DFT Analyses of Structures that Limit SRF Cavity Performance

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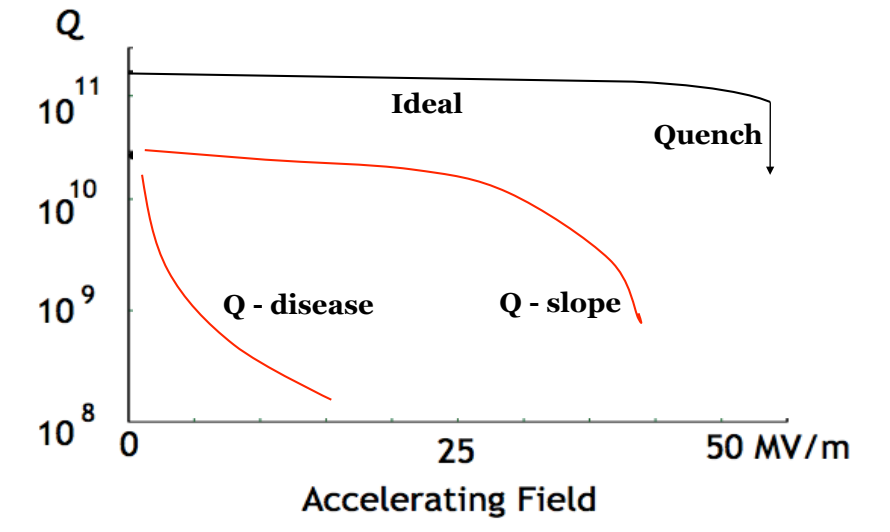
Overview

- Background - Impurities in niobium SRF cavities
- Methods - Modeling crystal structures with DFT
- Hydrogen in Niobium
  - Niobium hydride phases
  - Interactions with the ideal and defective lattice
  - Application to SRF cavity performance and processing
- Other impurities (**O**, N, C) in Niobium
  - Niobium Oxide phases
  - Effect on hydride phase formation
  - Application to SRF cavity performance and processing
  - An additional concern

Superconducting Radio-Frequency (SRF) Cavities
Limitations Related to Impurities in Niobium



- **Impurities** can
  - be dissolved in the metal and cause reduction of T_c and local heating
  - form precipitates with local magnetic moments or reduced T_c

- Resulting cavity behaviors include
  - **Q – disease,** caused by large hydride precipitates?
  - **Q – slope,** caused by smaller precipitates; dissolved oxygen, hydrogen, nitrogen, etc.; magnetic structures?

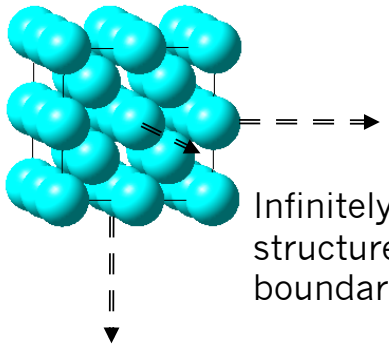
Impurity Absorption into Niobium
Cavity Forming and Processing Procedure

- Forming
  - Complex – shape and ultra high purity – source of many lattice defects
- Processing
  - **Bulk electropolish** (~150 μm) of inner surface - remove damage layer from forming
  - Wash - remove chemical residues from EP
  - **800 °C bake** - outgas hydrogen absorbed during chemical processing
  - Tune - shape changes during processing
  - **Fine electropolish** - smooth surface
  - Wash - remove chemical residues from EP
  - Rinse - remove dust (prevent field emission)
  - Assemble
  - **120 °C bake** - it works (why?)
  - Test performance

Density Functional Theory Modeling
Creating a Model

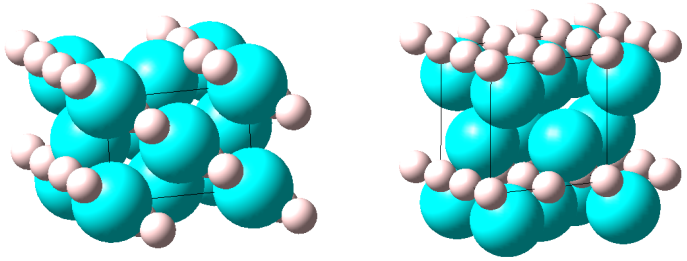
bcc Niobium

Build a crystal structure



Infinitely expand structure with periodic boundary conditions

NbH (β niobium hydride)



Compare properties of different structures with the same stoichiometry

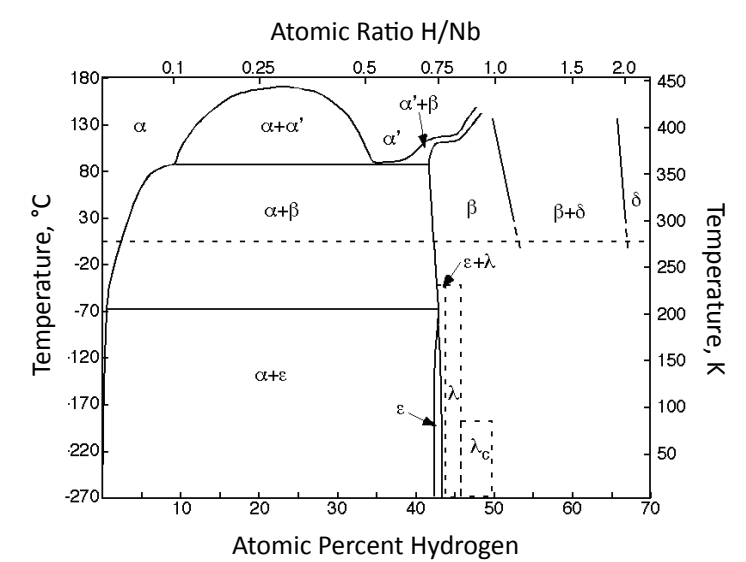
- Properties of interest include:
  - Energies – electronic, vibrational, strain
  - Geometry
  - Charge distribution
  - Magnetic moments
  - Phonons

Density Functional Theory Modeling
Calculations

- Solve the electronic structure problem for the model system
- Hohenberg, Kohn, Sham – obtain properties from electron density instead of many-electron wavefunction: $E = T(\rho) + V(\rho) + Exc(\rho)$
  - $T(\rho)$ – kinetic energy
  - $V(\rho)$ – potential energy
  - $Exc(\rho)$ – exchange-correlation energy - unknown form
    -> describe with parameterized 'functionals'
- Parameters
  - Vienna Ab Initio Simulation Package (VASP)
  - Plane wave basis set w/400 eV cutoff
  - PAW pseudopotentials to describe atomic cores
  - PBE-GGA exchange-correlation functional
  - 0.25/Å gamma-centered Monkhorst-Pack *k*-point mesh
- Bader Method to assign local properties

Hydrogen in Niobium

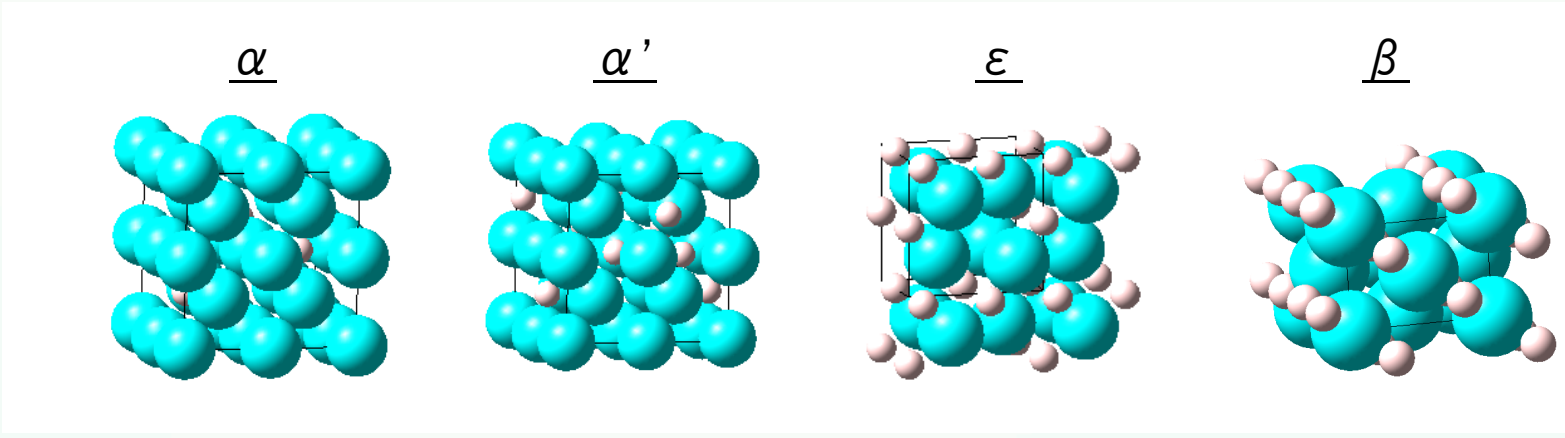
- The niobium – hydrogen phase diagram is very complex
  - α, α' – interstitial hydrogen dispersed in bcc niobium
  - β, ε – ordered hydrogen interstitials in fco niobium
  - δ – ordered hydrogen interstitials in fcc niobium – fluorite structure
  - λ, λ_c – experimentally unconfirmed phases

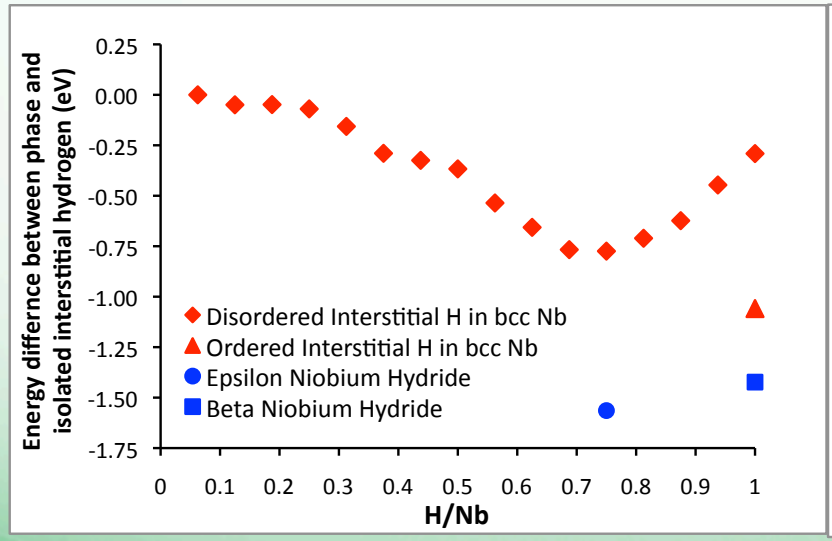


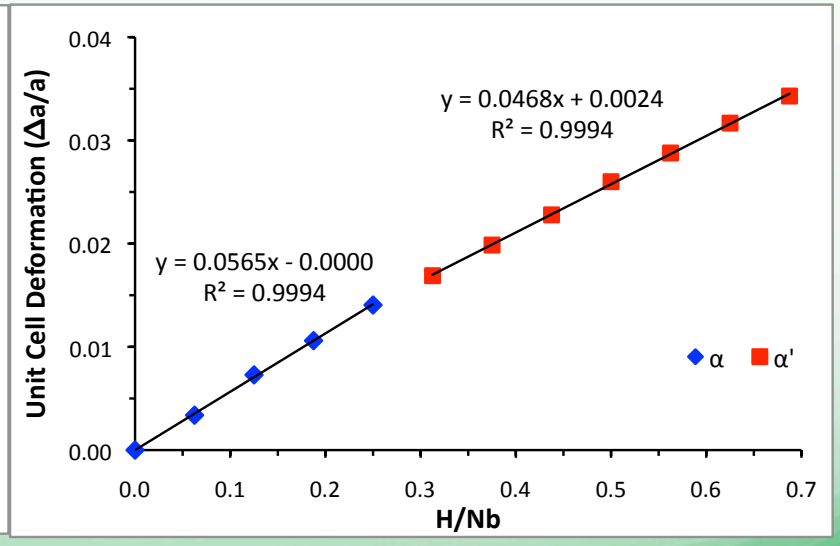
R.E. Ricker, G.R. Myneni, J. Res. Natl. Inst. Stand. Technol., 115, 1 (2010).

- What do we have in SRF cavities and how is it affected by processing?

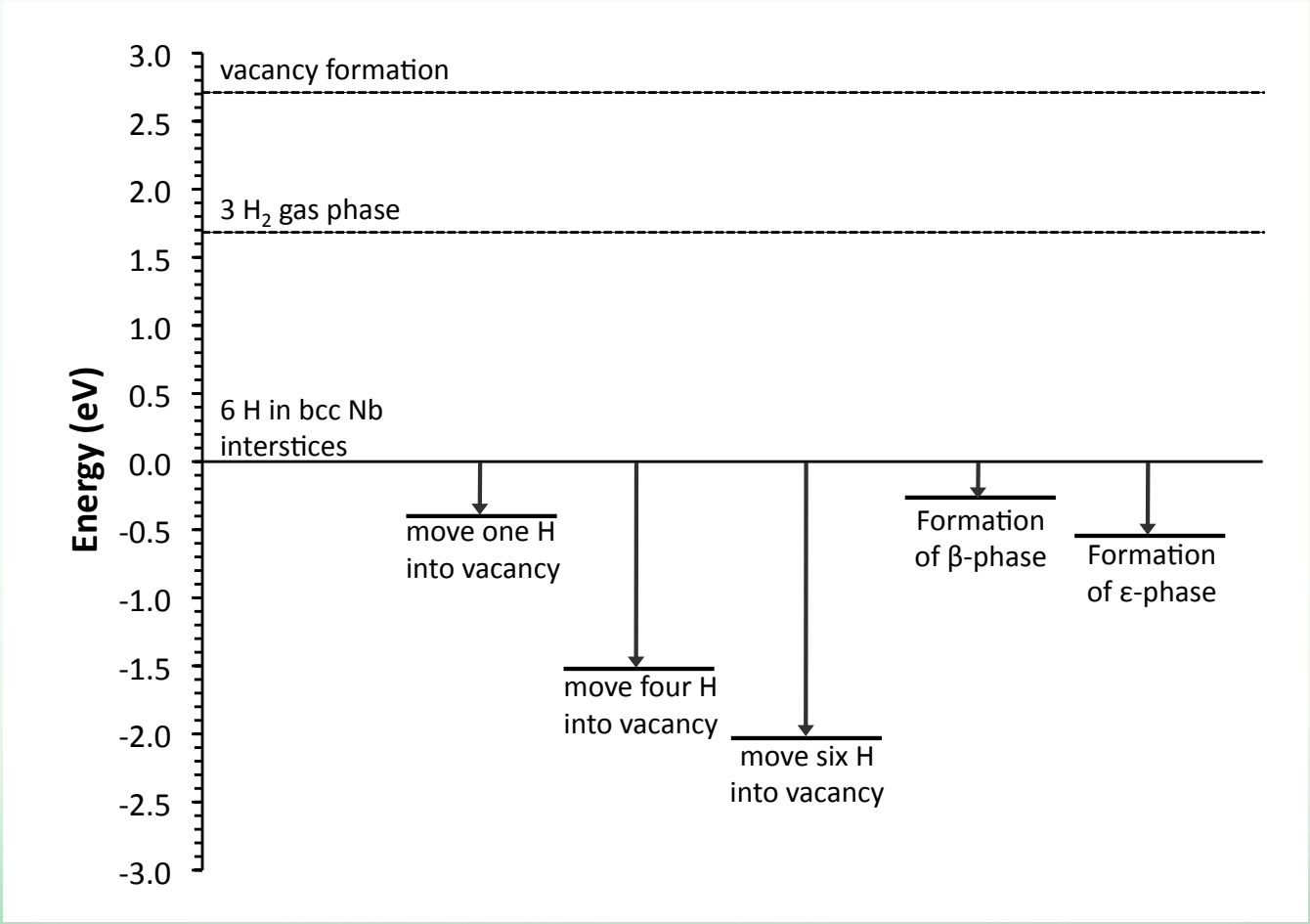
Hydrogen in Niobium
Phase Models







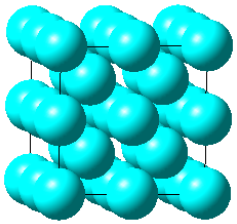
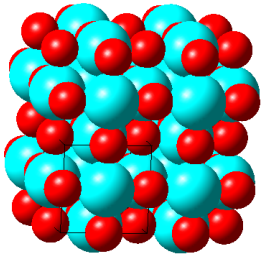
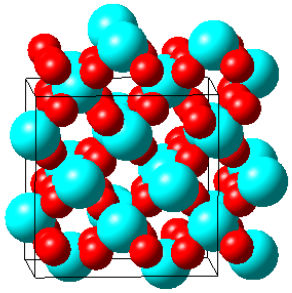
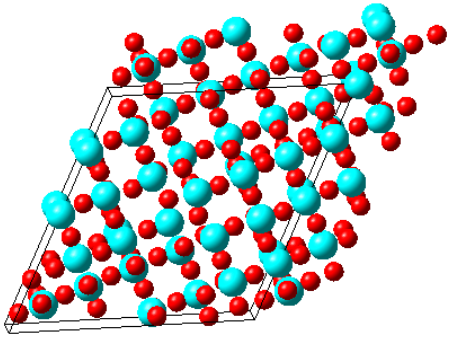
Hydrogen in Niobium
How do Phases Form?



Application to SRF Cavities

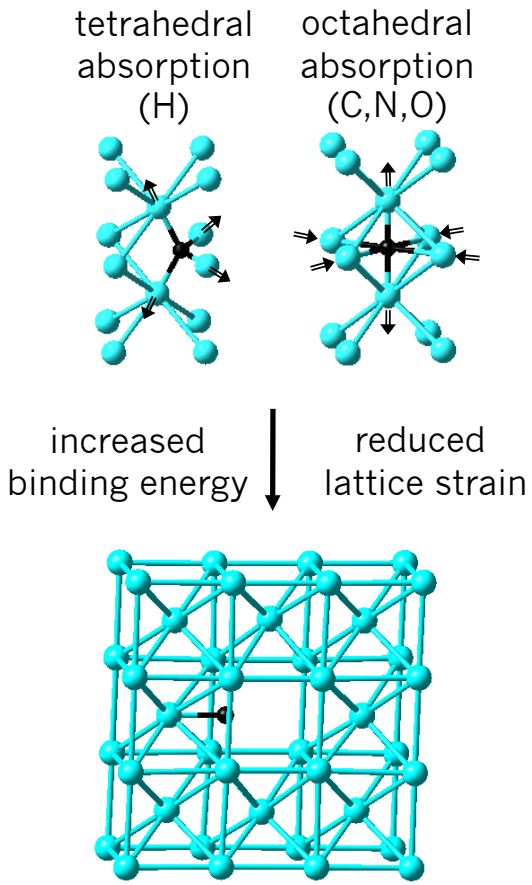
- Hydrogen in niobium could be a source of Q-slope and Q-disease.
  - Ordered hydride phases suffer from a greatly reduced superconducting T_c
  - Does the size of the precipitate matter? Large precipitates -> Q-disease; small precipitates, interstitial hydrogen -> Q-slope?
- Niobium hydride phase modeling showed
  - The driving forces for phase formation are evident in both lattice strain and energetic analyses of the presented models
  - Niobium lattice point defects can serve as nucleation centers for phase formation

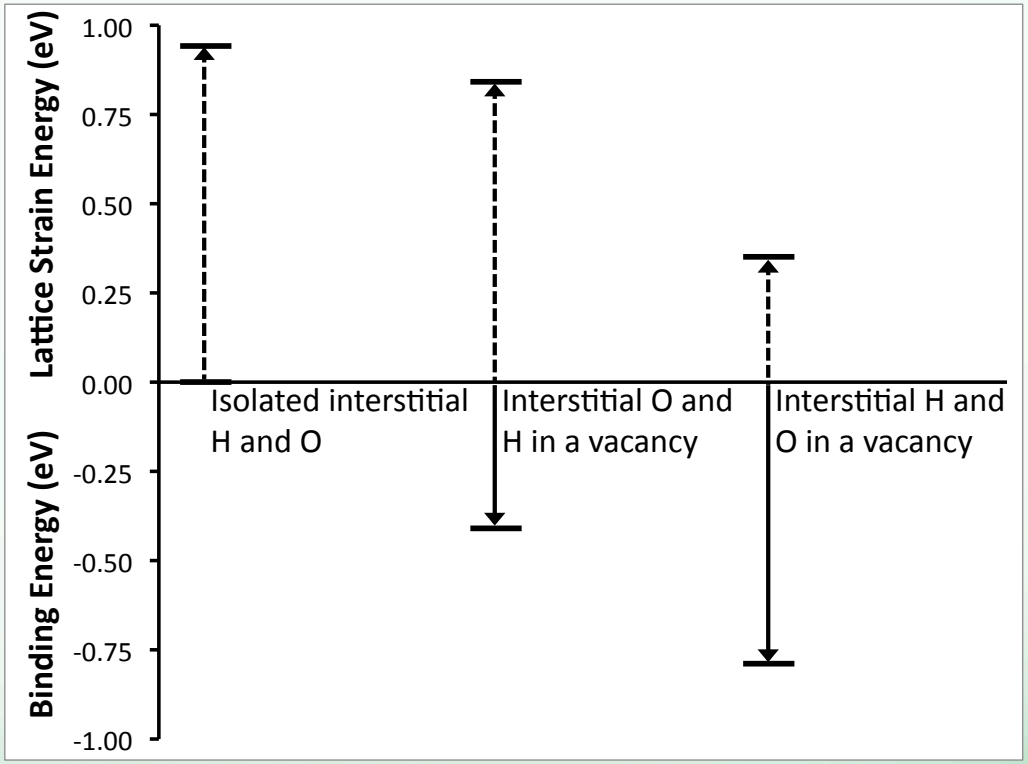
Other Impurities in Niobium
Oxide Layers

Nb – cubic	NbO – cubic	NbO_2 – tetragonal	Nb_2O_5 – monoclinic
			
3.3 Å; 90°	4.2 Å; 90°	9.7, 9.7, 6.0 Å; 90°	20.7, 3.8, 19.6 Å; 90, 65, 90°

- Thermodynamic ordering of oxide layers on the niobium surface
- Strained and defective interfaces
- Surface layer can be highly defective or amorphous
- Interfaces can be trapping centers for other impurities such as H

Other Impurities in Niobium
Relation to Hydrogen





Application to SRF Cavities

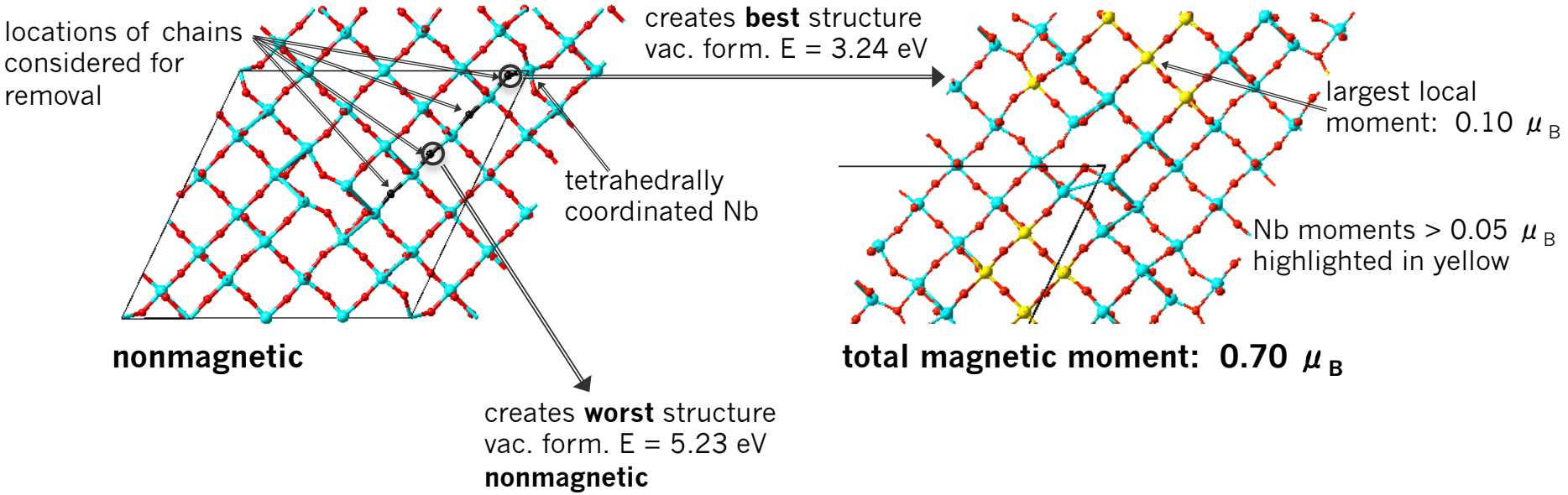
- The success of the 120 °C bake may be related to the interaction between impurities and lattice defects.
- Suggested mechanism:
  - -> Hydrogen is liberated from both the ordered hydride phases and the niobium site vacancies
  - -> Hydrogen diffuses into the niobium bulk
  - -> Some oxygen diffuses from the oxide phases or niobium interstitial sites and becomes trapped by the niobium vacancies in the near surface region
  - -> Hydrogen is prevented from returning to those phase nucleation centers
  - -> Hydrogen may also become trapped by sites in the niobium bulk

Oxygen in Niobium
An Additional Concern

Create a chain of oxygen vacancies (1.4%)

Beginning Structure – P2 Nb_2O_5

Energetically Best Structure



Summary

- Hydrogen in Niobium
  - Phase properties and driving forces for phase formation
  - Nucleation of phases by niobium lattice defects

    -> Removal of nucleation sites -> prevention of hydrides

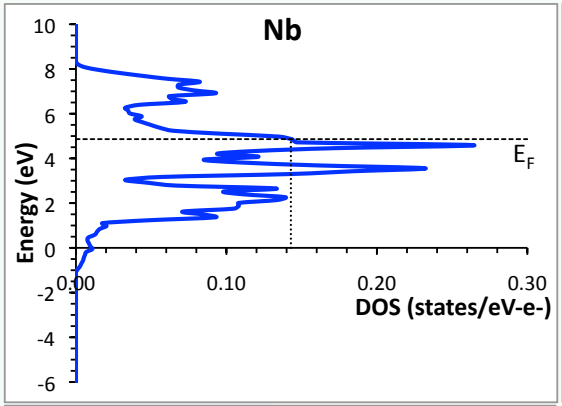
- Other impurities (**O**, N, C) in Niobium
  - Oxide structures
  - Interactions between impurities and the niobium lattice during the 120 °C bake

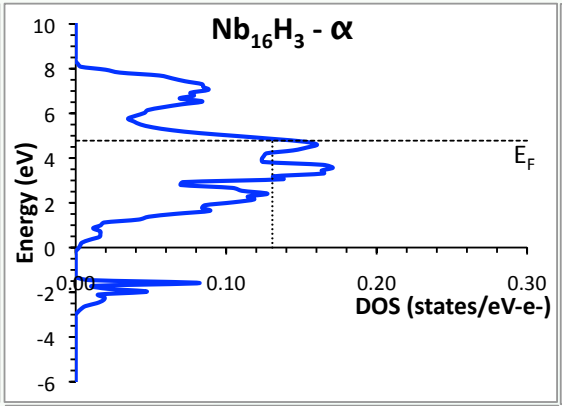
    -> dissociation/prevention of hydrides
  - Magnetism in defective oxides

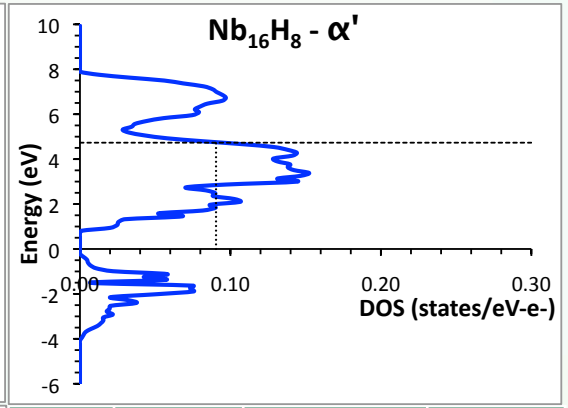
Acknowledgments

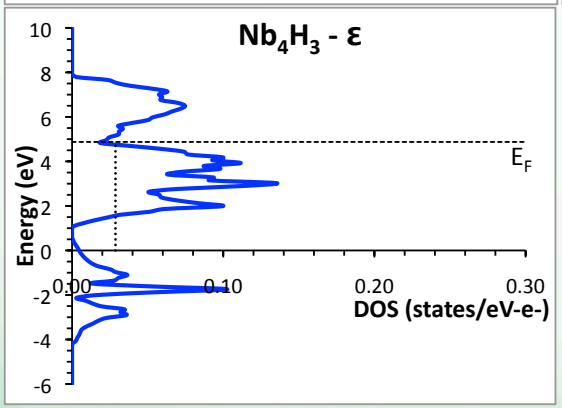
- Lance Cooley and Superconducting Materials Group members
- David Seidman and group members
- Computing resources at Fermilab

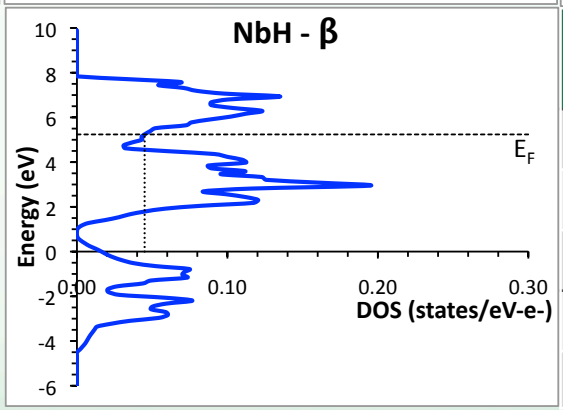
Hydrogen in Niobium
Electron and Phonon States





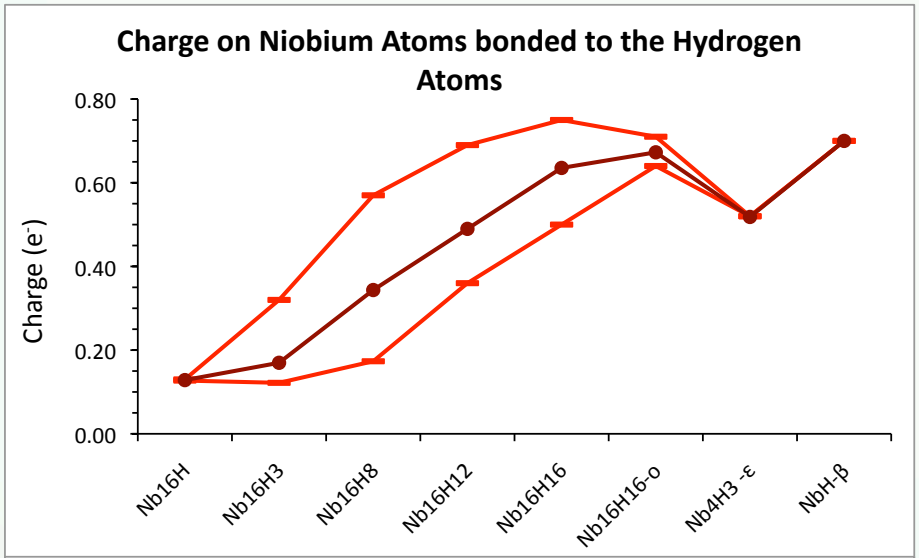


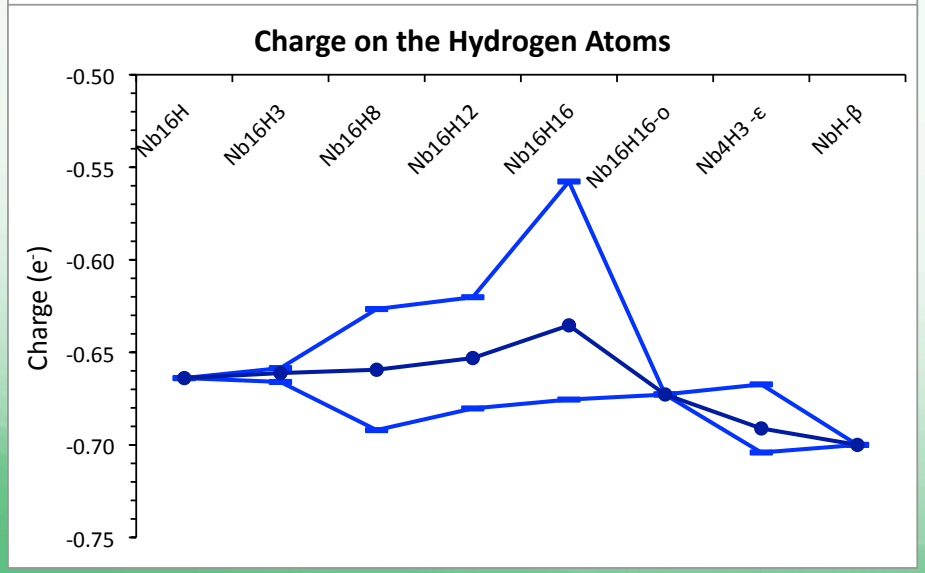




	E_F (eV)	DOS @ E_F (states/eV)	$\langle\omega\rangle_{log}$ (MeV)
Nb	4.86	0.14	17.9
α	4.78	0.13	28.5
α'	4.73	0.09	42.6
ε	4.88	0.03	62.2
β	5.24	0.04	69.4

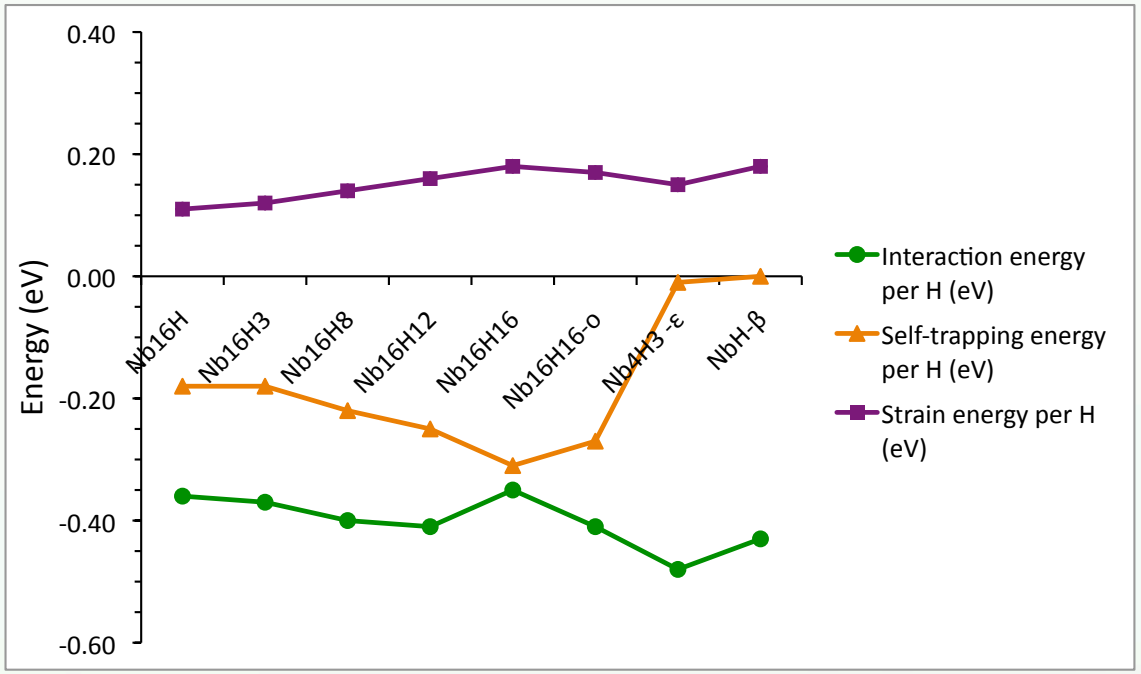
Hydrogen in Niobium
Local Charges





- The highest, lowest, and average charges are shown
- The charge on Nb atoms increases with increasing H concentration
- The charge on the H atoms slightly decreases with increasing H concentration and is the lowest for the ordered phases
- The charges on the Nb and H atoms are ~ constant for the ordered phases and equal and opposite for the beta phase

Hydrogen in Niobium
Energy Breakdown



- Interaction energy and self-trapping energy decrease with increasing H concentration; self-trapping energy is zero for the ordered configurations
- Lattice strain energy increases with increasing H concentration, is ~ equal for the disordered and ordered hydrogen configurations of the same concentration