, . . .
- Made from ultra pure niobium (>99.98%)
  - Type II superconductor with T_c = 9.8 K
- Operation in the superconducting state decreases losses due to surface resistance by ~10^6

Motivation: Losses in SRF Cavities

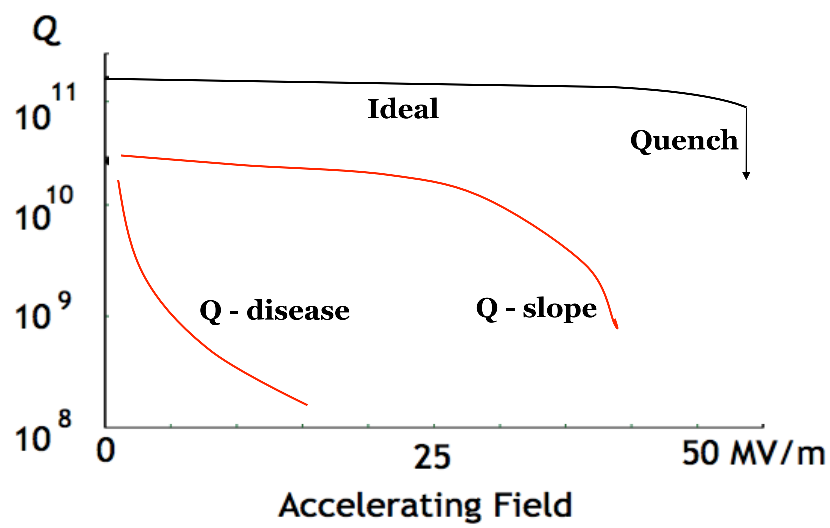


- R_S is dependent on material properties and operating conditions
- Only top few 100 nm matters



P. Schmüser, Prog. Part. Nucl. Phys. 49 (2002)

Motivation: Losses in SRF Cavities

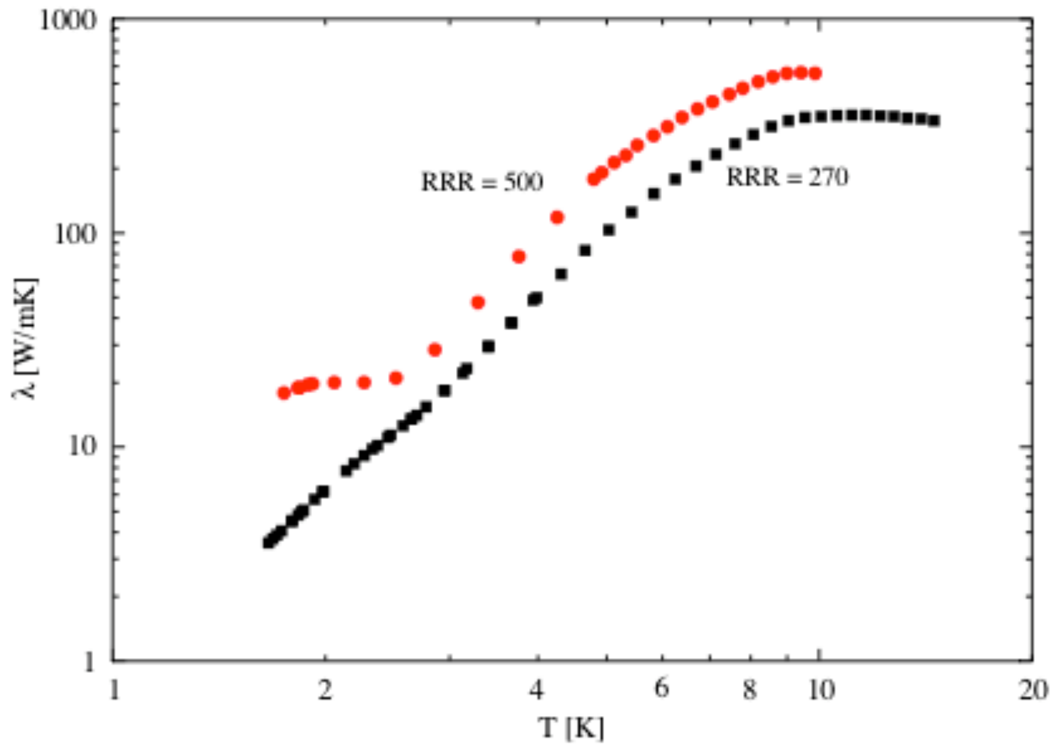


$$Q = \frac{stored\ energy}{dissipated\ power / rf\ \text{cycle}}$$

$$= \frac{G}{R_s}$$

- Electron field emission
- Multipacting
- Q-disease
- Q-slope

Motivation: Recovery from Loss



T. Schilcher, TESLA-Report, TESLA 95-12, DESY (1995)

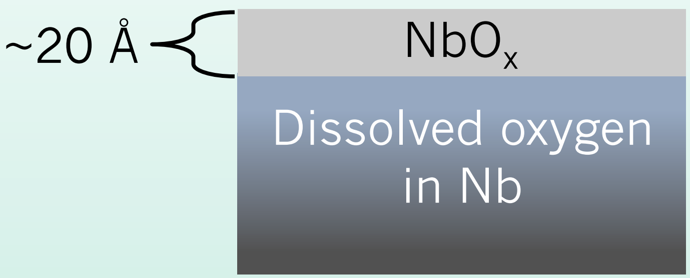
- Resistance -> dissipation -> need quick heat removal
- Thermal conductivity in the bulk is important

Motivation: Empirically Developed Cavity Processing Procedures

- Some important techniques
  - **Buffered chemical polishing** of outer surface – increase heat transfer
  - **Bulk electropolishing** (~150 μm) of inner surface – remove damage layer from forming
  - **600-800 °C bake** – eliminate Q-disease
  - **Tumbling** – smooth surface
  - **High pressure rinse** – remove dust (prevent field emission)
  - **100-160 °C bake** – mitigate Q-slope
  - **Nitrogen treatment** – increase Q
- Much recent research into physical mechanisms occurring during these steps and the resulting cavity performance

Motivation: Impurities in Niobium

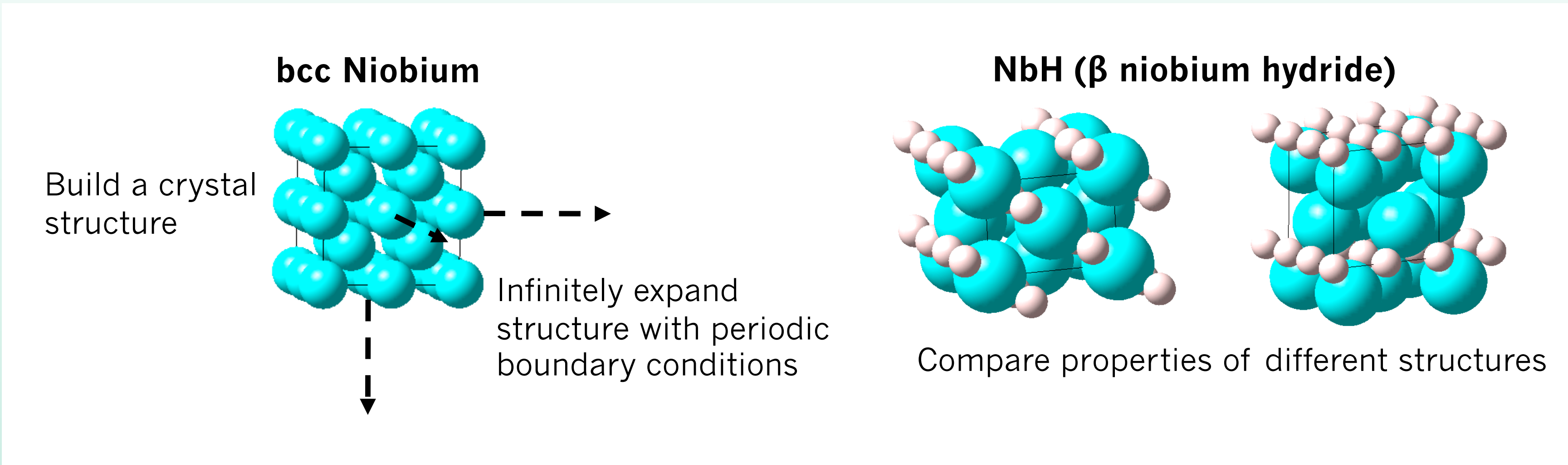
- The surface oxide could be a source of Q-slope



  - Supply of dissolved oxygen in the bcc niobium – lowers T_c by ~0.9 K per at. %
  - Surface layer can be highly defective or amorphous

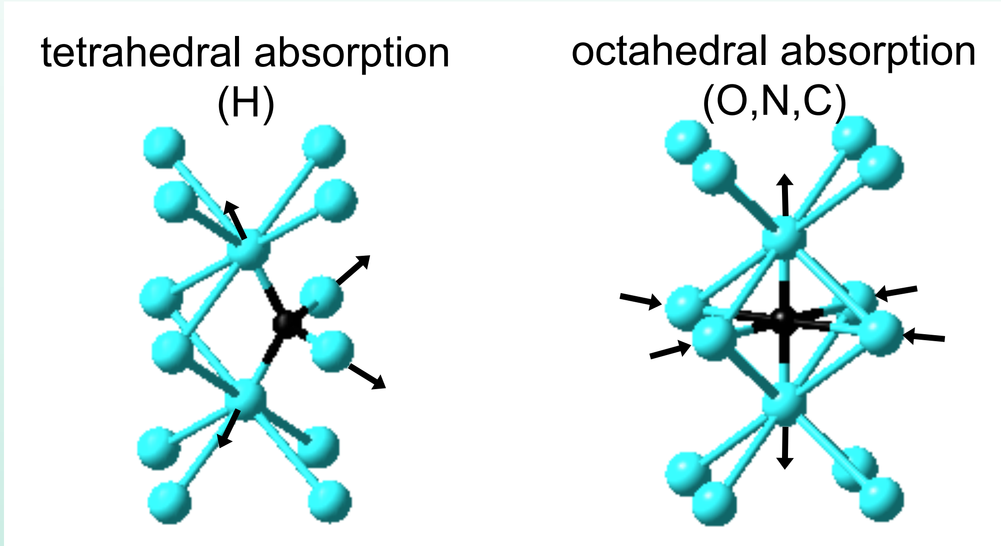
- Dissolved N and C may have a similar effect as dissolved O
- Hydrogen could be responsible for Q-slope and Q-disease
  - Ordered hydride phases have a superconducting $T_c < 2K$
  - Precipitates larger than ξ may be the culprit of Q-disease, while smaller precipitates may contribute to Q-slope
    - Considering the proximity effect and that hydrides are metallic, $\xi \sim 0.5\ \mu m$

Density Functional Theory Modeling



- Solve the electronic structure problem for the model systems using density functional theory in VASP
- Assess properties such as binding energy, charge distribution, and niobium lattice strain

Properties of the Interstitial Impurities



	$Nb_{128}H$	$Nb_{128}O$	$Nb_{128}N$	$Nb_{128}C$
Charge on interstitial atom (e^-)	-0.65	-1.35	-1.63	-1.76
Binding energy (eV)	-2.41	-7.02	-7.39	-8.48
Lattice strain energy (eV)	0.11	0.83	0.83	0.96

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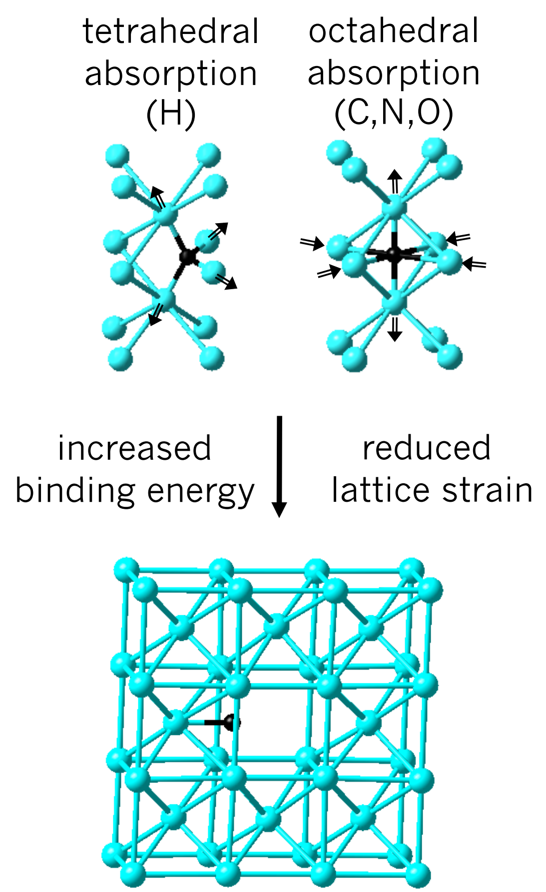
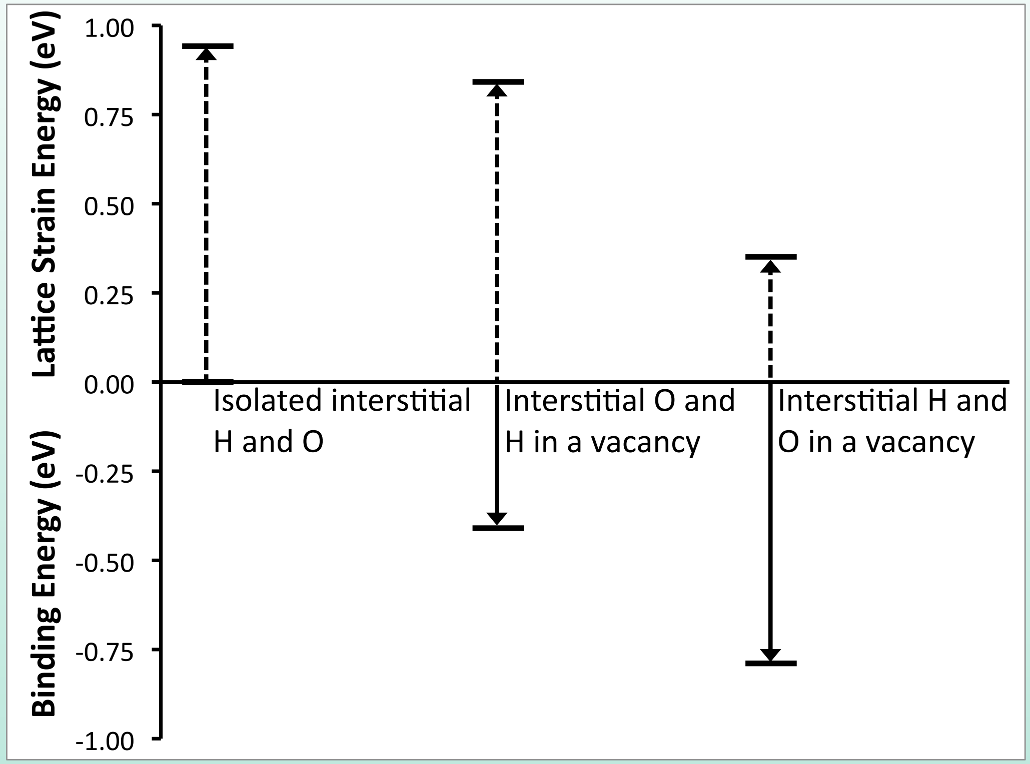
Impurities Around Niobium Lattice Vacancies





- Impurities are attracted to lattice defects to alleviate lattice strain

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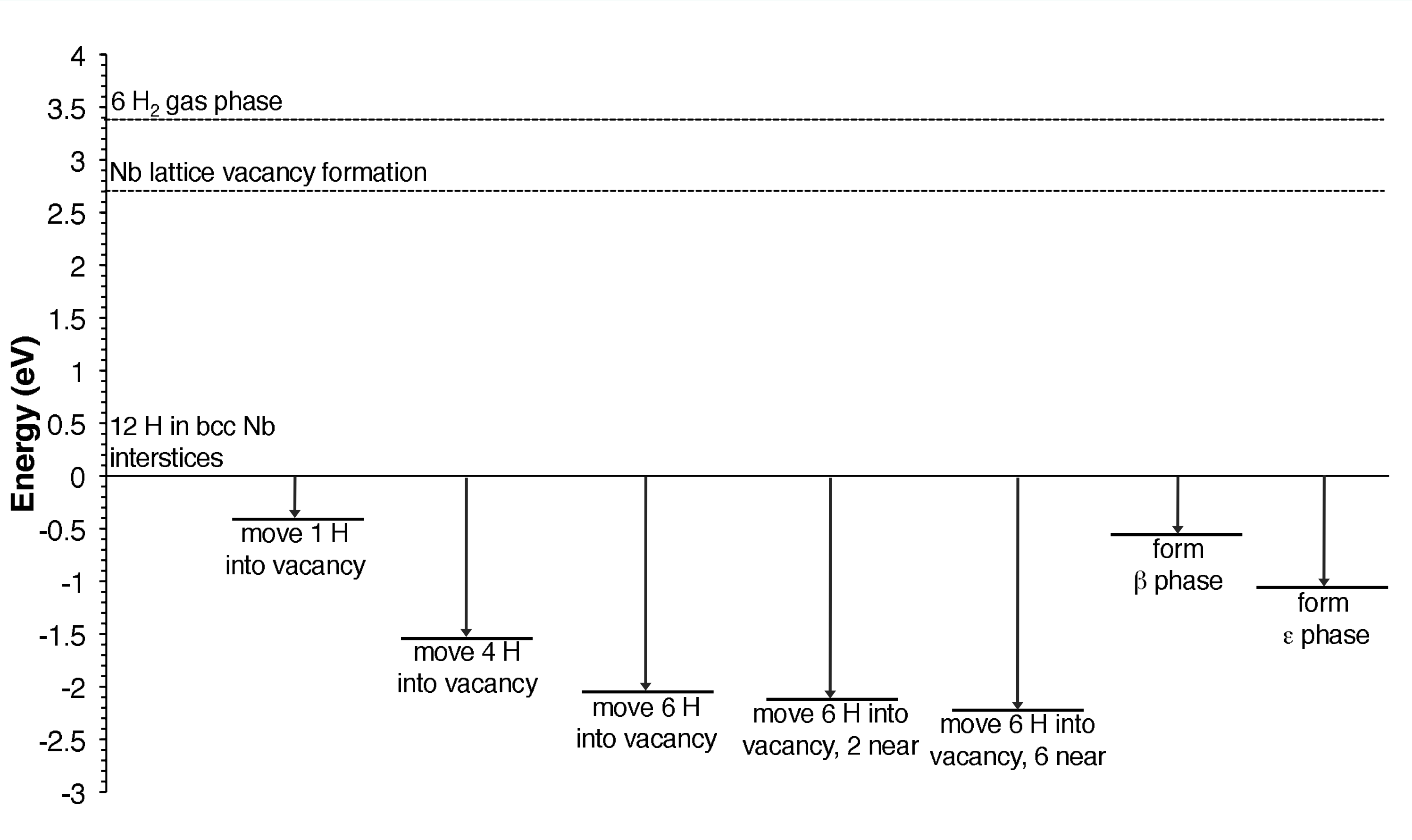
Niobium Lattice Vacancies Can Nucleate Ordered Impurity Phases



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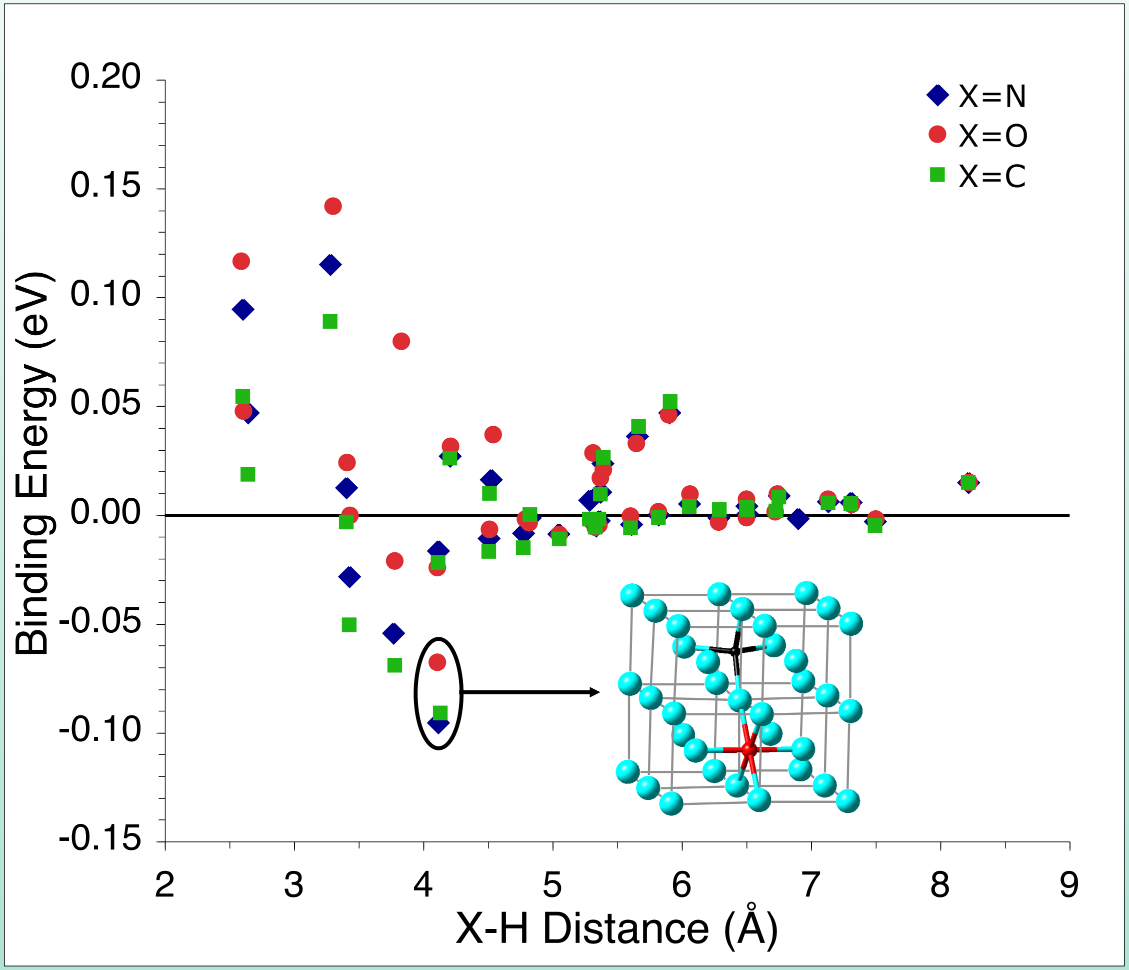
Impurities Can Work Together to Prevent Detrimental Phases from Forming



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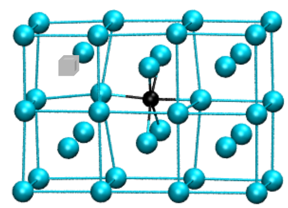
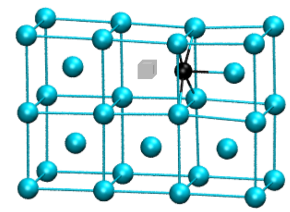
Application to SRF Cavities

- Proposed mechanism for the low temperature anneal:
  - -> Hydrogen is liberated from both the ordered hydride phases and the niobium site vacancies
  - -> Some oxygen diffuses from the oxide phases or niobium interstitial sites and becomes trapped by the niobium vacancies in the near surface region
  - -> Hydrogen is trapped by other impurities or defects rather than an ordered phase
- Application to cavity processing procedure:
  - -> Control the recovery state of the niobium to reduce hydride phase nucleation centers
  - -> Dope the niobium with O, N, C to trap H atoms

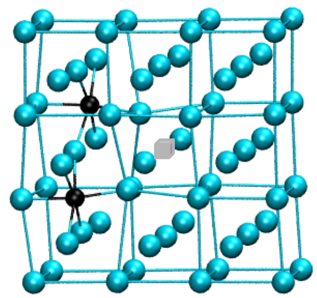
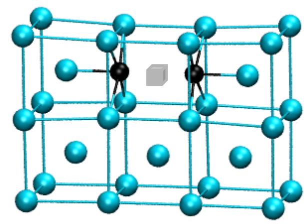
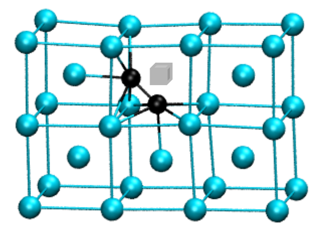
Difference Between Impurities Around Niobium Lattice Vacancies

		
	Binding Energy (eV)	
C	**-0.39**	0.00
N	**-0.29**	-0.25
O	-0.22	**-0.79**
H	n.a.	**-0.32**

- Preferred binding site correlates with ground state electron configuration of impurity atom.

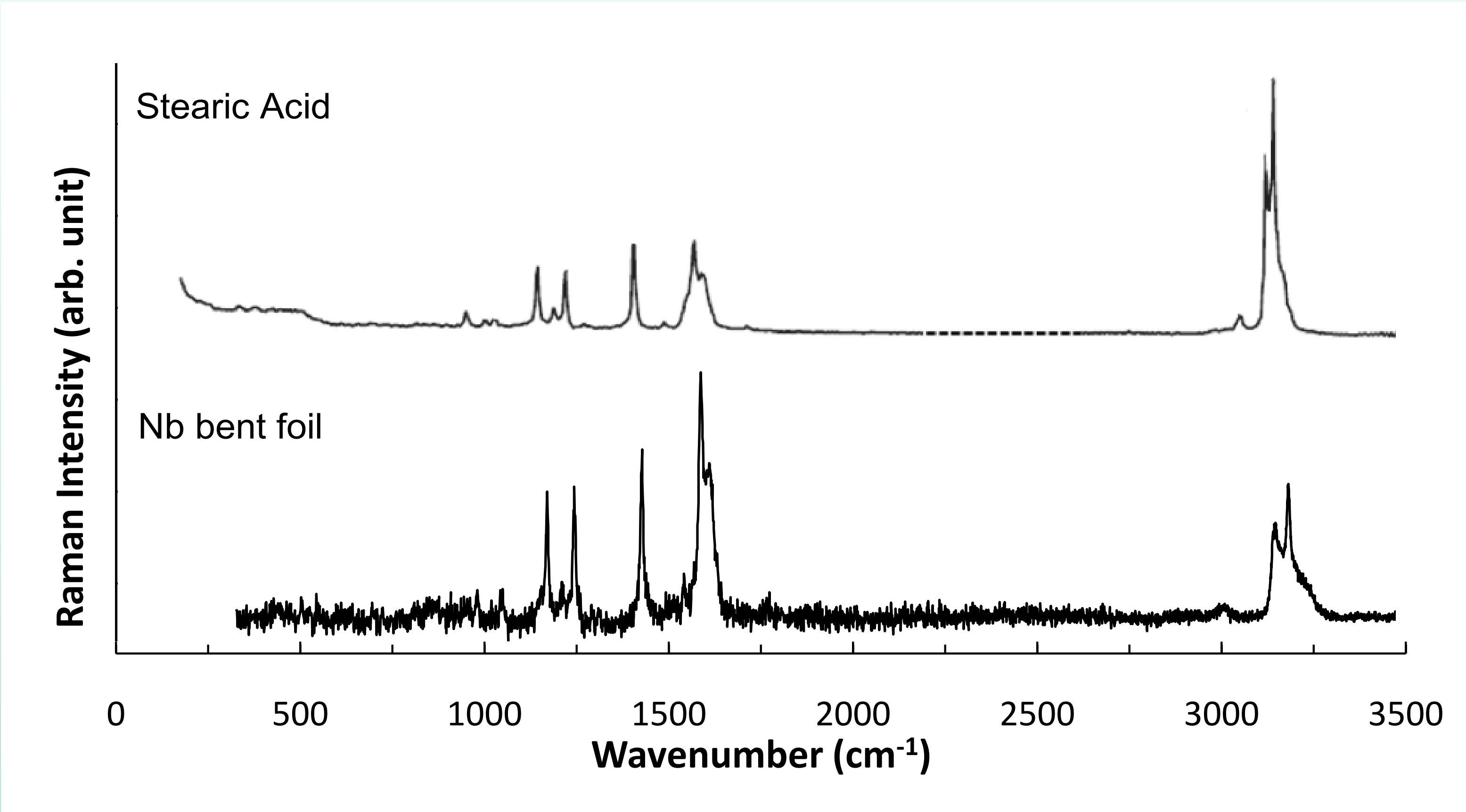
Difference Between Impurities Around Niobium Lattice Vacancies

Two Impurities Near Vacancy

			
	Binding Energy (eV)		
C	**-0.89**	-0.14	-0.46
N	-0.57	**-0.61**	n.a.
O	-	**-1.65**	n.a.
H	n.a.	**-0.70**	n.a.

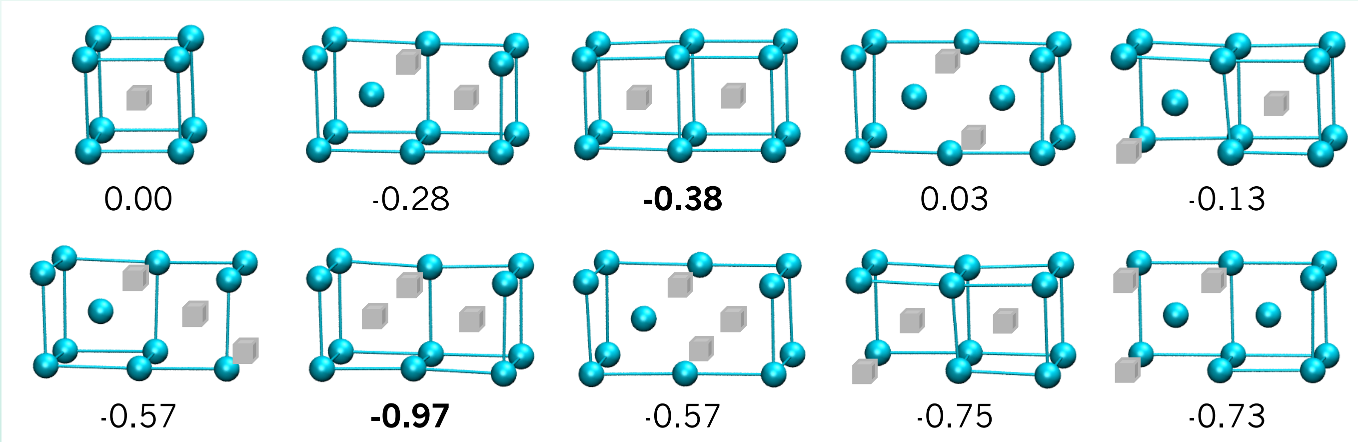
- C is special! Can it form longer chains in extended defects?

Raman Spectrum of Hydrocarbon Chains in Niobium



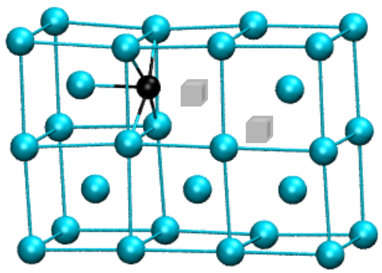
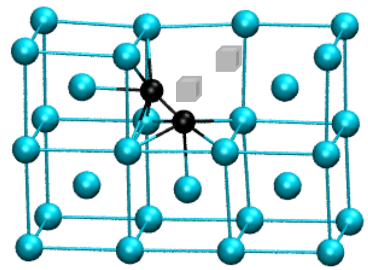
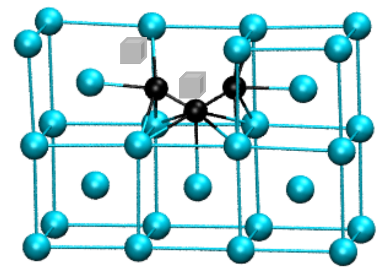
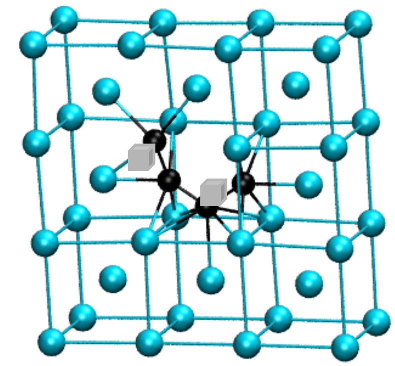
C. Cao, et al. 2013 Phys. Rev. ST Accel. Beams 16 064701

Niobium Lattice Di- and Tri- Vacancies



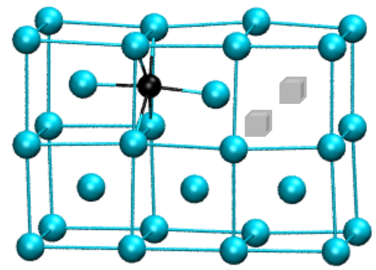
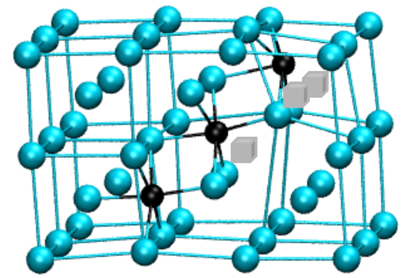
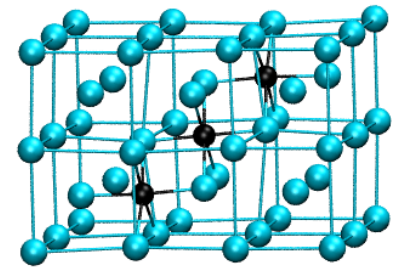
- The formation energy of tri-vacancy clusters is approximately equal to the sum of the constituent vacancy pairs

Carbon Chains in Niobium

				
BE_C (eV)	-0.35	-0.88	-0.51	0.07
BE_{NbC} (eV)	-0.03	-0.24	0.45	1.35

- Longer chains quickly become unfavorable
- C-H in Nb spontaneously dissociates
- Is a surface or surface-like defect, such as a grain boundary, required for chain formation?

Carbon Clustering in Niobium

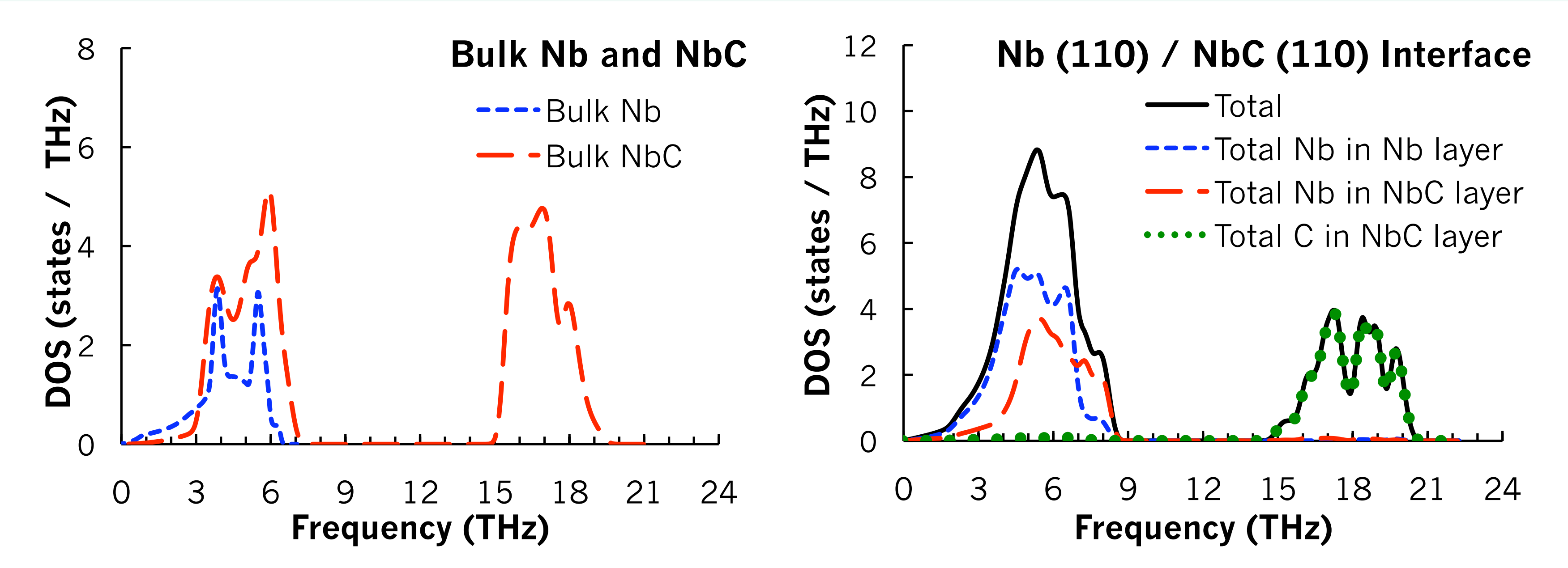
			
BE_C (eV)	-0.77	-1.84	-0.32
BE_{NbC} (eV)	-0.45	-0.88	0.64

- Favorable for C to cluster
- C can form Cottrell atmospheres around niobium lattice vacancy-type defects

Application to SRF Cavities

- Decrease in DOS at the Fermi level for interstitial C is similar to interstitial O
  - -> This may allude to a similar decrease in T_c
  - -> Effect is mitigated as C absorbs near Nb lattice vacancy-type defects
- Lower solubility of C in Nb than the other interstitial impurities and strong attraction to vacancy-type defects indicates that C will likely be found near these sites
- NbC is an electron-phonon superconductor with an 11 K T_c, so its formation is not detrimental like NbH

Interface Properties



- Broadening of acoustic states at the interface alludes to possible changes in superconductivity
  -> needs further investigation

Summary

- First-principles calculations have shed light on important physical processes occurring in the material of SRF cavities
  - The interactions between H, O, and niobium lattice vacancy-type defects play an important role in the low temperature anneal
  - O, N, and C can trap H and prevent detrimental hydride phase formation
  - Subtle differences in the interactions between O, N, and C with niobium lattice vacancy-type defects may have important effects on niobium's properties
  - The interfaces between niobium and impurity precipitates may affect superconductivity

Acknowledgements

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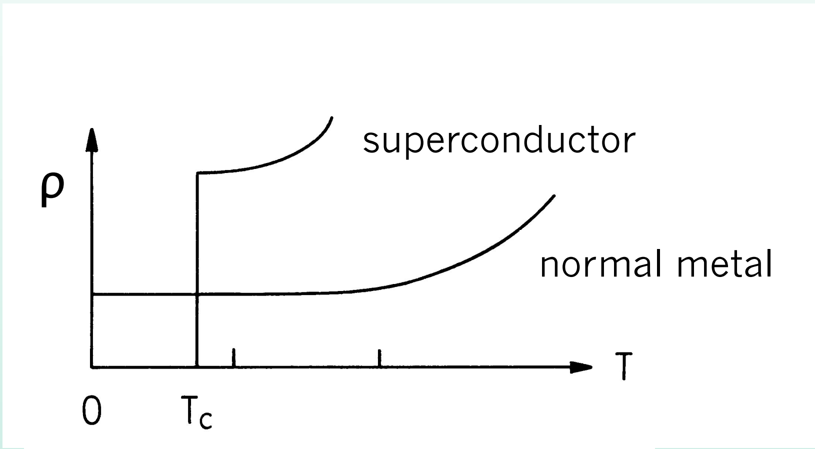
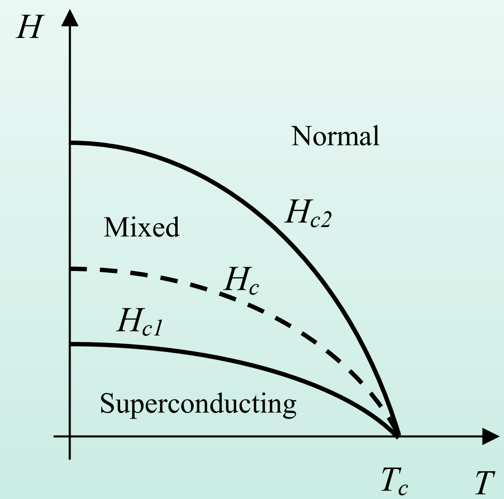
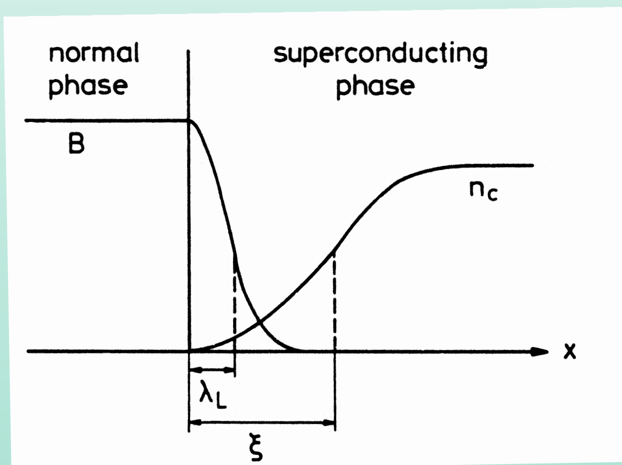
Thank you!

Superconductivity Review







$B = \mu_0 H$

Niobium

T_c = 9.2 K

B_{c1} = 174-190 mT

B_c = 200 mT

B_{c2} = 390-450 mT

λ = 32-44 nm

ξ_0 = 30-60 nm

Superconducting Radio-Frequency (SRF) Cavities

$$R_{BCS} = \frac{A}{T}\sigma_n\omega^2\left(\lambda_L\sqrt{\frac{l+\xi_0}{l}}\right)^3\exp\left(\frac{-BT_c}{T}\right)$$

Material Properties

σ_n: normal state conductivity; T_c: superconducting transition temperature

λ_L: London penetration depth; l: electron mean free path

ξ_0: superconducting current coherence length for the pure material

Operating Conditions

T: temperature; ω: frequency