Electronic and Atomistic Modeling of Qubit Materials & Interfaces

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- Numerous Collaborators

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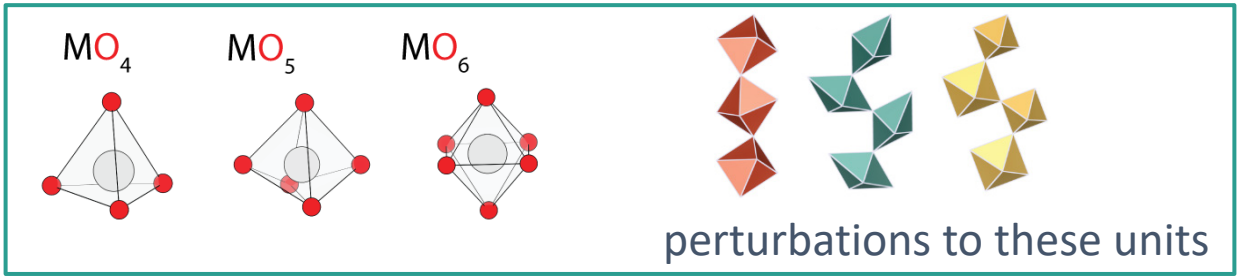
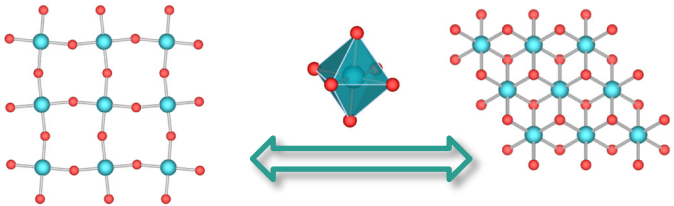
U.S. Department of Energy | Office of Science
3M
ACCESS
Argonne National Laboratory
DOD HPC Modernization Program
NERSC

Picoscale structure (100 pm = 1 Å)

- Local structure ~ geometry of these units

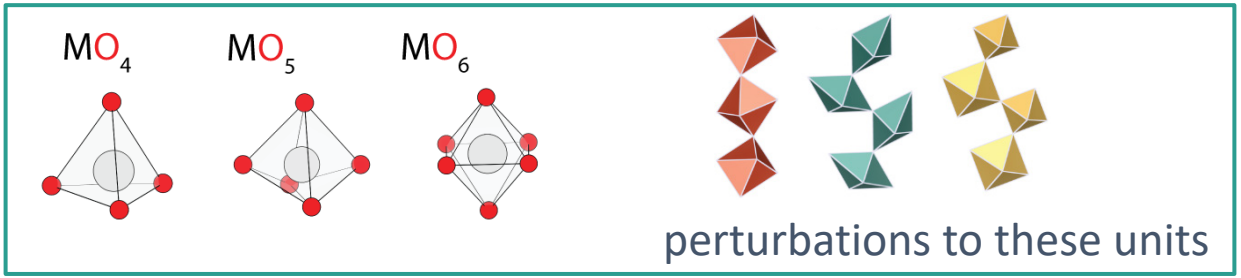


- Crystal structure ~ how one or more of these units tile space to from an extended solid



Picoscale structure (100 pm = 1 Å)

- Local structure ~ geometry of these units



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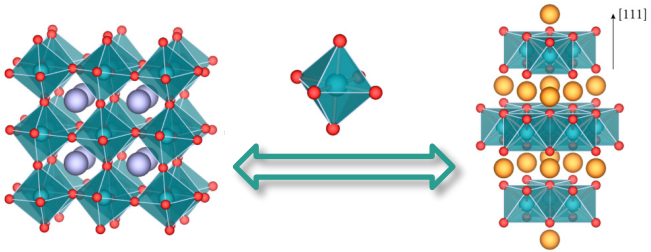
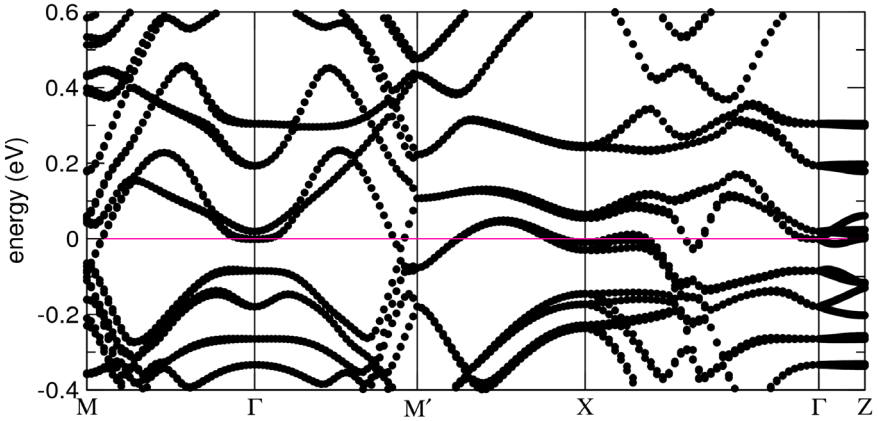
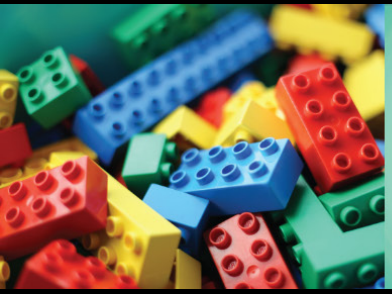




$$E[n(\mathbf{r})] = F[n(\mathbf{r})] + \int V_{ext}(\mathbf{r})n(\mathbf{r})d\mathbf{r}$$

heterostructures and superlattices



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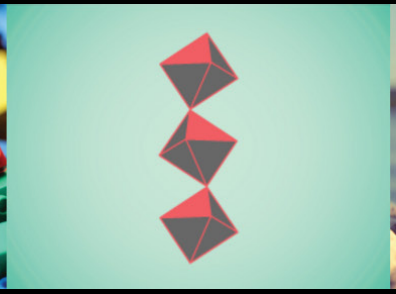
polyhedral-property control



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harmonizing contraindicated properties

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materials informatics

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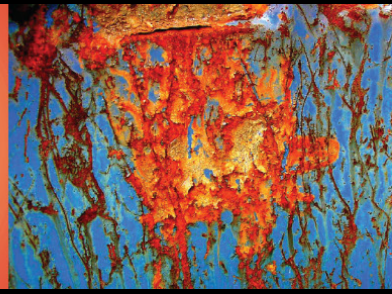
corrosion and electrochemistry



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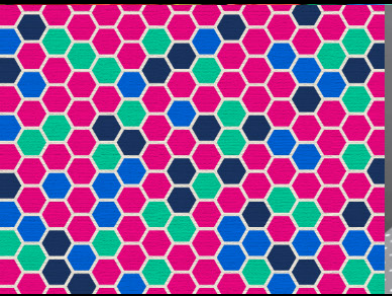
quantum materials and molecules



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transition metal compounds

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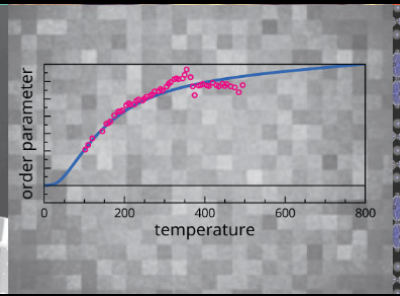
ultrafast/metastable transitions



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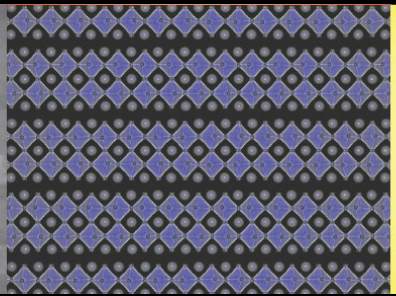
ferroics and multiferroics



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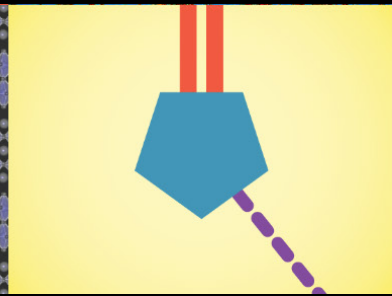
nonlinear optical crystals



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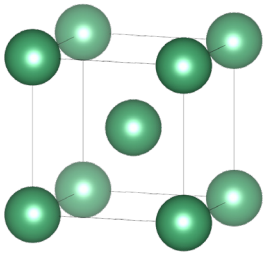
Lecture Outcomes

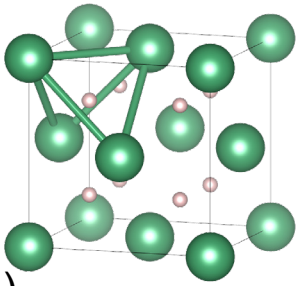
- Begin to bridge the gap between theory and experiment, fostering a deeper understanding of qubit materials and interfaces and their practical applications

Use systems charts to guide material-property correlation studies	Create atomistic models of materials and interfaces used for superconducting qubits	Understand principles of electronic and atomistic modeling	Analyze and interpret modeling results from electronic and atomistic calculations



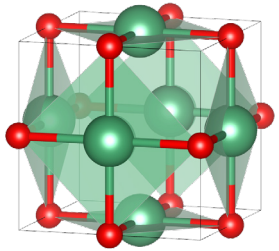
Nb ($Im\bar{3}m$)

- Niobium and its hydrides



NbH_2 ($Fm\bar{3}m$)

- Niobium and its oxides



NbO ($Pm\bar{3}m$)

Agenda

Use systems charts to guide material-property correlation studies

- SC Qubit Materials and Systems Charts – Introduction
- Modeling Materials
  - Model Formulation
  - Electronic Structure Models
  - Atomistic Models
  - From Phenomenological to Microscopic
- Use Cases
  - Nb and its hydrides
  - Nb and its oxides
- Co-Design and Integration with Experimentation – Summary

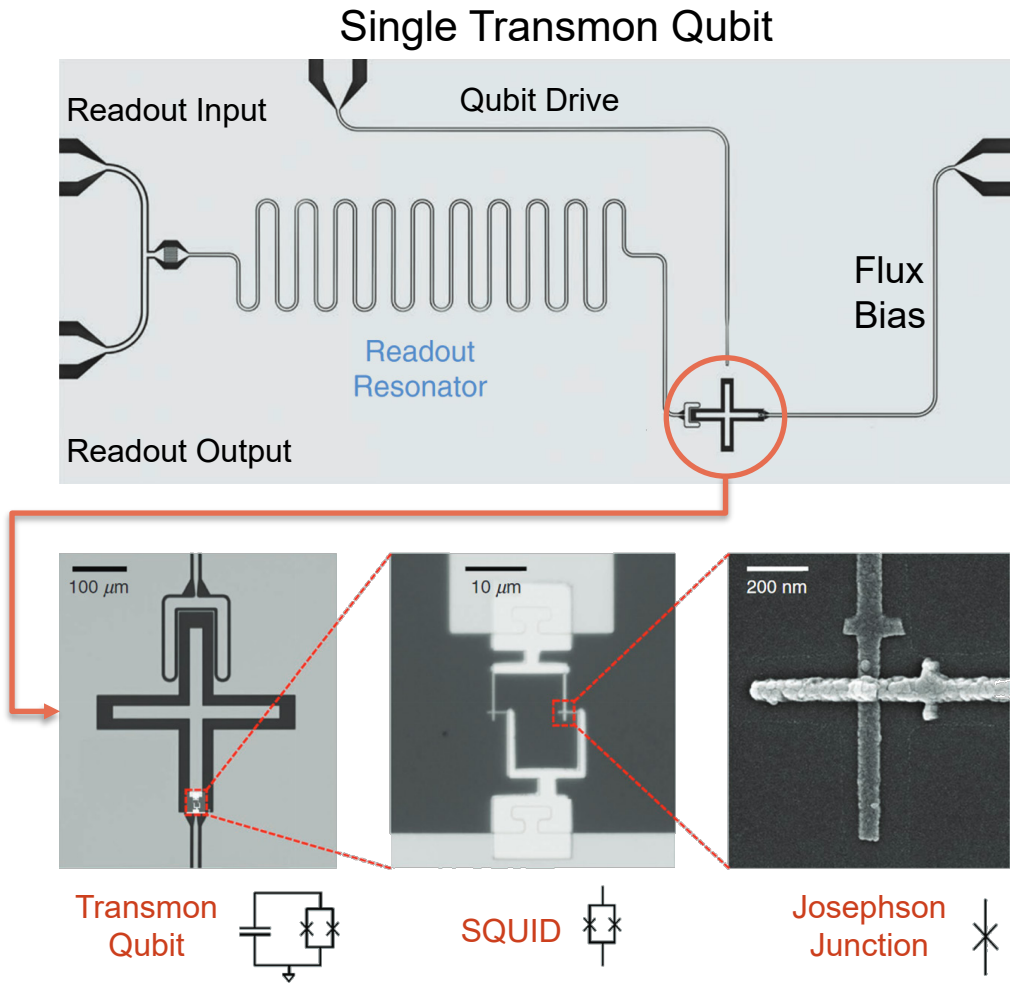
SC Qubit Architecture

Primary Materials

- Superconducting Films (Al, Nb, Ta)
- Insulating Substrate (Si, Sapphire)
- Josephson Junction (S-I-S)

Secondary Materials

- Silicon and metal oxides
- Intermetallic phases (Nb-Si)
- Adhered contaminants
- Interstitial contaminants
  - Hydrogen, Oxygen, Carbon, …



Materials Contributions to Losses (T_1) from CPW Resonators

Two-level systems

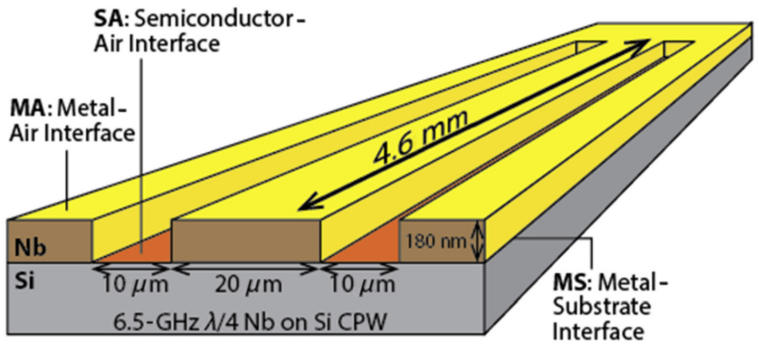
- Electric dipoles (charge noise)
- Magnetic moments (flux noise)
- Quasiparticles (broken pairs)

Quasiparticles

- Coupling directly to qubit

Thermal losses

- Dielectric loss at CPW interfaces
- Quasiparticles



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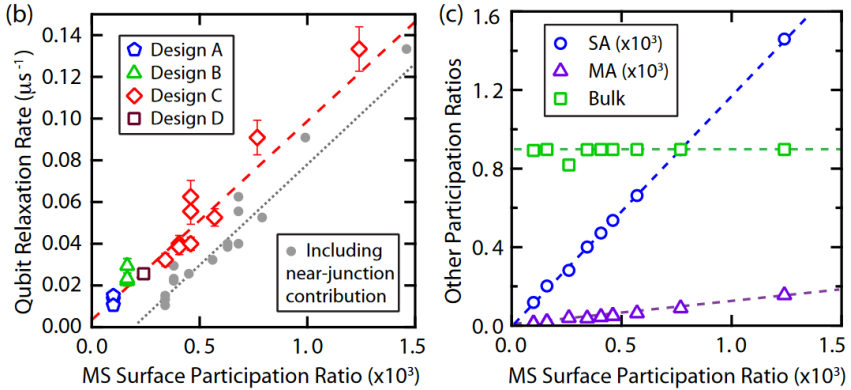
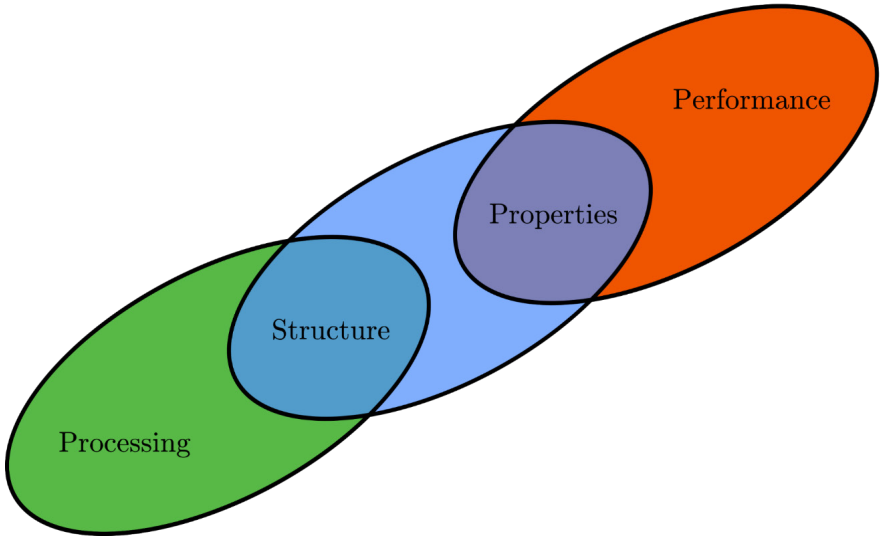


C. Wang, C. Axline, Y. Y. Gao, T. Brecht, Y. Chu, L. Frunzio, M. H. Devoret, and R. J. Schoelkopf, Surface Participation and Dielectric Loss in Superconducting Qubits, Appl. Phys. Lett. 107, 162601 (2015).

Simplify complexity using the materials science paradigm

- Processing
- Structure
- Properties
- Performance



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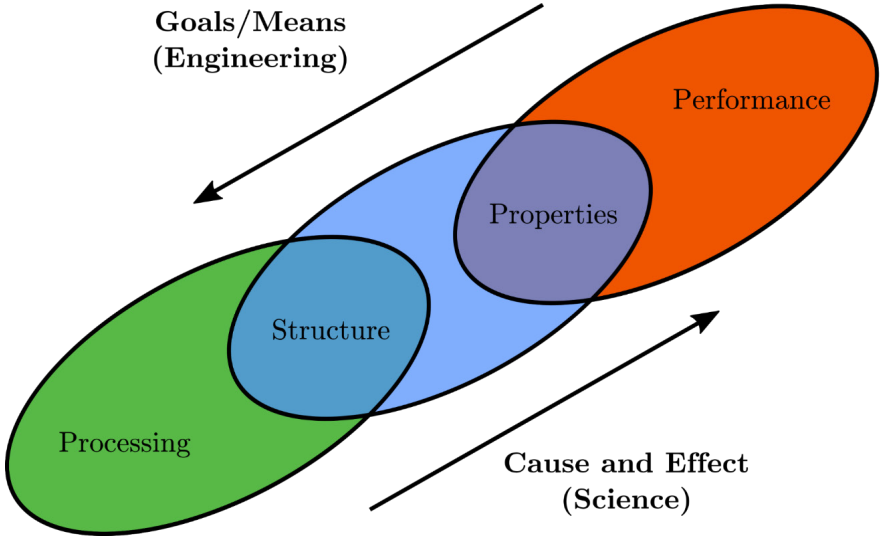
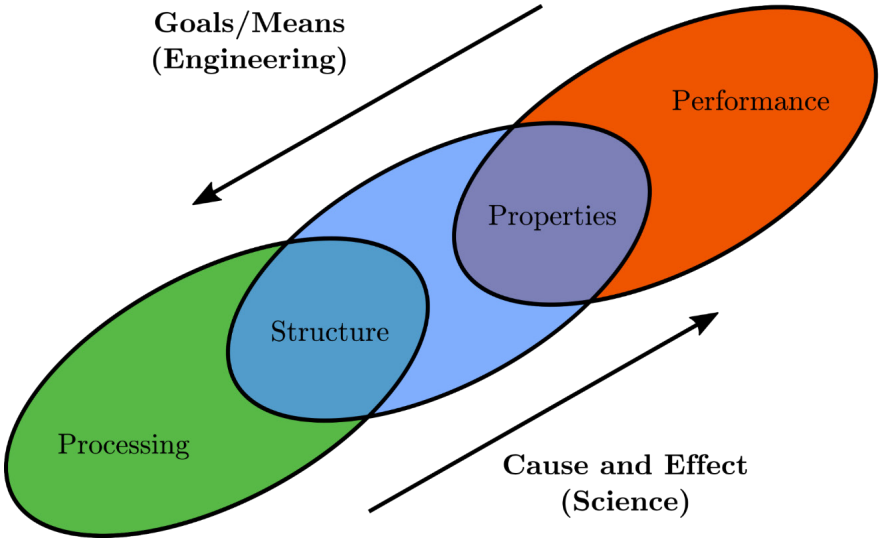
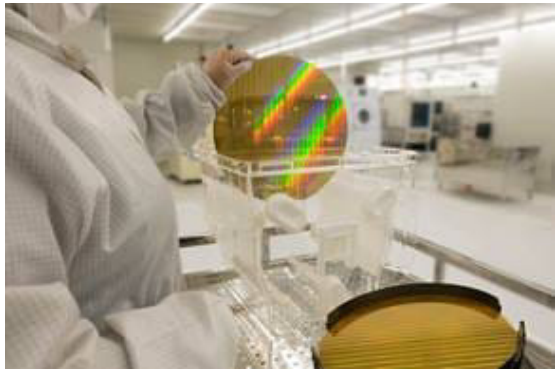


Simplify complexity using the materials science paradigm

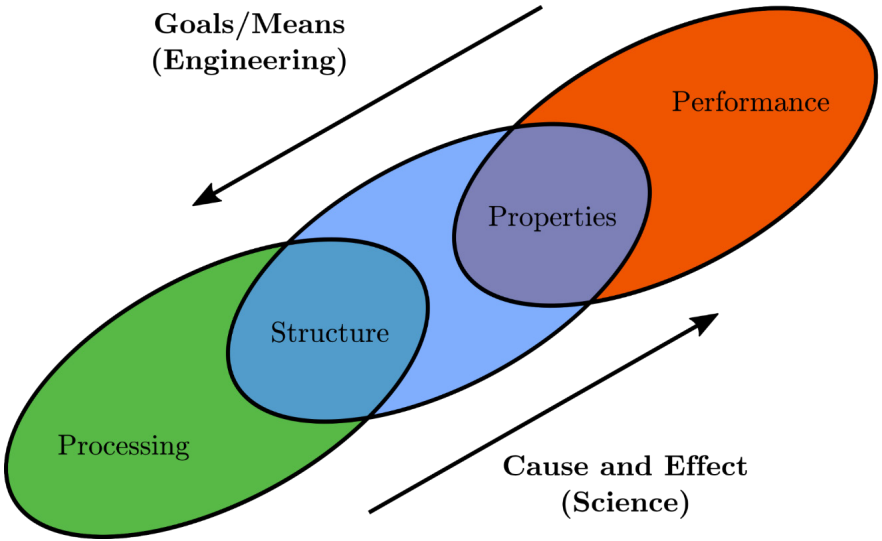
- **Processing:** The way a material is made (thermal, chemical, physical)
- Structure
- Properties
- Performance





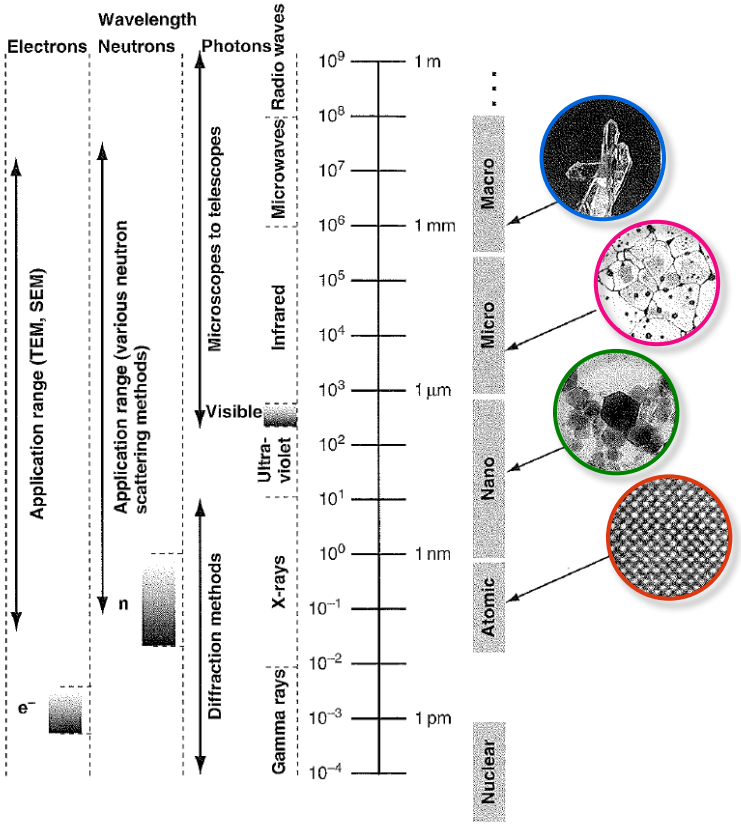
Simplify complexity using the materials science paradigm

- Processing: The way a material is made (thermal, chemical, physical)
- **Structure:** The way the material is organized
- Properties
- Performance



Internal structures of materials

- The way in which of atoms, molecules, phases, etc. assemble across length scales



Quartz crystal

Grains in a $SrTiO_3$ ceramic

Nanocrystalline $Mn_{0.5}Zn_{0.5}Fe_2O_4$ particles

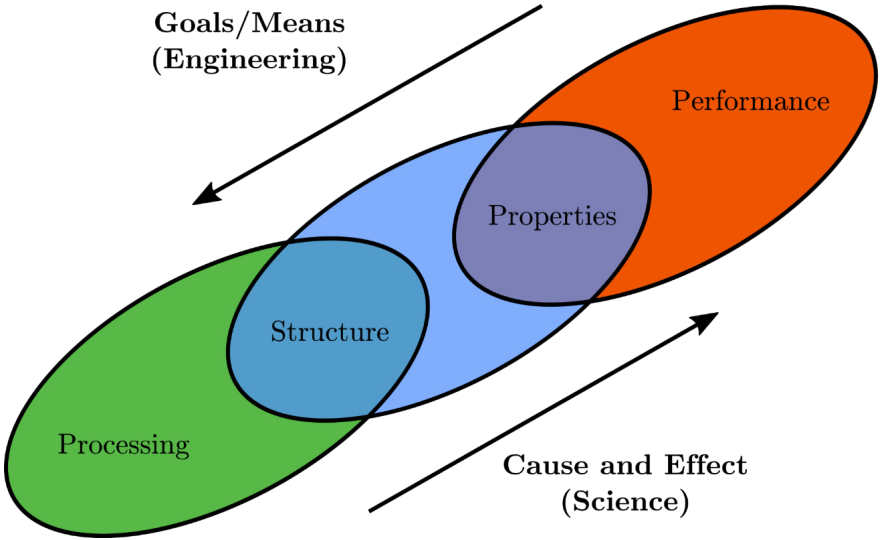
Atomic resolution image of $BaTiO_3$

Structure of a material depends on processing history, not just composition, and often exhibits hierarchical order

From de Graef and McHenry, *Structure of Materials* (2012)

Simplify complexity using the materials science paradigm

- Processing: The way a material is made (thermal, chemical, physical)
- Structure: The way the material is organized
- **Properties**: The way the material behaves
- Performance

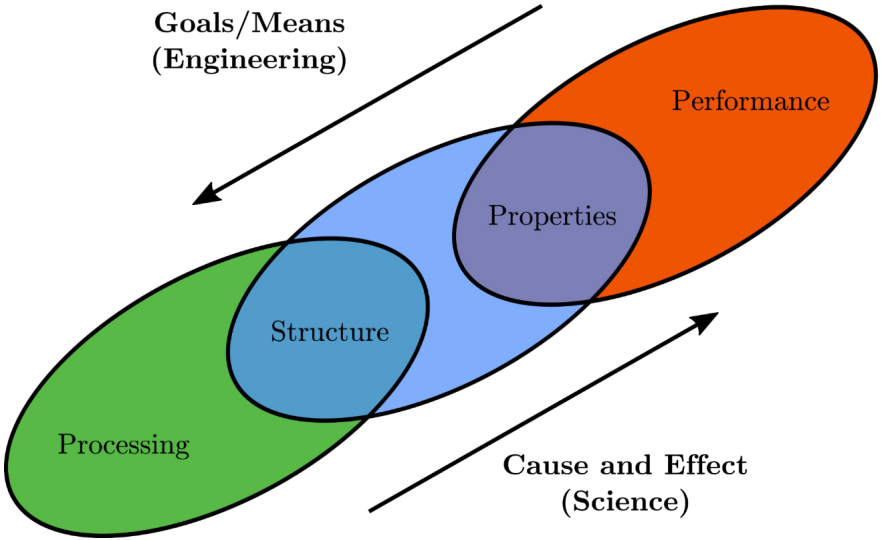


A quantifiable attribute of a material and informs us about how we expect a material to respond (displace) to a stimulus (force)

- **Mechanical** – stiffness, piezoelectricity
- **Electrical** – electrical conductivity
- **Optical** – transparency, emission
- **Magnetic** – ferromagnetic, diamagnetic
- **Chemical** – corrosion resistance
- **Thermal** – heat capacity, conductivity

Simplify complexity using the materials science paradigm

- Processing: The way a material is made (thermal, chemical, physical)
- Structure: The way the material is organized
- Properties: The way the material behaves
- **Performance**: How well a material does what it is intended to do



MSE Tools of the Trade

- Theory
- Characterization
- Computation/Modeling
- Data Science/AI

Apply systems approach to simplify complexity

- *System engineering* developed by G.M. Jenkins (1970s)

- **Nature of systems**
  - Complex grouping of components
  - Divisible into subsystems (flow-block diagrams)
  - Subsystems interactive: output of 1 is input of 2
  - System is a part of hierarchy of systems (strong influence of higher levels)
  - System has **objective(s)** influenced by the wider system; overall objective is compromise between conflicting objectives
  - System must be **designed** to function at maximum efficiency

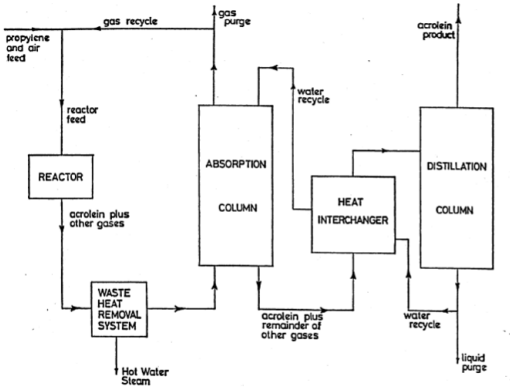


Figure 4.1 Simplified flow-block diagram of an acrolein plant as an example of a simple system with interacting subsystems.

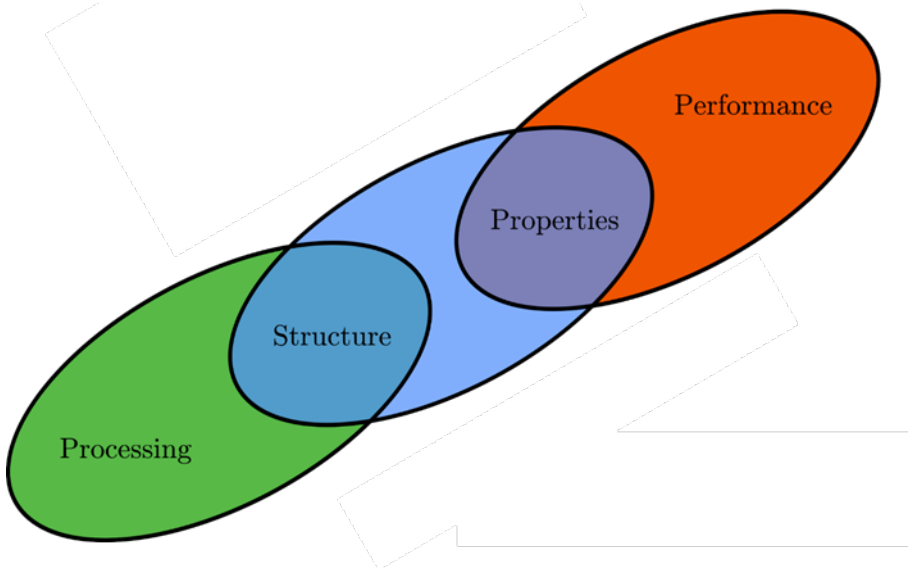
- Apply systems approach to materials, integrating processing, structure, property, and performance (G.B. Olson)
  - Science 277,1237-1242 (1997)

CHiMaD

SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

Using materials science paradigm – Systems Design Charts

- Consider the material, interface(s), or device(s) as a system
- Identify connections between processing-structure-properties-performance
  - Understanding the strength of connections requires domain expertise



Using materials science paradigm – Systems Design Charts

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- Guidelines
  - Processing is sequential (use arrows to show direction)
  - Structures can interact with one-way arrows
  - “Links” represent the reciprocal interactions
  - Properties are quantitative / measurable
  - Performance is what an end-user may request for a component or application

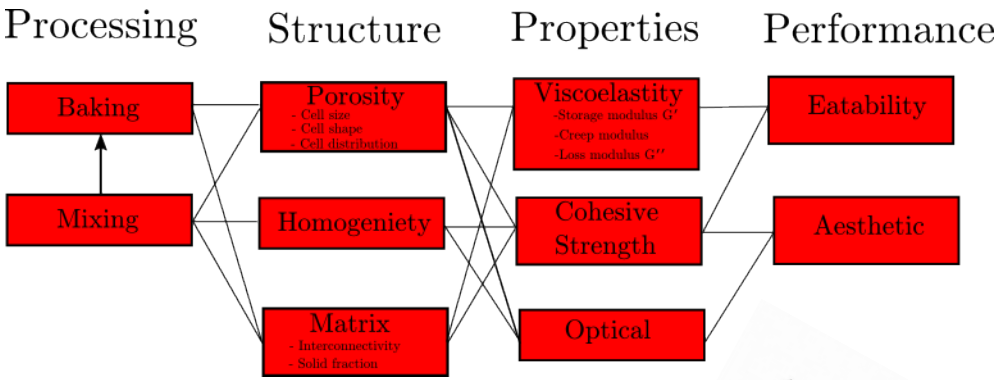
Using materials science paradigm – Systems Design Charts

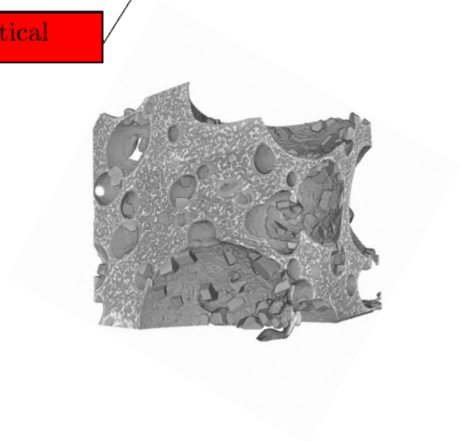
- Consider the material, interface(s), or device(s) as a system
- Identify connections between processing-structure-properties-performance
  - Understanding the strength of connections requires domain expertise

PROCESSING — **STRUCTURE** — **PROPERTIES** — **PERFORMANCE**

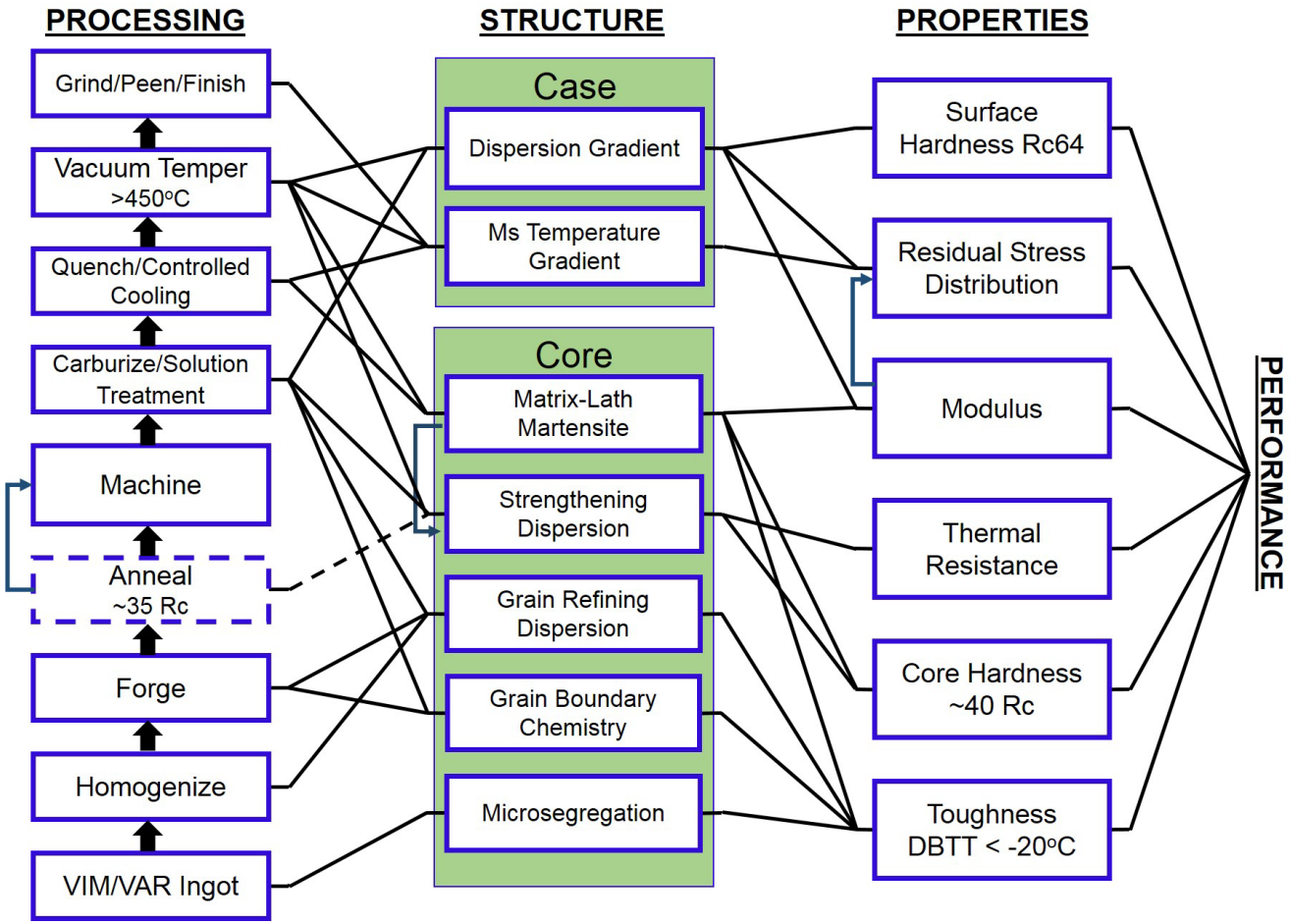
- Systems design chart for chocolate cake
  - Processing?
  - Structures?
  - Properties?
  - Performance?

Simplified Systems Design Chart for Cake





System Design Charts Get Complex! – C64 Gear Steel



Pub. No.: US 2009/0199930 A1
Pub. Date: Aug. 13, 2009

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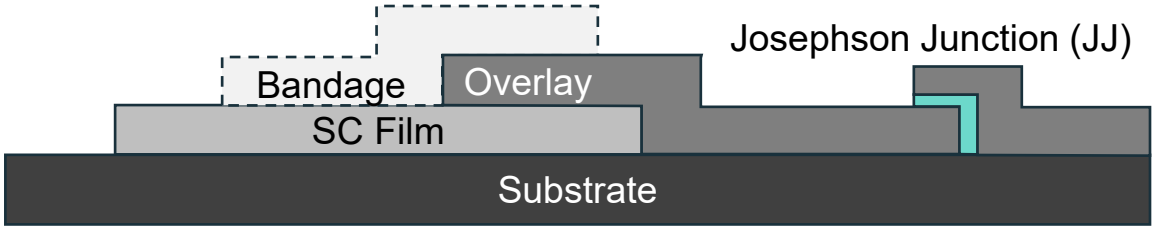
Superconducting Qubits as a Complex System

Materials

- Substrates
- SC Films
- Dielectrics

Interfaces



Metrics

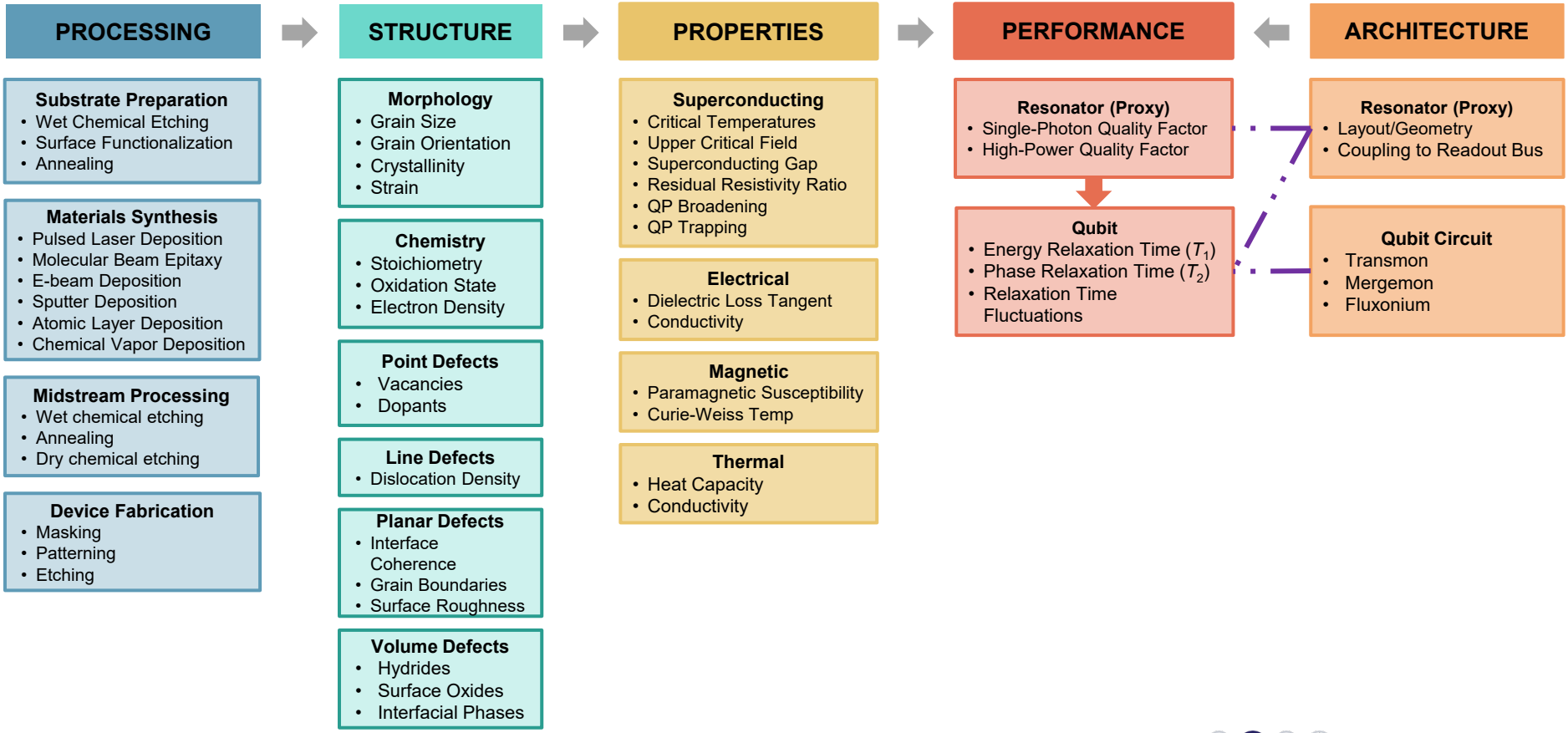
- Resonator Q
- Qubit Coherence Times (T_1/T_2)
- Coherence Time Fluctuations

PROCESSING → STRUCTURE → PROPERTIES → PERFORMANCE ← ARCHITECTURE

More recommendations for system design charts

- Be as specific as possible
- Charts can and should evolve as we understand more about the system
- Subsystems are usually your focus, but also consider the whole system first
- Consider what models, tools, experiments the links represent

Systems Design Chart



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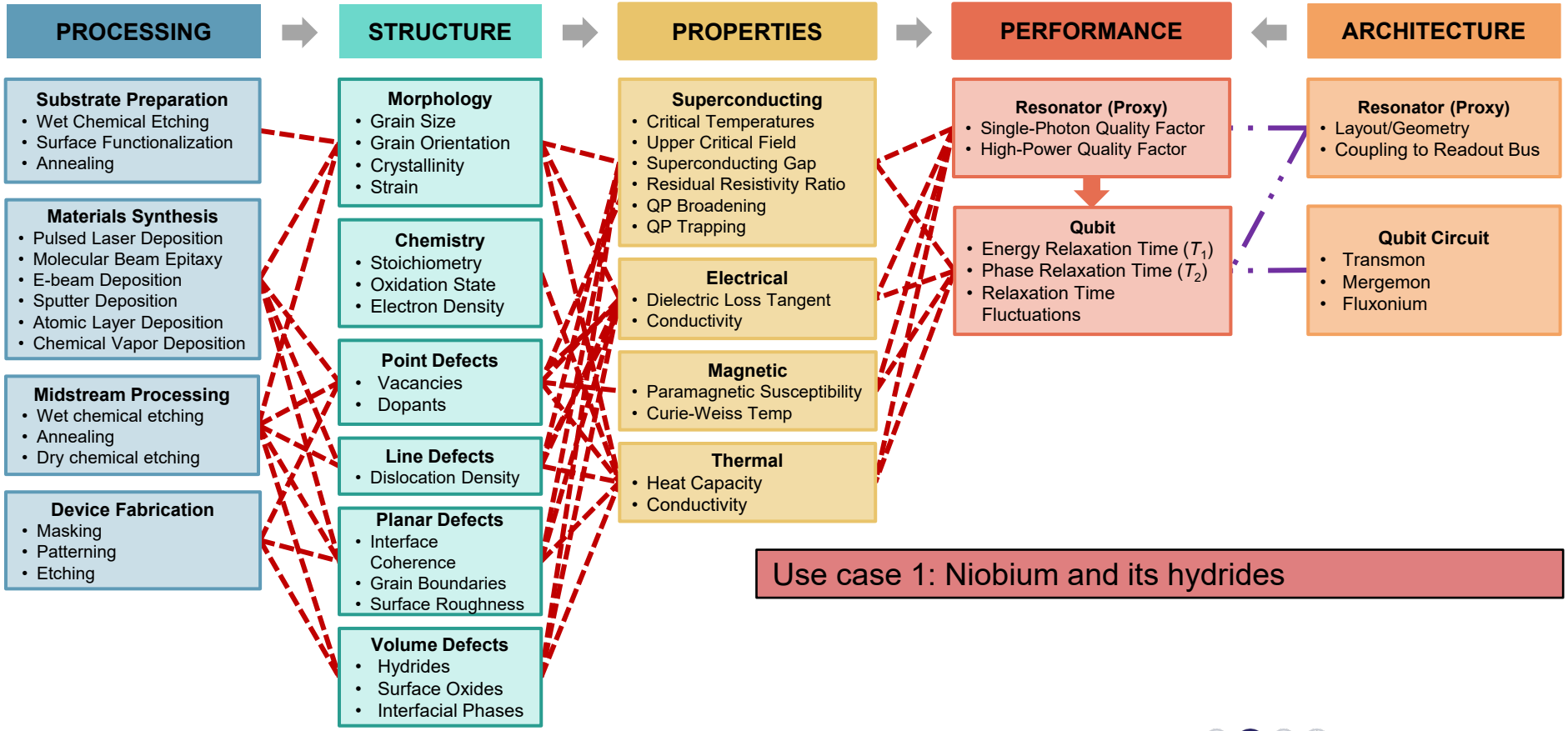
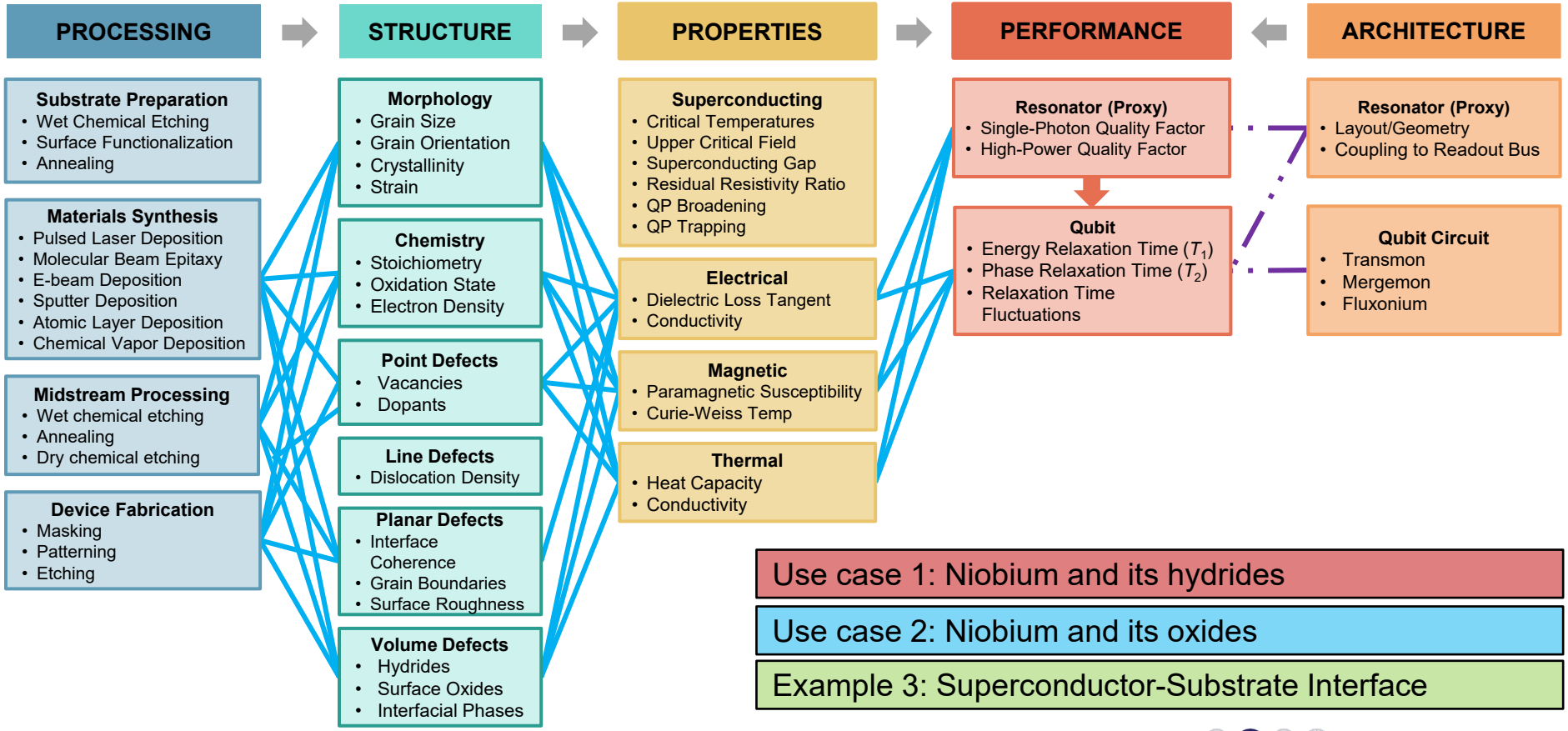


Use case 1: Niobium and its hydrides

Systems Design Chart

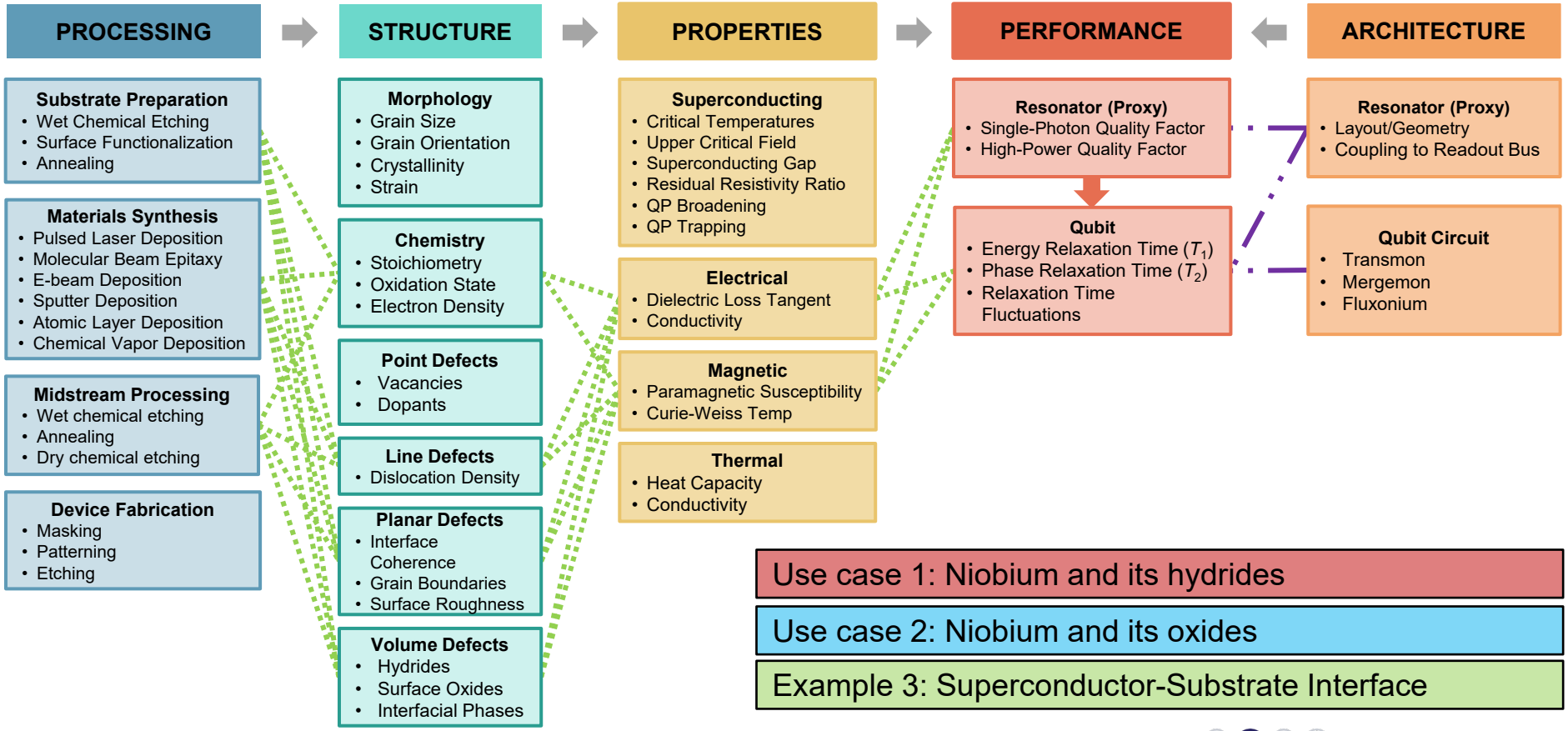


Use case 1: Niobium and its hydrides

Use case 2: Niobium and its oxides

Example 3: Superconductor-Substrate Interface

Systems Design Chart

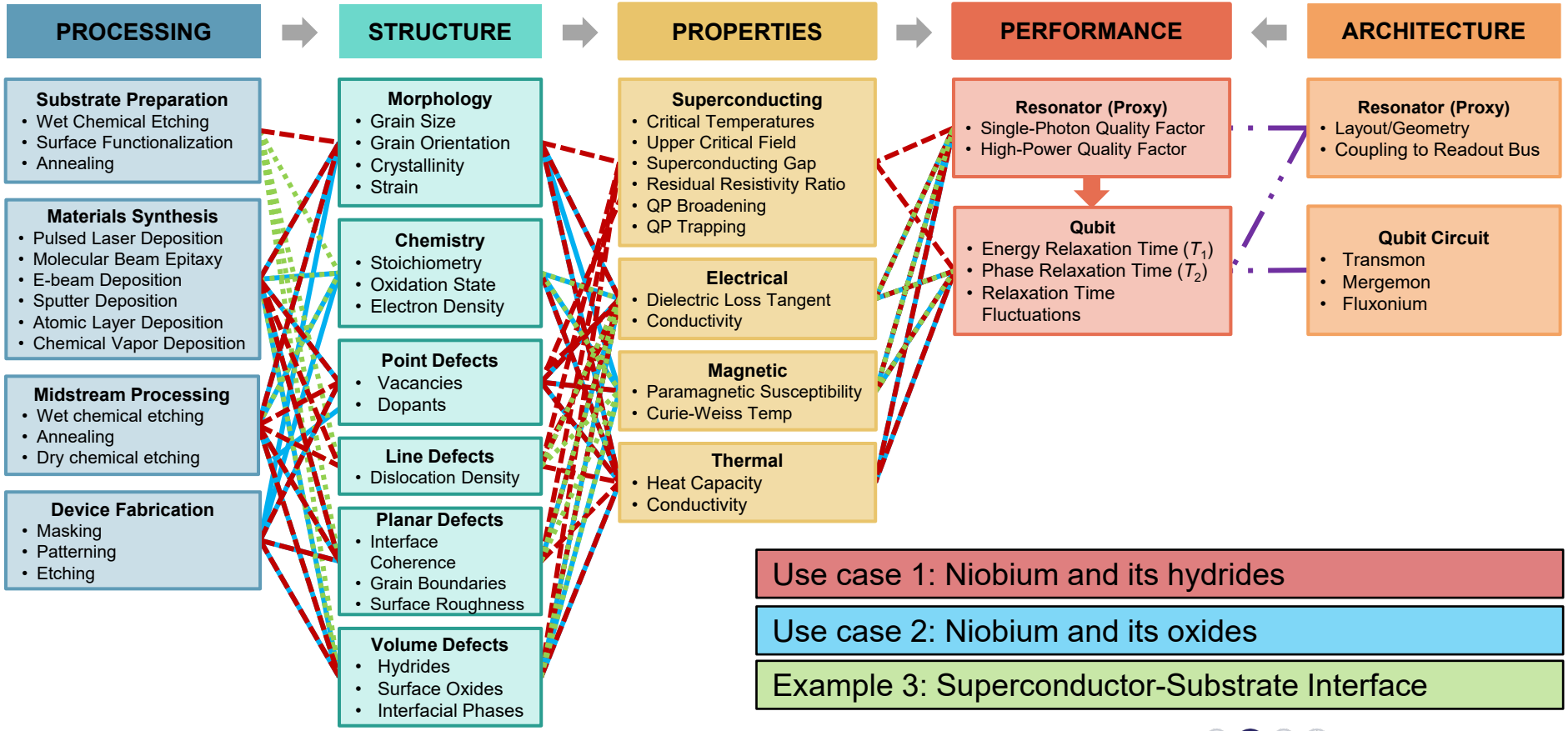


Use case 1: Niobium and its hydrides

Use case 2: Niobium and its oxides

Example 3: Superconductor-Substrate Interface

Systems Design Chart



Use case 1: Niobium and its hydrides

Use case 2: Niobium and its oxides

Example 3: Superconductor-Substrate Interface

Agenda

- SC Qubit Materials and Systems Charts – Introduction

- Modeling Materials
  - Model Formulation
  - Electronic Structure Models
  - Atomistic Models
  - From Phenomenological to Microscopic

- Use Cases
  - Nb and its hydrides
  - Nb and its oxides

- Co-Design and Integration with Experimentation – Summary

Create atomistic models of materials and interfaces used for superconducting qubits

Understand principles of electronic and atomistic modeling

Theory, modeling, and simulation

- **Theory**
  - Attempt to find a fundamental description of a physical process
  - Coherent group of general propositions used as principles of explanation for a class of phenomena

- **Model**
  - An idealization of real behavior
  - Approximate description based on empirical and/or physical reasoning
  - Distinction from theory: Model attempts to create idealization of real behavior to a given accuracy, not a fundamental description that is strictly true

models describes a part of a real system by using a similar but simpler structure; they providing a starting point for theory

Model representation

- Models always have an external representation of some kind
  - Representation is approximate
  - Each representation is useful for some purposes

Electronic Structure Model

S. Griffin (2023): [arXiv: 2307.16892]

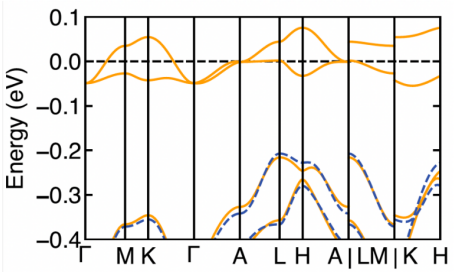
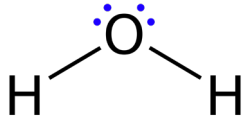


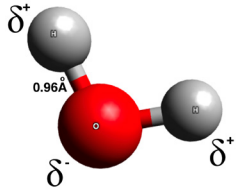
FIG. 4. Calculated spin-polarized electronic band structure in smaller energy range around the Fermi level showing the isolated two-band Cu-*d* manifold. The Fermi level is set to 0 eV and is marked by the dashed line.

Atomic Structure Model

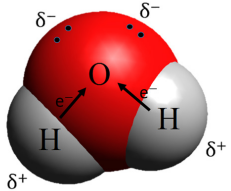
Lewis Structure



Ball-Stick



Space Filling



Equation Models

Classification Models

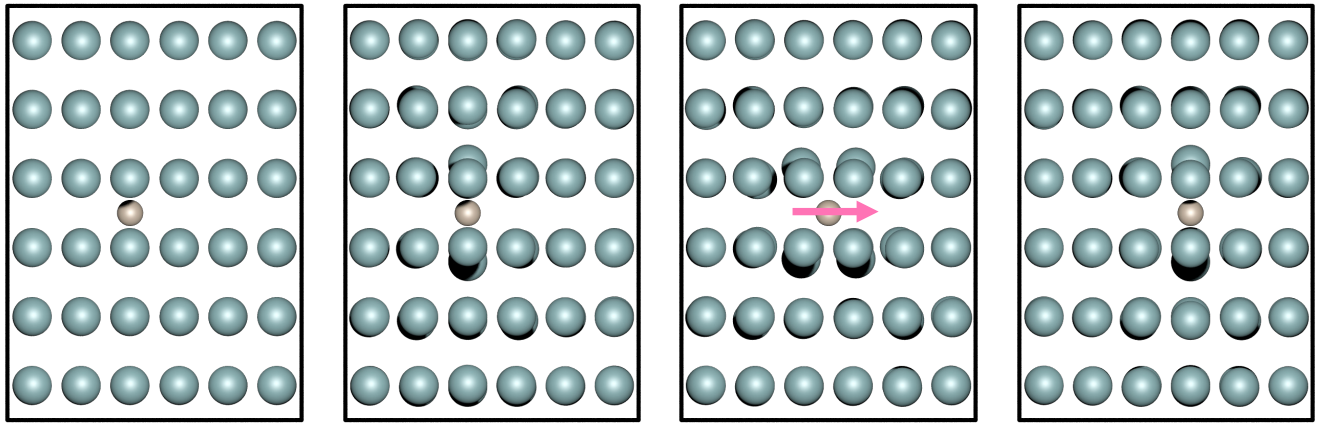
Theory, modeling, and simulation

- **Simulation**
  - Study of the dynamical response of a system
  - Subjecting models to inputs and constraints that simulate real events

  - *Does not mimic reality, but mimics a model of reality*

- Accuracy depends on many factors
  - Numerical methods and their accuracy
  - Inadequacies of the model (assumptions, principles) upon which simulation is based

Interstitial Oxygen Diffusion in Nb

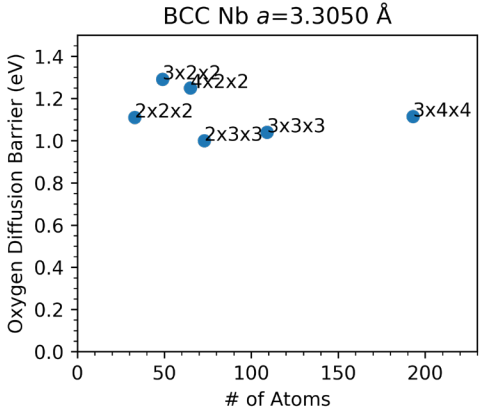


Initial State
Pre-Relaxation

Initial State
Post-Relaxation

Transition State
Post-Relaxation

Final State
Post-Relaxation



Calculated
diffusion barrier:
1.1 eV

- Successful materials modeling relies on
  - Adequate familiarity with the underlying mathematics and numerical analysis principles
  - Solid understanding of the materials physics or chemistry of the problem to be solved

Theory, modeling, and simulation

- **Simulation**
  - Study of the dynamical response of a system
  - Subjecting models to inputs and constraints that simulate real events

  - *Does not mimic reality, but mimics a model of reality*

- Accuracy depends on many factors
  - Numerical methods and their accuracy
  - Inadequacies of the model (assumptions, principles) upon which simulation is based

- Cannot separate simulations from the underlying models!

Building physical and testable models

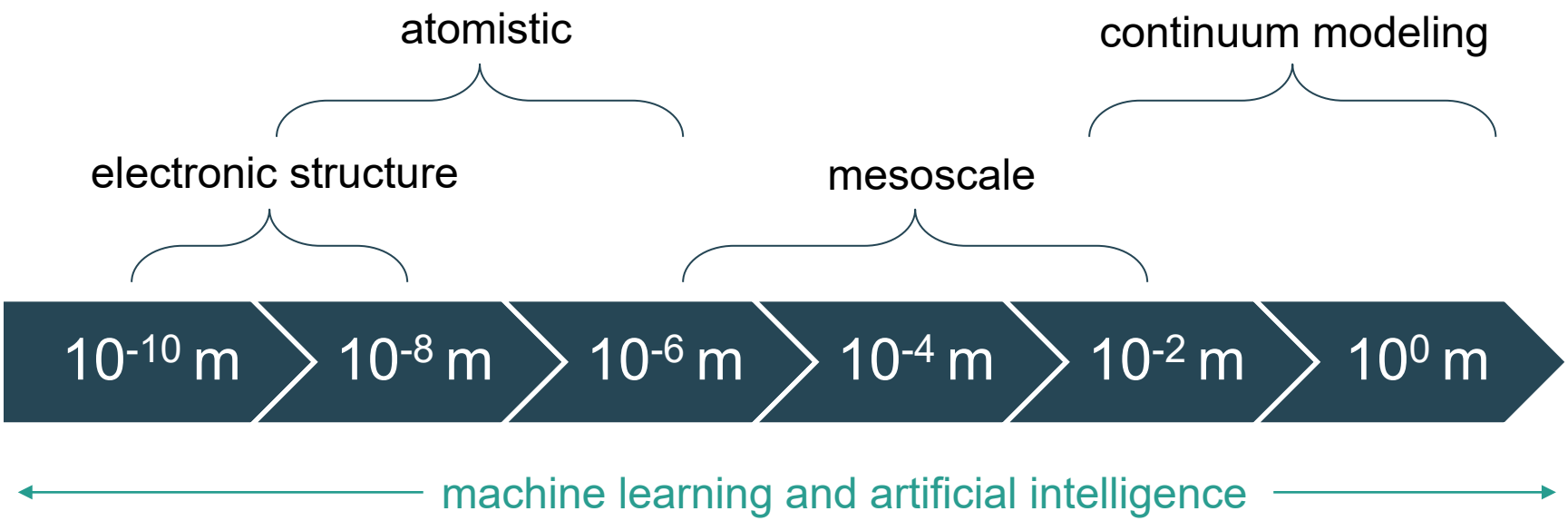
- Simulations are not reality, they represent a model of reality

- Cost/benefit analysis
  - Just because you can calculate something, it does not mean it's always the best approach
  - It is sometimes simpler and better to do a measurement

- Garbage In = Garbage out (GIGO)

> ***"COMPUTERS ARE USELESS. THEY CAN ONLY GIVE YOU ANSWERS."***
>
> – Pablo Picasso

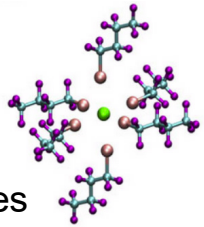
Length scales and methods



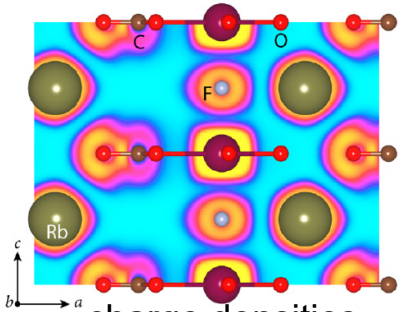
Types of methods

- **Electronic structure**
  - Calculate where the electrons are in materials
  - Relies on quantum mechanics, wave functions and methods to solve Schrodinger equations

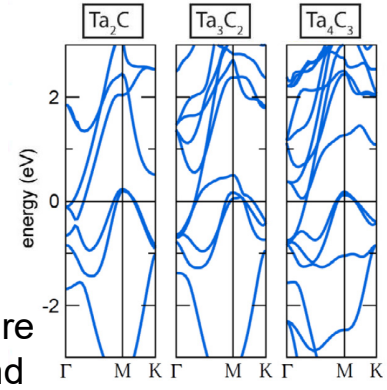
- **Atomistic**
  - Follow individual atoms in materials
    - Molecular statics
    - Quasi-harmonic theory
    - Molecular dynamics
    - (Kinetic) Monte Carlo



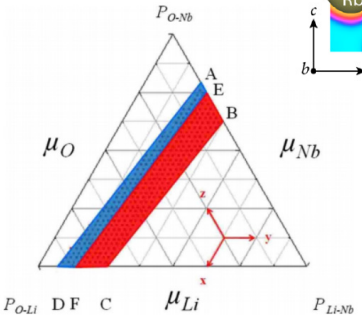
structures



charge densities



band structure
electronic and
optical properties



total energy
relative stability of configurations
and concentrations

Types of methods

- **Mesoscale**
  - Track other entities (grains size, magnetization,…)
    - Cellular automata (CA)
    - Monte Carlo
    - Phase fields
- **Continuum modeling**
  - General differential equation solving
  - Numerical methods of ODEs/PDEs
  - Thermal transport
- **Data-driven methods**
  - Unsupervised learning
  - Supervised learning
  - Neural networks
  - Symbolic regression

Metropolis Monte Carlo – generates configurations according to the desired statistical mechanics distribution

✓ There is no time, the method cannot be used to study evolution of the system

✓ Equilibrium properties can be studied

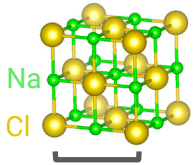
Kinetic Monte Carlo (KMC) – can address kinetics of a system

✓ Use transition rates that depend on the energy barrier between the states, with time increments formulated so that they relate to the microscopic kinetics of the system

Methodology: Density Function Theory (DFT) Simulations

Macroscopic
(visible scale)

Modelling



Microscopic
building blocks
(atomic scale)

5.7Å (1Å = 10^{-10}m)

From theory to computation

N-electron potential energy

Electron-electron interactions

$$E[n] = \int d\mathbf{r} n(\mathbf{r}) V_n(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \frac{n(\mathbf{r}) n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

$$- \sum_i \int d\mathbf{r} \phi_i^*(\mathbf{r}) \frac{\nabla^2}{2} \phi_i(\mathbf{r}) + E_{xc}[n]$$

DFT total energy

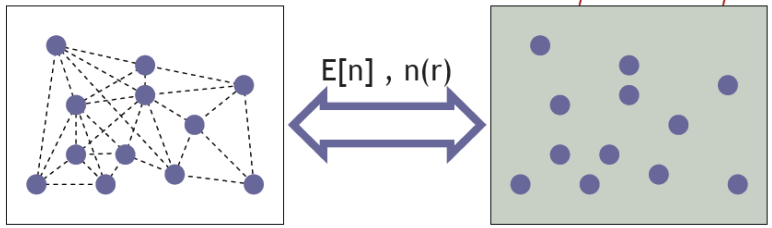
N-electron kinetic energy

Exchange-correlation energy

- Solve a set of Schrodinger-like equations for the electronic states to obtain the ground state density (and properties) of a material

DFT approach (band theory)

$\mathcal{H}\Psi = \mathcal{E}\Psi$ $\quad\quad$ $\hat{H}\phi = \epsilon\phi$



interacting electrons

non-interacting electrons

$$E[n(\mathbf{r})] = F[n(\mathbf{r})] + \int V_{ext}(\mathbf{r})n(\mathbf{r})d\mathbf{r}$$

kinetic energy, Hartree terms, quantum mechanical (exchange-correlation) and electromagnetic terms

the atomic structure and any external fields are contained in this term

- The ground-state density of electrons interacting with each other can be calculated as the ground-state density of an auxiliary system of non-interacting electrons (Kohn & Sham, 1965)

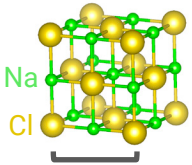
Popularity of DFT for materials modeling

- Transferability – method applies to many material classes
- Simplicity – direct link between elementary QM (independent particles) and materials physics and chemistry
- Reliability
  - Accuracies can be as good as a few percent
  - Approximations (uncontrolled but often very good)
- Software sharing
  - Efficient numerical methods to perform the minimization
- Reasonable starting point for higher level methods

Methodology: Density Function Theory (DFT) Simulations

Macroscopic
(visible scale)

Modelling



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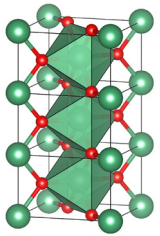
DFT total energy

$$- \sum_i \int d\mathbf{r} \phi_i^*(\mathbf{r}) \frac{\nabla^2}{2} \phi_i(\mathbf{r}) + E_{xc}[n]$$

N-electron kinetic energy

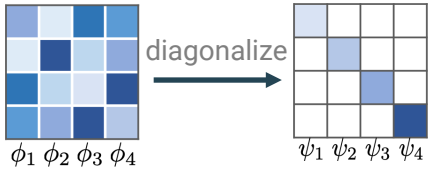
Exchange-correlation energy

Workflow of DFT simulations



Crystal structure
and composition

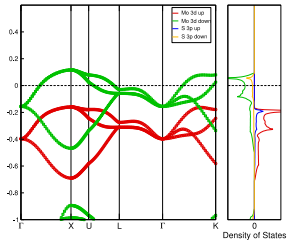
mature electronic structure tools



Solving the ground state
electronic wave function

- Energy
- Magnetism
- Band gap
- Elasticity
- …

Properties of interest



Result analysis

What we can calculate with DFT (accessible properties)

- Total energy in the ground state
  - Cohesive energies
  - Relative stability of different phases/structures
  - Heats of formation
  - Surface and interface energies
  - Adsorption energies, diffusion barriers, etc.

- Structural Optimization
  - Cell shape and size
  - Atomic positions

- Electronic properties
  - Electron density plots
  - Atomic charges and magnetic moments
  - Kohn-Sham band structure/ eigenvalues (not real-world structure, but often compared)

Material	Expt	Theory	Delta	Type
LaBi	6.57	6.648	1.2%	alloy
CaF_2	5.4626	5.496	0.6%	halide
Ag	4.086	4.112	0.6%	metal
V	3.028	3.019	-0.3%	metal
ZrN	4.62	4.634	0.3%	misc
NbO	4.2103	4.2344	0.6%	oxide
GaAs	5.653	5.663	0.2%	semiconductor
$CoSi_2$	5.36	5.3	-1.1%	silicide

Chris J. Pickard

Accuracy: 1-2% for a weakly correlated material
Except for E_{coh} and band gaps

What we can calculate (energy derivatives)

- First-order
  - Atomic forces, stress tensor
  - Macroscopic polarization (Berry Phase approach)
  - Magnetoelectric coupling (recent development)

- Second-order
  - Optical and static dielectric tensor
  - Elastic constants and piezoelectric tensor
  - Born effective charges and IR intensities
  - Phonon dispersion plots

- Third-order
  - Non-linear optical susceptibilities
  - Raman intensities

Accuracy: 5-10%
Except for high-frequency dielectric constant

Building models

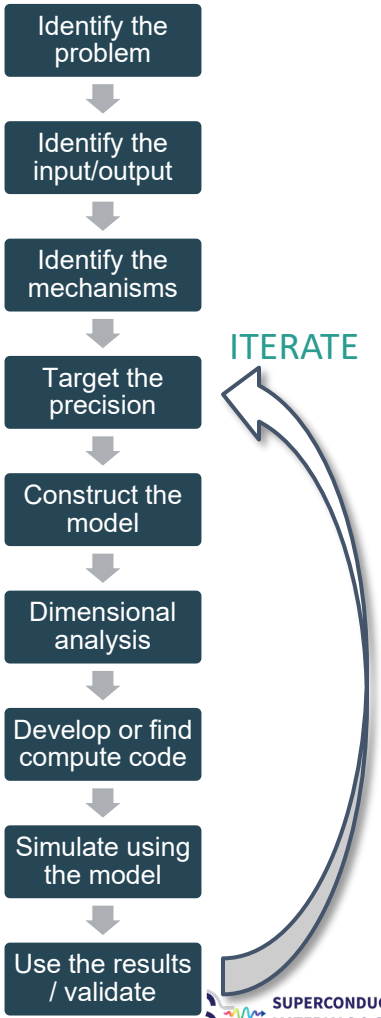
- Standard steps which are often not explicitly recognized
- Approach is often used even implicitly

DISCLAIMER:
Inaccurate answers from numerical methods do not necessarily imply errors in the model

and

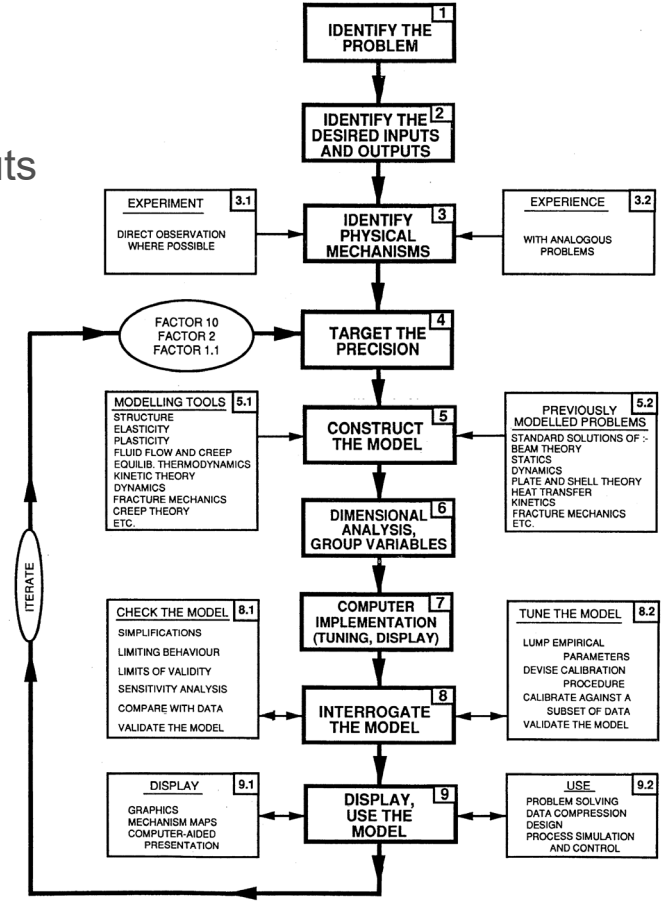
Accurate numerical solutions do not imply a correct model

- Models should be no more complicated than necessary
- "Everything should be made as **simple** as possible, **but no simpler**."



Steps in physical model formulation

- Step 1 : Identifying the problem
- Step 2 : Identifying the desired inputs and outputs
- Step 3 : Identifying the physical mechanisms
- Step 4 : Targeting the precision
- Step 5 : Constructing the model
- Step 6 : Dimensional analysis
- Step 7 : Computer implementation
- Step 8 : Interrogating the model
- Step 9 : Displaying the results
- Step 10: Validate



M.F. Ashby Mat Sci Tech **8**, 102 (1992)

Step 1: Identifying the problem

- Pertinent length scales and materials structure
- E-M Fields

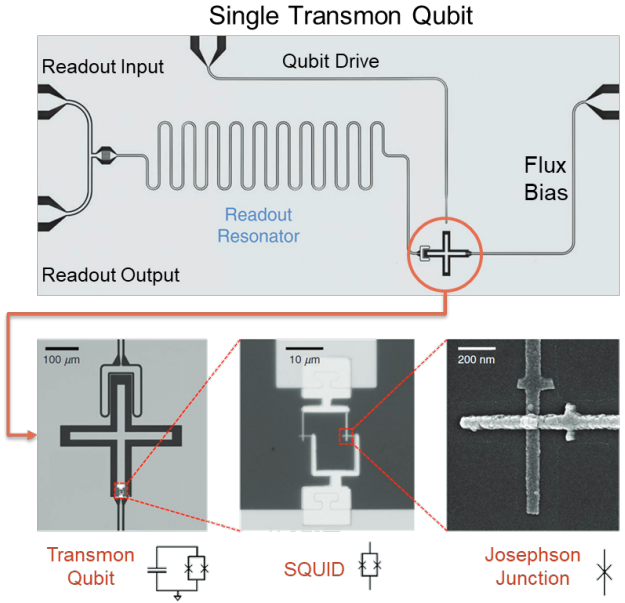
10^{-2} m

- Localized materials defects

10^{-10} m → 10^{-8} m

- Extend materials defects

10^{-6} m



- Hydrogen interstitials
- Role of oxygen vacancies
- Processing RRR
- Quasiparticles
- …

Step 2: Identifying desired inputs and outputs

- What are the essential ingredients of the model?
  - Composition, structure, boundary conditions, temperature, time, etc.
- What are the less important quantities that could be added later?
  - Start simple and then add complexity
- Remember that the output…
  - Is only as good as the input
  - Could be used as input for a higher-level model

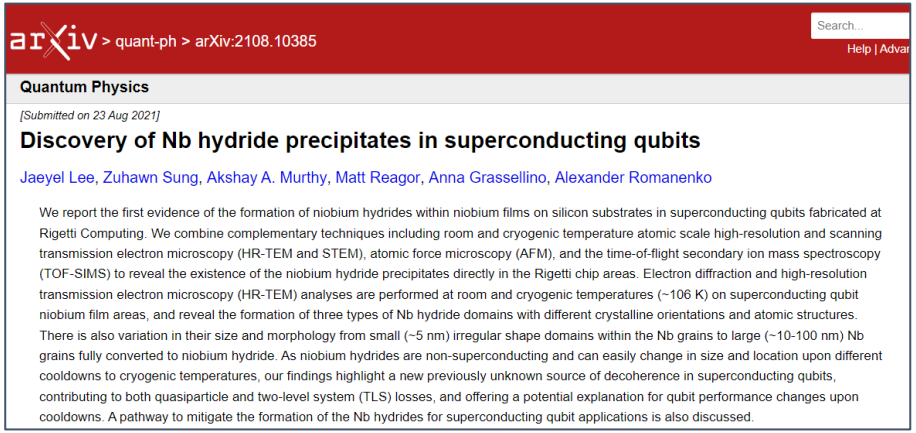
Agenda

Analyze and interpret modeling results from electronic and atomistic calculations

- SC Qubit Materials and Systems Charts – Introduction
- Modeling Materials
  - Model Formulation
  - Electronic Structure Models
  - Atomistic Models
  - From Phenomenological to Microscopic
- Use Cases
  - Nb and its hydrides
  - Nb and its oxides
- Co-Design and Integration with Experimentation – Summary

Nb and its hydrides (NbH_x)

- Recent discovery – hydrides in Nb films on Silicon processed by Rigetti
  - 3 types of Nb hydrides with varying atomic structures, crystalline orientation, and morphology
  - Small irregularly shaped (~5 nm) to large distinctly shaped (~100 nm)



arXiv > quant-ph > arXiv:2108.10385

Search...

Help | Advar

Quantum Physics

[Submitted on 23 Aug 2021]

Discovery of Nb hydride precipitates in superconducting qubits

Jaeyel Lee, Zuhawn Sung, Akshay A. Murthy, Matt Reagor, Anna Grassellino, Alexander Romanenko

We report the first evidence of the formation of niobium hydrides within niobium films on silicon substrates in superconducting qubits fabricated at Rigetti Computing. We combine complementary techniques including room and cryogenic temperature atomic scale high-resolution and scanning transmission electron microscopy (HR-TEM and STEM), atomic force microscopy (AFM), and the time-of-flight secondary ion mass spectroscopy (TOF-SIMS) to reveal the existence of the niobium hydride precipitates directly in the Rigetti chip areas. Electron diffraction and high-resolution transmission electron microscopy (HR-TEM) analyses are performed at room and cryogenic temperatures (~106 K) on superconducting qubit niobium film areas, and reveal the formation of three types of Nb hydride domains with different crystalline orientations and atomic structures. There is also variation in their size and morphology from small (~5 nm) irregular shape domains within the Nb grains to large (~10-100 nm) Nb grains fully converted to niobium hydride. As niobium hydrides are non-superconducting and can easily change in size and location upon different cooldowns to cryogenic temperatures, our findings highlight a new previously unknown source of decoherence in superconducting qubits, contributing to both quasiparticle and two-level system (TLS) losses, and offering a potential explanation for qubit performance changes upon cooldowns. A pathway to mitigate the formation of the Nb hydrides for superconducting qubit applications is also discussed.

https://arxiv.org/abs/2108.10385

- Hydrides lead to loss of performance in SRF Cavities (Alex's lecture): Q disease [Supercond. Sci. Technol. 26 035003 (2013)]
- Hydrides are metallic and non-superconducting
  - Small hydrides, proximity-induced superconductivity
  - Large hydrides, regular metal conductivity
- Additional QPs due to proximity breakdown under high fields (H>Hb)

Steps in physical model formulation

- Step 1 : Identifying the problem
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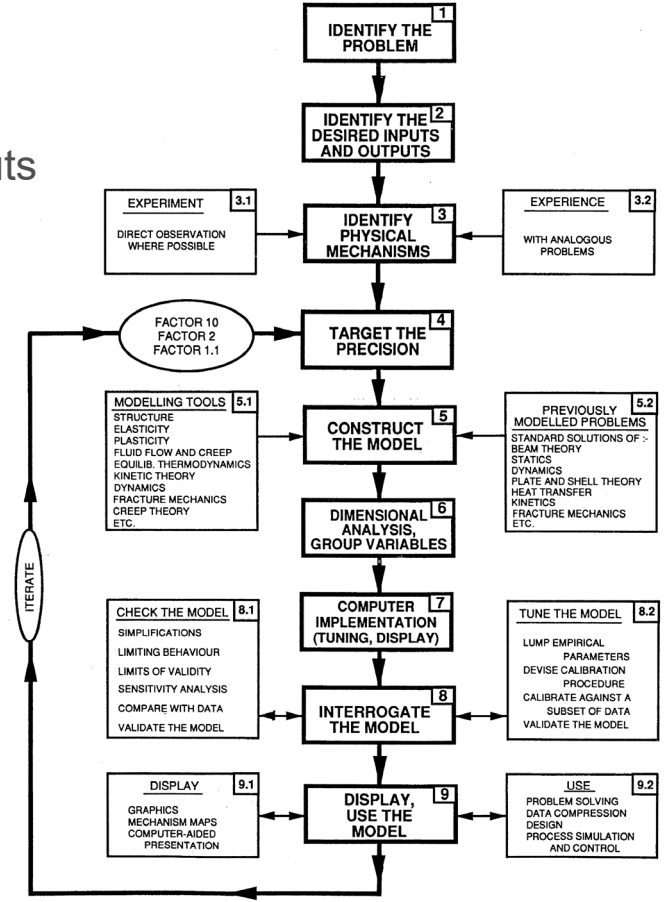

M.F. Ashby Mat Sci Tech **8**, 102 (1992)

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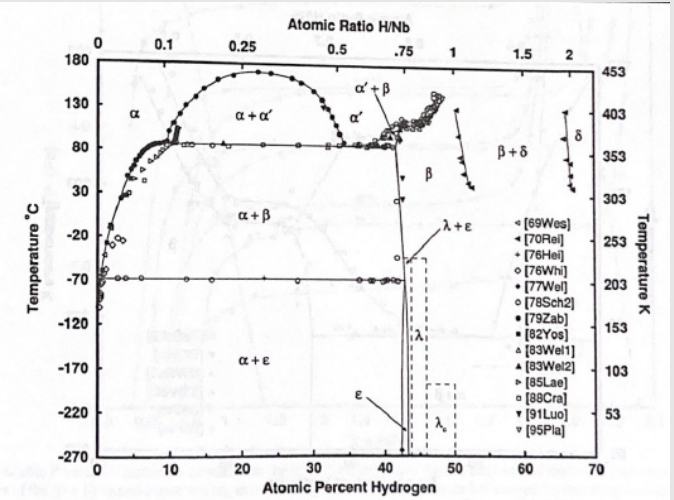


F. D. Manchester and J. M. Pitre, in *Phase Diagrams of Binary Hydrogen Alloys*, edited by F. D. Manchester (ASM International, 2000), pp. 115-137

1. Which are the relevant hydride phases?
2. Are bulk or interface structure/properties important?
3. What are the electronic/magnetic properties of the Nb/NbH grain boundaries?
   - Input – structure
   - Output – electronic properties
4. Can we understand and predict hydride nucleation and growth?
   - Input – structure
   - Output – elastic stiffness tensors

Building atomistic model – a short diversion

- BCC crystal has 12 tetrahedral sites and 6 octahedral sites

Structures and densities can be visualized in VESTA

- Structure can be rendered in 3D using minimal information (atomic species and their occupied Wyckoff sites) and a structure visualization program like VESTA

Windows

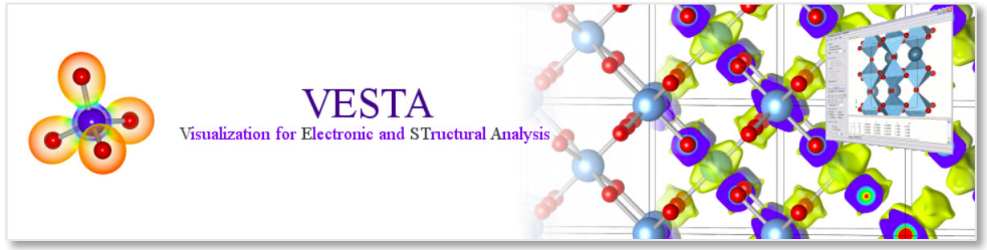
- VESTA.zip (ver. 3.5.8, built on Aug 11 2022, 14.3MB)
  For 32-bit version of Windows.
- VESTA-win64.zip (ver. 3.5.8, built on Aug 11 2022, 17.2MB)
  For 64-bit version of Windows.

macOS

- VESTA.dmg (ver. 3.5.8, built on Aug 11 2022, 25.3MB)
  Requires OS X 10.9 or newer, Intel CPUs that are capable of 64 bit instruction sets.

Linux x86_64

- VESTA-gtk3.tar.bz2 (ver. 3.5.8, built on Aug 11 2022, 23.8MB)
- vesta-3.5.8-1.x86_64.rpm (built on Aug 11 2022, 40.9MB)
  Requires GTK 3.22 or newer.
  Distributions where VESTA is known to work:
  - Redhat Enterprise Linux 7 or later
  - Ubuntu 18.04 or later



Choose the VESTA version for your OS and follow the install directions or extract the files

You can use this (or equivalent software) for constructing input structures and analyzing crystal structures

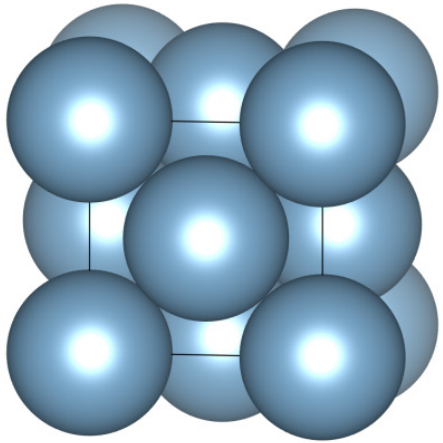
http://jp-minerals.org/vesta/en

VESTA demo (later for homework)

- Opening files
- Drawing bonds
- Measuring angles and distances
- Applying periodic boundary conditions
- Creating supercells

Face Centered Cubic (FCC) structure

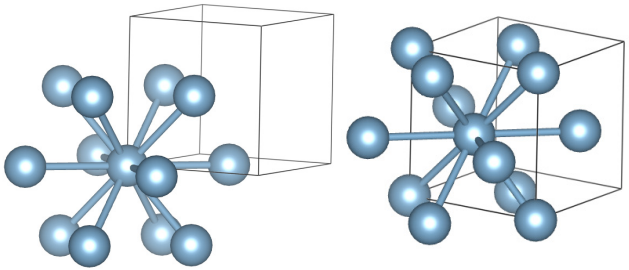
- Atoms touch each other along the face diagonals



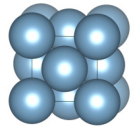
Example: Al, Cu, Au, Pb, Ni, Pt, Ag

Coordination # = 12

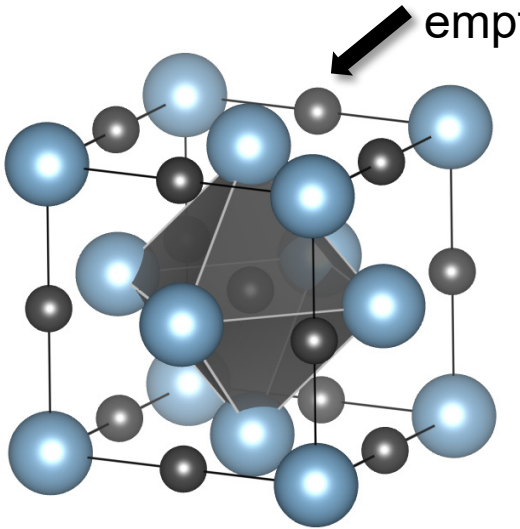
Cubic-close packing forms an **antiprism**



Octahedral and tetrahedral voids in cubic close-packed structures



- Full list of site positions



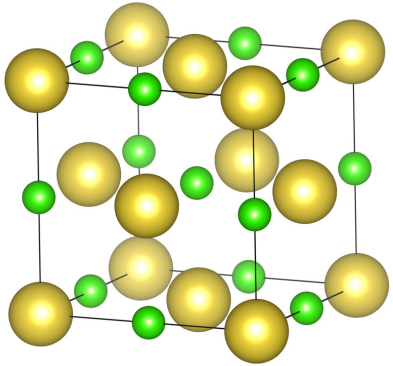
octahedral voids
SG=$Fm\bar{3}m$ (No. 225)

Atom	x	y	z
Anion	0	0	0
hole	1/2	1/2	1/2

Atom	x	y	z
Anion	0	0	0
	1/2	1/2	0
	1/2	0	1/2
	0	1/2	1/2
hole	1/2	1/2	1/2
	1/2	0	0
	0	1/2	0
	0	0	1/2

AB crystal structures

- NaCl structure
  - Equal number of cations and anions
  - CCP array of Cl^- anions
  - Na^+ cations fill 100% of octahedral voids filled
  - Tetrahedral interstices remain empty

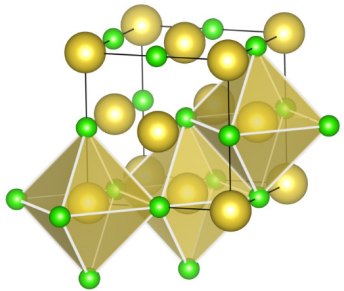


- Alternative description
  - Can be considered as two interpenetrating FCC lattices (one cation FCC lattice and one anion FCC lattice)

NaCl
SG=$Fm\bar{3}m$ (No. 225), $a = 5.63$ Å

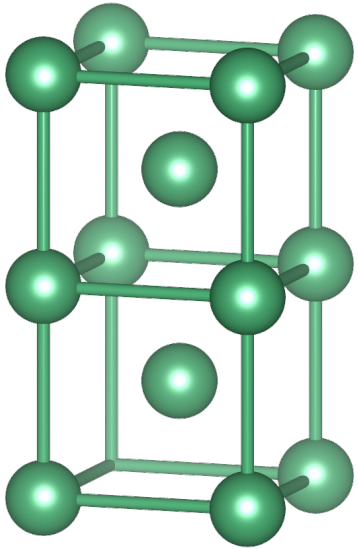
Atom	x	y	z
Na	0	0	0
Cl	1/2	1/2	1/2

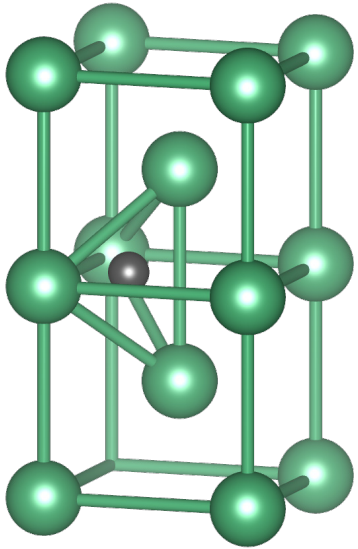
- Examples
  - Alkali metal hydrides
  - Alkali halides except for CsX (X=Cl, Br, I)
  - Alkaline earth oxides, sulfides, selenides, and tellurides Mg-Ba except MgTe
  - Carbides and nitrides MC and MN and some phosphides
  - Many alloy phases

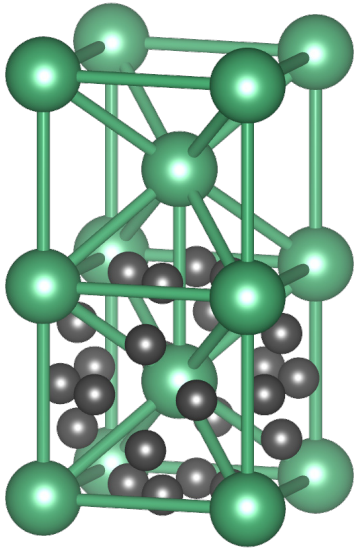


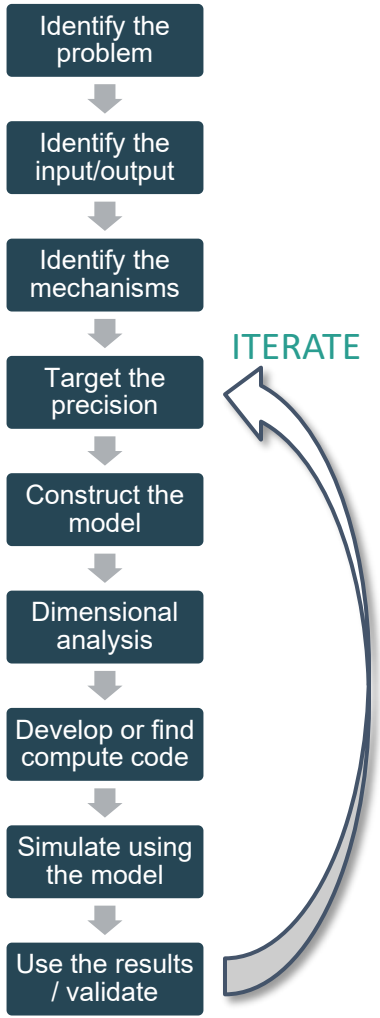
Build atomistic model

- BCC crystal has 12 tetrahedral sites and 6 octahedral sites
- Hydrogen can occupy any of the 12 tetrahedral sites, and its concentration governs which Nb hydrides can form in the Nb matrix



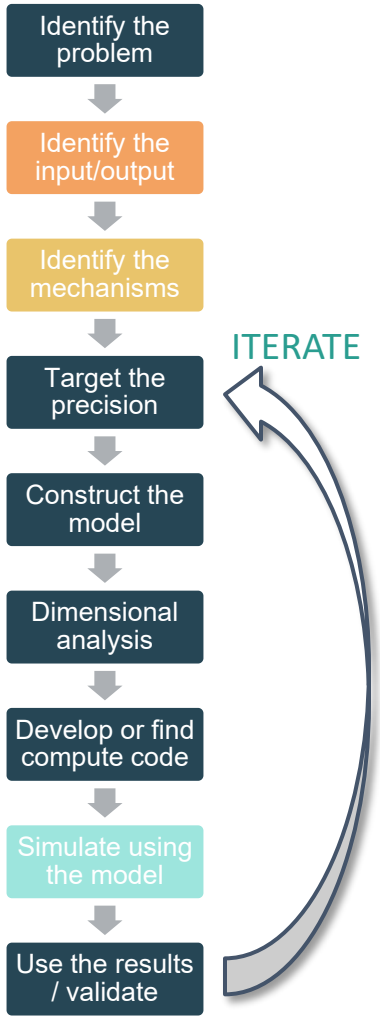





Identify the problem
Identify the input/output
Identify the mechanisms
Target the precision
Construct the model
Dimensional analysis
Develop or find compute code
Simulate using the model
Use the results / validate
ITERATE

- Hydride-induced decoherence in Nb superconducting planar resonators and superconducting qubits
- Various hydride structures
  - Bulk (single phase)
  - Interfaces (two-phase)

- Electronic structure



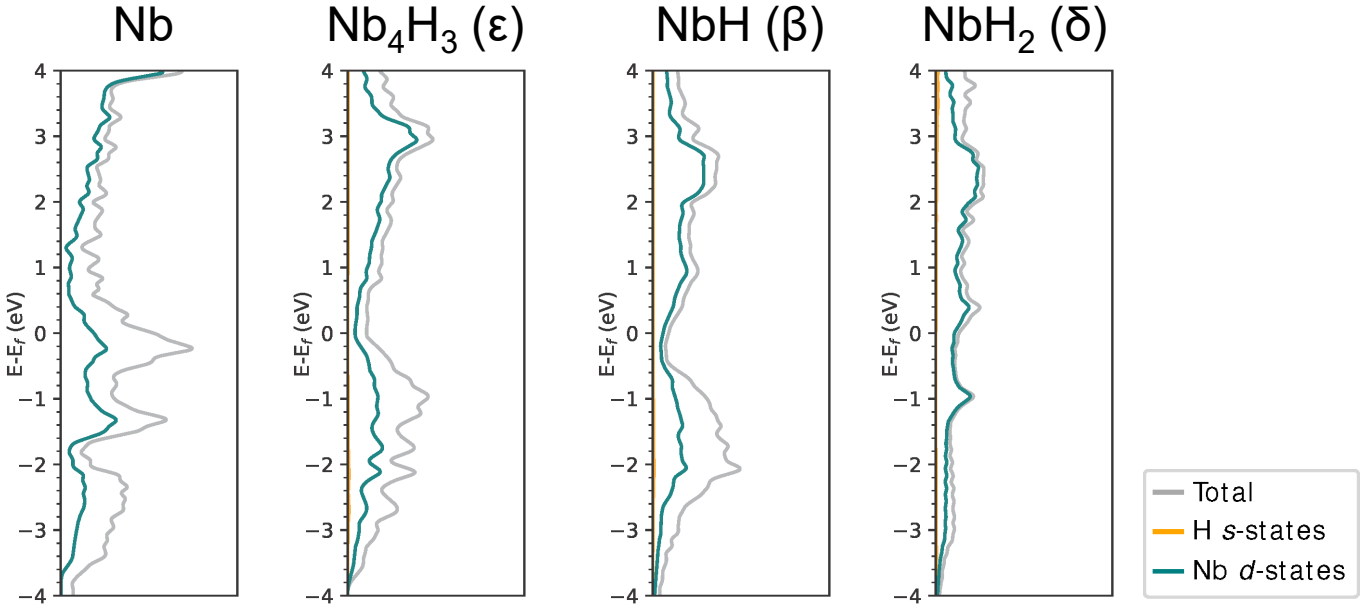
- Microwave dissipation emerges due to Nb hydrides being poor or non-superconductors

Quality factor Q_0 of SRF cavities is determined by the surface resistance via the formula:

$$Q_0 = \frac{\omega U}{P_{\text{diss}}} = \frac{\omega \mu_0 \int_V H^2 \mathrm{d}V}{\int_A R_s(H) H^2 \mathrm{d}A} \qquad (1)$$

where ω is the angular frequency, U is stored energy calculated from the integral of the field over cavity volume, and P_{diss} is the power dissipated in cavity walls calculated as an integral of surface resistance over cavity walls. Extremely low surface resistance in superconducting state and hence very high quality factors $Q_0 > 10^{11}$ are achievable in such structures.

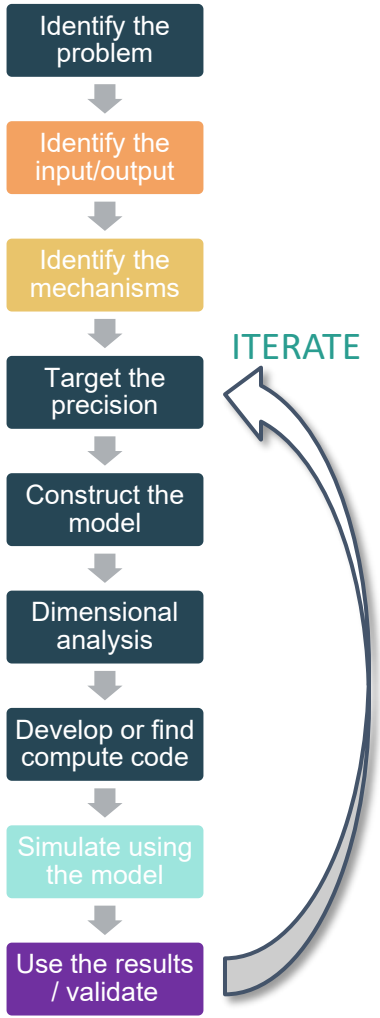
Electronic density of states of bulk NbH_x



- Nb_4H_3 (ε) is the low temperature stable hydride phase
- Metallic character persists with increasing hydrogen content but poor SCs
- Superconducting character lost with increasing content
- Hydrides are nonmagnetic

- Hydride-induced decoherence in Nb superconducting planar resonators and superconducting qubits
- Various hydride structures
  - Bulk (single phase)
  - Interfaces (two-phase)

- Electronic structure



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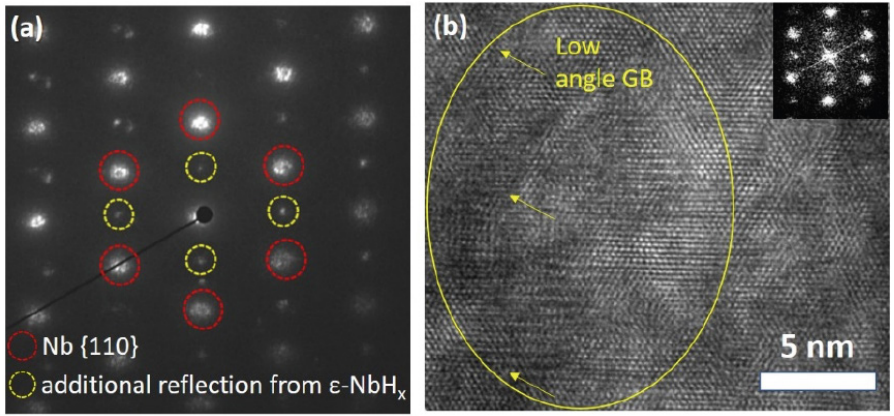
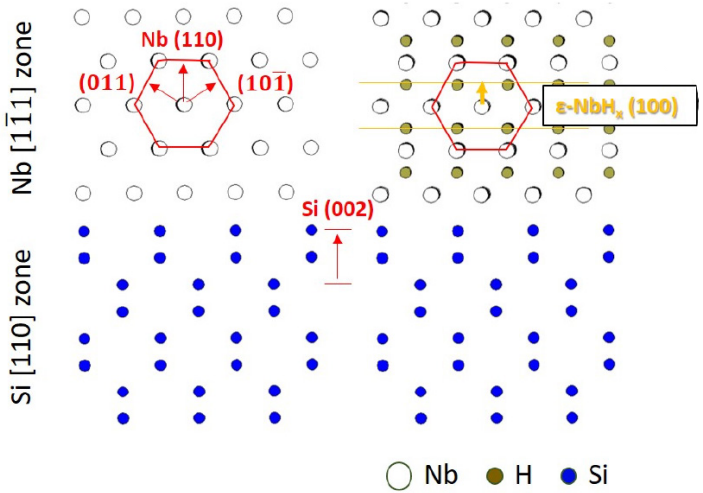
Nb hydride precipitates in superconducting qubits

- Nb hydrides analyzed in detail using HR-TEM
- Nb hydrides in Nb grains within the superconducting coplanar resonators
- Hydride volume fraction is estimated to be 0.1~1%



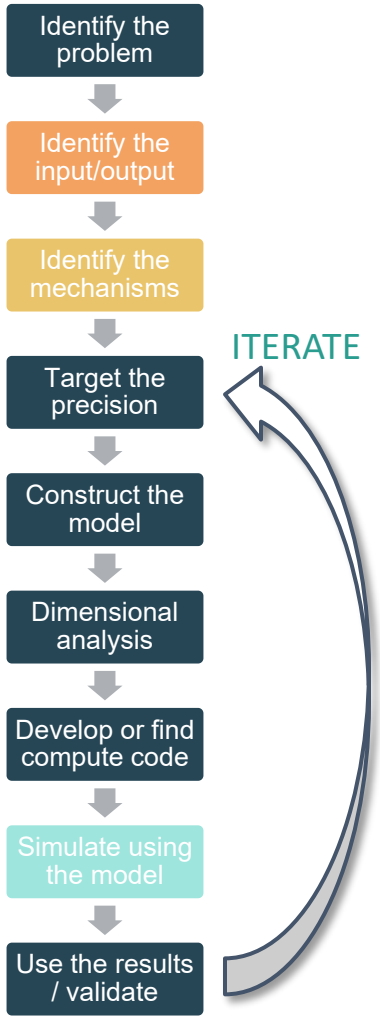
https://arxiv.org/abs/2108.10385



(100) plane of ε-NbH_x is parallel to the (110) Nb in the film

- Hydride-induced decoherence in Nb superconducting planar resonators and superconducting qubits
- Various hydride structures
  - Bulk (single phase)
  - Interfaces (two-phase)

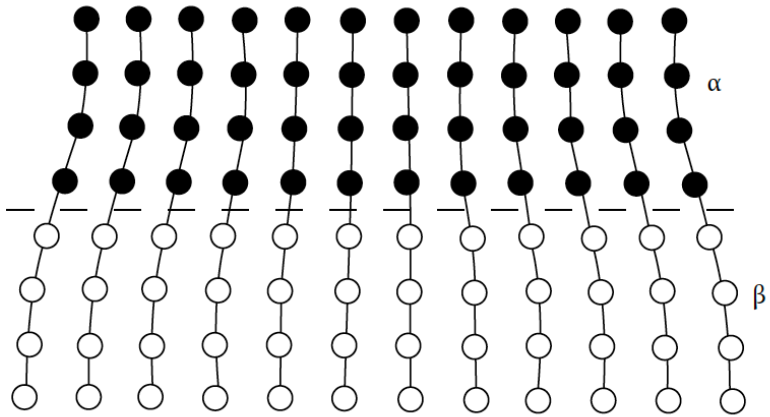
- Elastic moduli



- Nucleation and growth
- Balancing interfacial energies

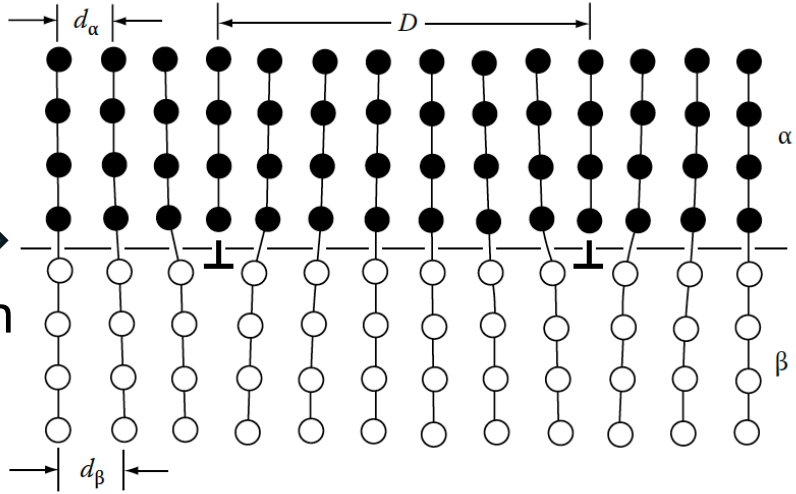
Are the interfaces coherent?

Coherent



Growth

Semicoherent or incoherent

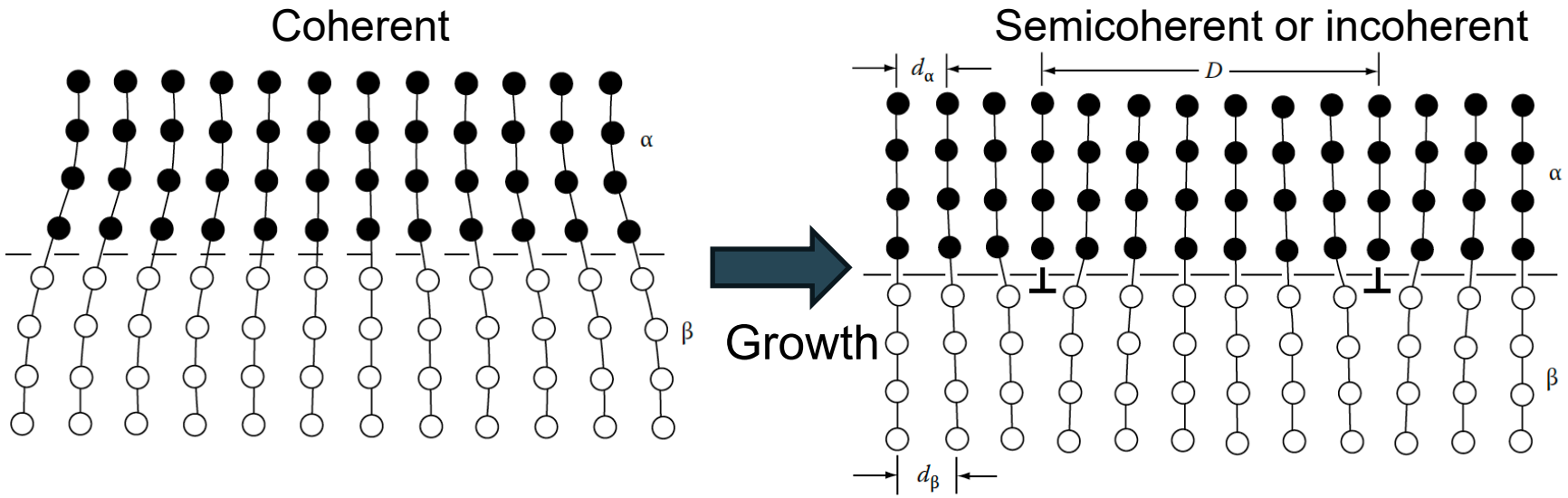


A coherent interface with slight mismatch leads to coherency strains (or lattice distortions) in the adjoining lattices.

A semicoherent interface. The misfit parallel to the interface is accommodated by a series of edge dislocations.

Porter and Easterling and Courtesy Peter Voorhees

Are the interfaces coherent?

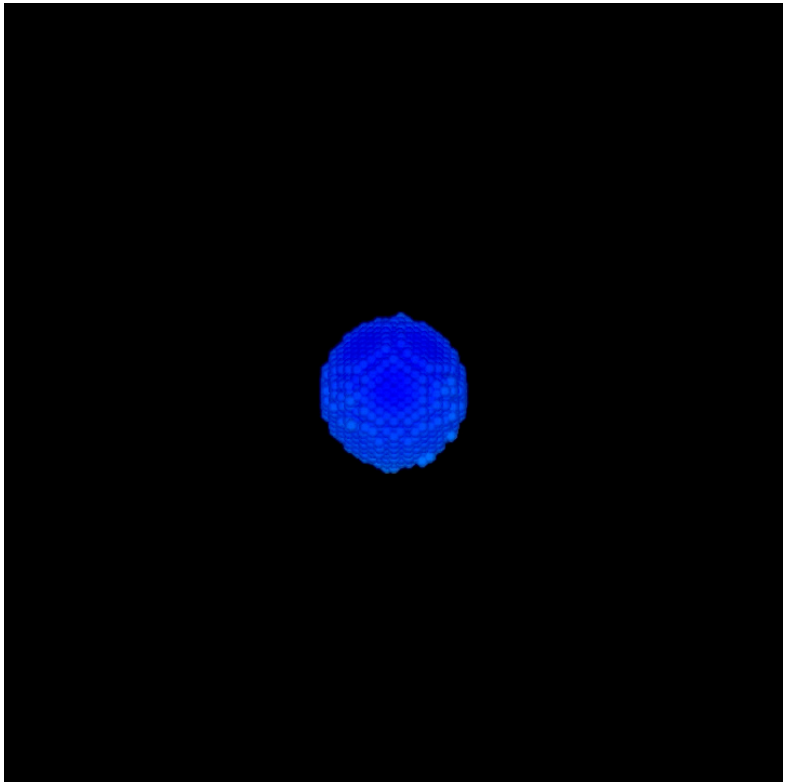


The transition occurs at critical a particle size $R_c \sim \frac{3\Delta\sigma}{4\mu\epsilon^2}$

For Nb hydrides $R_c \sim 2$ nm

Porter and Easterling and Courtesy Peter Voorhees

How a coherent precipitate becomes incoherent?



- MD simulation shows a TiC precipitate (20% lattice misfit)
- The precipitate is completely encased in dislocations

Hydride Mitigation Strategies

- Post-annealing of Nb films above 600 °C to degas H
  - Supercond. Sci. Technol. 30(9) 094004 (2017)

- Challenge – Nb silicides can form at Nb/Si interfaces

PHYSICAL REVIEW MATERIALS **6**, 064402 (2022)

Stability, metallicity, and magnetism in niobium silicide nanofilms

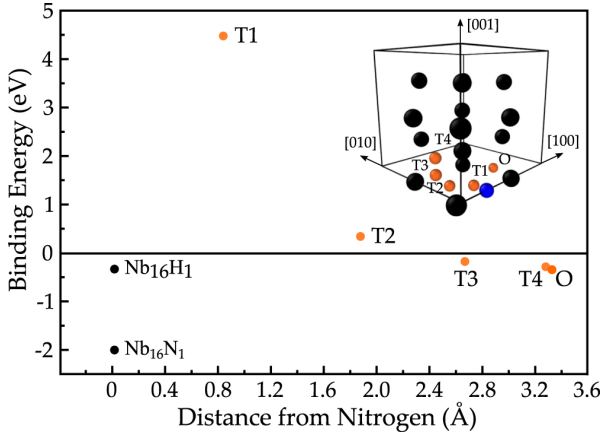
Xuezeng Lu,[1] Dominic P. Goronzy,[1,2] Carlos G. Torres-Castanedo,[1] Paul Masih Das,[1] Maryam Kazemzadeh-Atoufi,[1] Anthony McFadden,[3] Corey Rae H. McRae,[4,5] Peter W. Voorhees,[1] Vinayak P. Dravid,[1,6] Michael J. Bedzyk,[1,7,8] Mark C. Hersam,[1,9,10] and James M. Rondinelli[1,*]

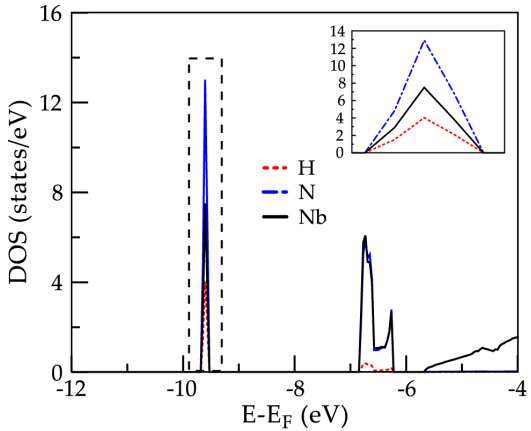
- Use nitrogen during processing to control nucleation
  - Supercond. Sci. Technol. 31(11) 115007 (2018)

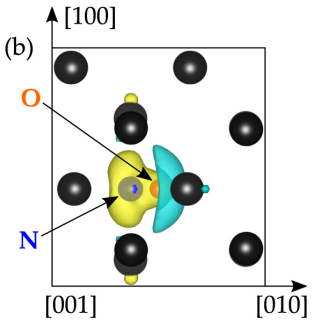
- Modify grain boundary structure (size, texture, etc.) to nucleation
  - J. Appl. Phys. 121(19) 193903 (2017)

Suppression of Hydrides with Nitrogen

- DFT calculations identify why there are low hydride concentrations observed near nitrogen treated niobium surfaces
  - Hydrogen binding is suppressed (short-range effect limited ~2.5 Å away)
  - Hydrogen disrupts covalent bonding between Nb-H
  - Nitrogen increases the energy barrier for hydrogen diffusion







Supercond. Sci. Technol. 31 115007 (2018)

Papers for More Information

- *Suppression of hydride precipitates in niobium superconducting radio-frequency cavities*
  - Supercond. Sci. Technol. 26 105003 (2013)
  - https://doi.org/10.1088/0953-2048/26/10/105003

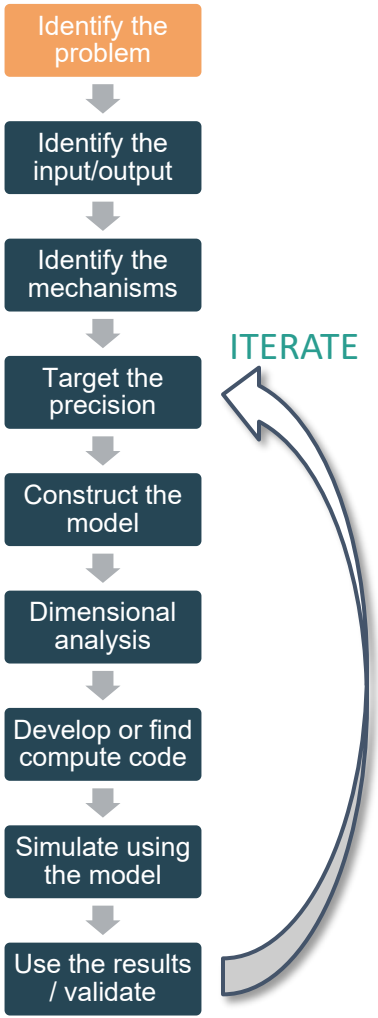
- *Revealing the role of nitrogen on hydride nucleation and stability in pure niobium using first-principles calculations*
  - Supercond. Sci. Technol. 31 115007 (2018)
  - https://doi.org/10.1088/1361-6668/aae147

- *Suppression of nano-hydride growth on Nb(100) due to nitrogen doping*
  - J. Chem. Phys. **152**, 214703 (2020)
  - https://doi.org/10.1063/5.0007042

Agenda

Analyze and interpret modeling results from electronic and atomistic calculations

- SC Qubit Materials and Systems Charts – Introduction
- Modeling Materials
  - Model Formulation
  - Electronic Structure Models
  - Atomistic Models
  - From Phenomenological to Microscopic
- Use Cases
  - Nb and its hydrides
  - Nb and its oxides
- Co-Design and Integration with Experimentation – Summary


Identify the problem
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Identify the mechanisms
Target the precision
Construct the model
Dimensional analysis
Develop or find compute code
Simulate using the model
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ITERATE

Magnetic Impurities as Loss Source in amorphous Nb_2O_{5-x}

- Reduced Nb pentoxides exhibit temperature dependent paramagnetism
  - Magnetic susceptibility increases with decreasing oxygen content
- Magnetic moments provide several channels for qubit decoherence:
  - Increased quasiparticle losses through Shiba mechanism*
  - Bloch relaxation of moments
  - Magnetic flux noise

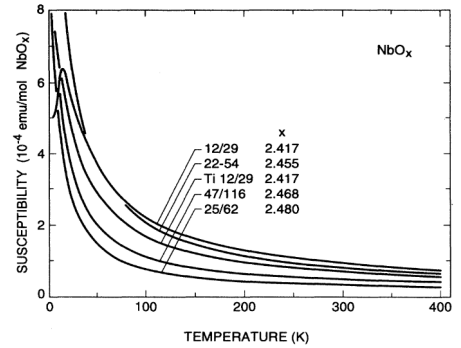
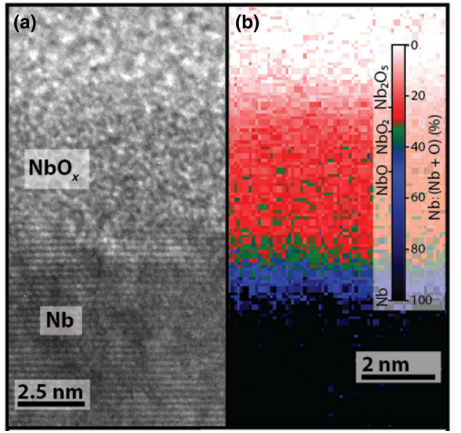


FIG. 13. Magnetic susceptibilities of $Nb_{25}O_{62}$, $Nb_{47}O_{116}$, $Nb_{22}O_{54}$, $Nb_{12}O_{29}$, and $Ti_{0.5}Nb_{11.5}O_{29}$ plotted per mole $(Nb,Ti)O_x$.

DOI: 10.1103/PhysRevB.44.6973

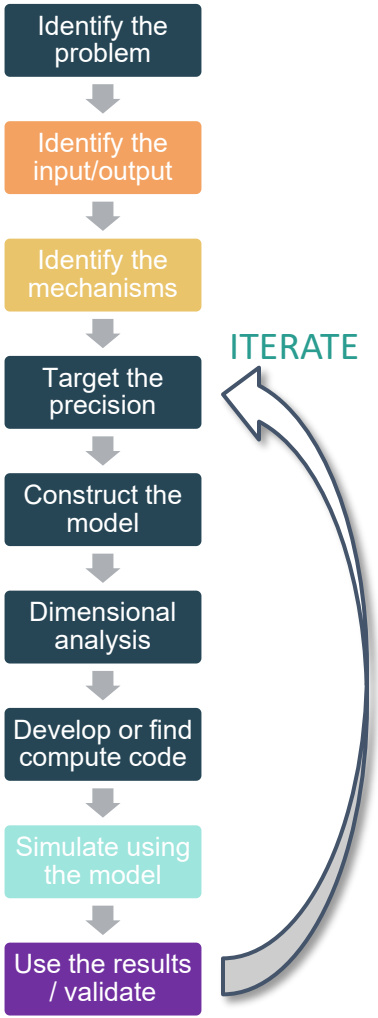


DOI: 10.1103/PRXQuantum.3.020312

Shiba theory applied to SRF cavities to model surface resistance impedance of s-wave superconductors with magnetic impurities [Phys. Rev. B 86, 024514 (2012)]

- Various NbO_x structures
  - Bulk Crystalline
  - Bulk Amorphous

- Electronic structure



The Shiba Theory for magnetic impurities in a superconducting host

$$\phi(v) = \frac{\varepsilon}{|\Delta|} = v\left(1 - \frac{1}{\tau_s|\Delta|}\frac{\sqrt{1-v^2}}{((1-\gamma)^2 - v)}\right)$$

Surface impedance in the Superconductor Resonator Frequency Limit

$$Z(\omega) = \frac{32\pi\omega}{c^4}\int_0^\infty dk \frac{Q_2(\omega,k)}{[k^2 + 4\pi Q_1(k)/c^2]^2}.$$

Parameters

Magnetic impurity density: τ_s^{-1}

Dissipation: $Q_2(\omega, k)$

Superconducting gap: $|\Delta|$

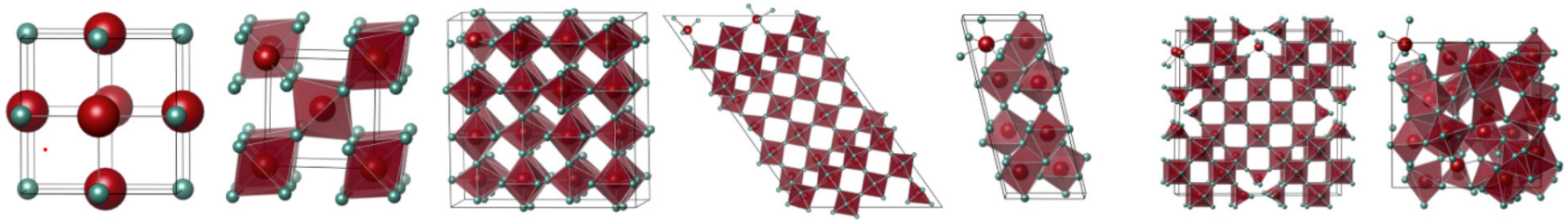
Energy scale

$\gamma \approx 0$ Weak exchange

$\gamma \approx 1$ Strong exchange

Courtesy S. Griffin (Molecular Foundry)

Nb Oxide Crystal Structures



NbO Pm3m	NbO_2 Rutile, $P4_2/mnm$	NbO_2 $I4_1/a$	N-Nb_2O_5 C2/m	B-Nb_2O_5 C2/c	M-Nb_2O_5 I4/mmm	Nb_2O_5 Amorphous
$4d^3$	$4d^1$	$4d^1$	$4d^0$	$4d^0$	$4d^0$	$4d^0$
Planar	Octahedral	Octahedral	Octahedral+ Tetrahedral	Octahedral	Octahedral+ Tetrahedral	4-, 5- and 6- coordinated
Paramagnetic	Paramagnetic	Paramagnetic	Diamagnetic	Diamagnetic	Diamagnetic	Diamagnetic

FIG. 1. Crystal structures of the Nb oxides considered in this work with their nominal valence configuration on the Nb atoms, the Nb coordination environment(s) and the resulting magnetic order in the stoichiometric case.

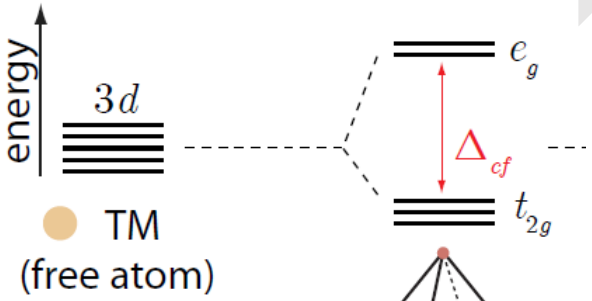
Sheridan, E., Harrelson, T. F., Sivonxay, E., Persson, K. A., Altoé, M. V. P., Siddiqi, I., Ogletree, D. F., Santiago, D. I., & Griffin, S. M. (2021). *Microscopic Theory of Magnetic Disorder-Induced Decoherence in Superconducting Nb Films*. https://arxiv.org/abs/2111.11684

Electronic structure of NbO_2

Niobium

Charge	Ionic Radius (Å)
3+	0.72
4+	0.68
5+	0.64

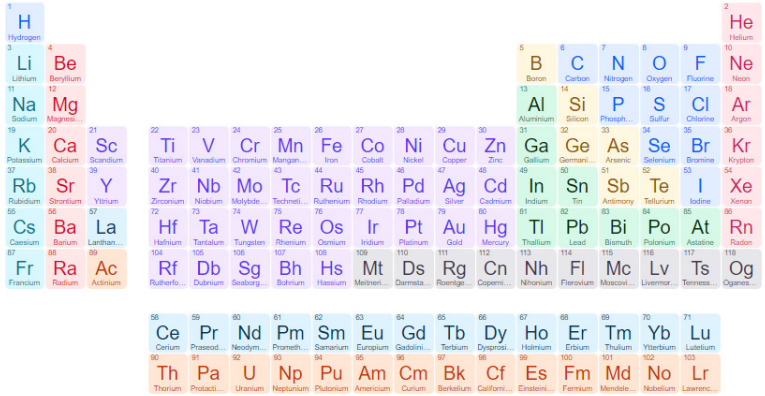
low-spin filling



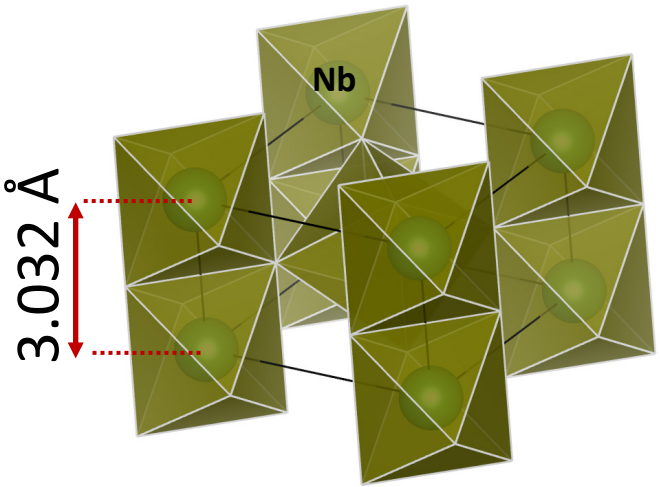
octahedral coordination

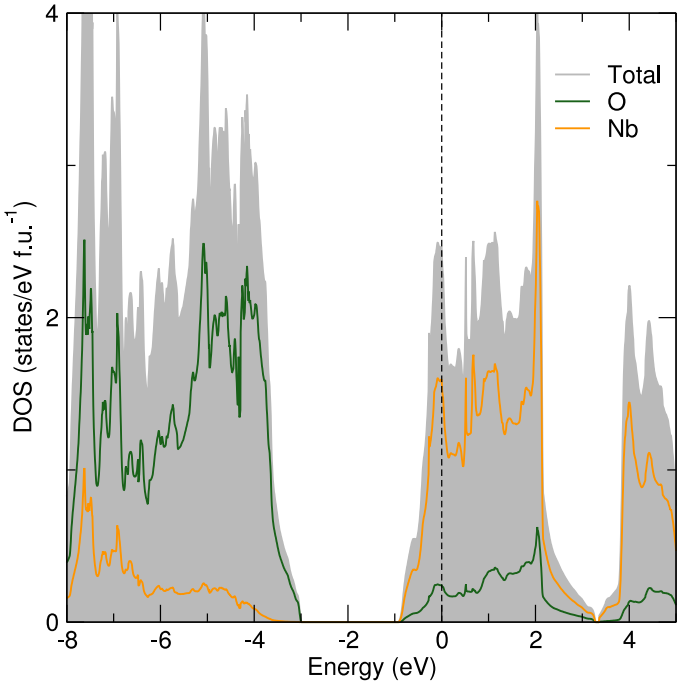
d^n	Class
2	Metal
1	Metal
0	Insulator

Periodic Table

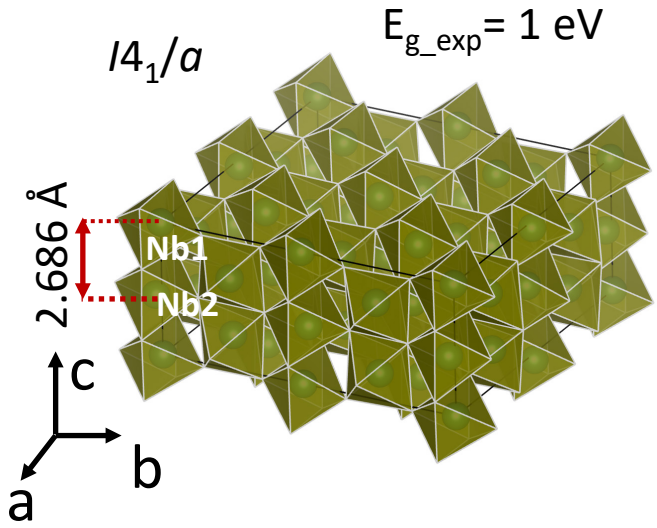


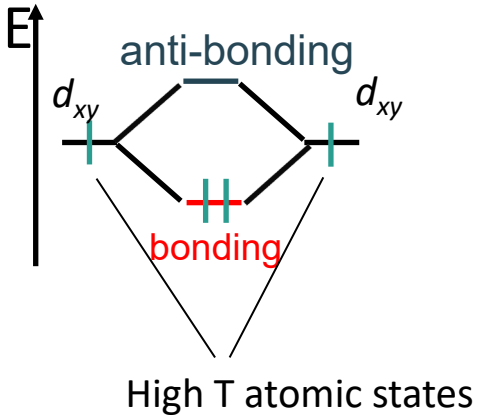
Electronic structure of NbO_2

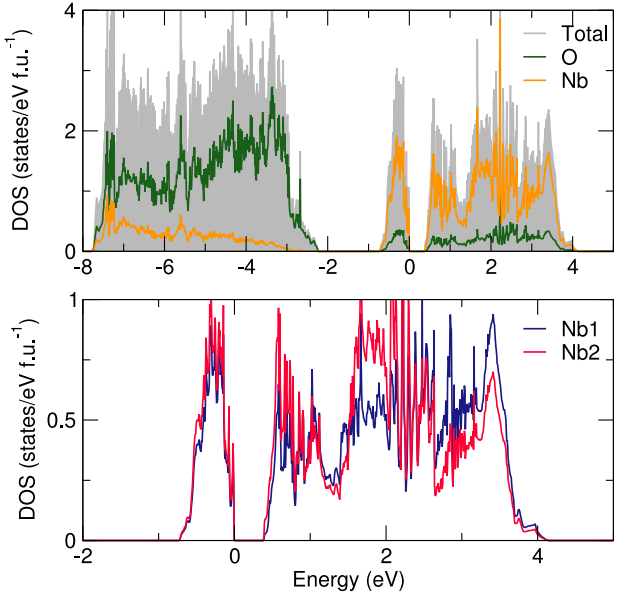




Electronic structure of NbO_2

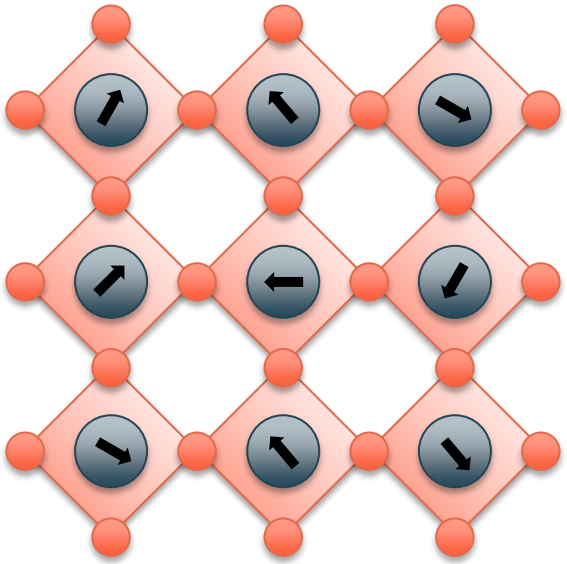




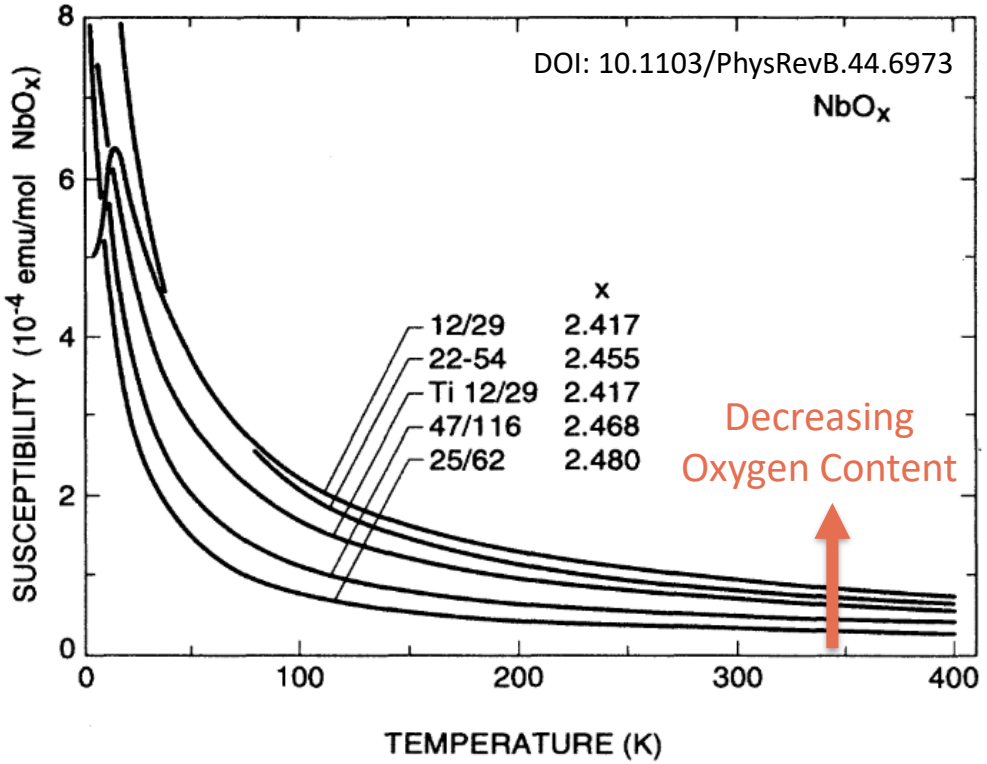


MIT = 1081 K

Paramagnetism in Reduced Nb Pentoxides (oxygen vacancies)

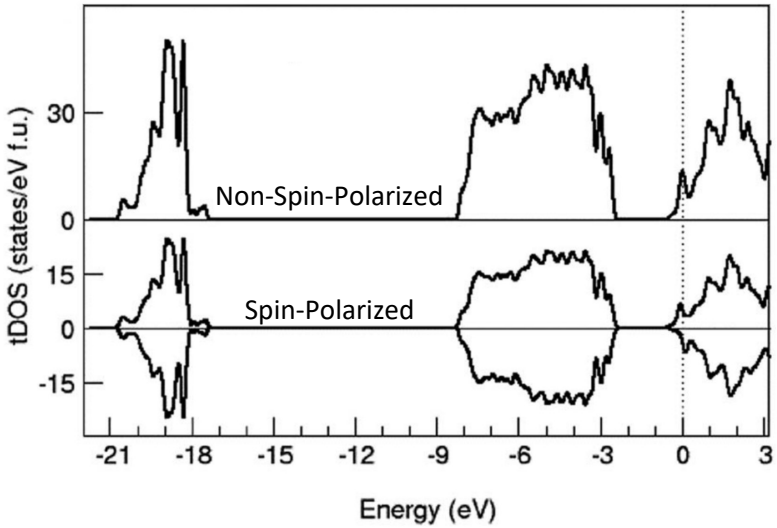


Paramagnetic moments
hosted on transition metal sites

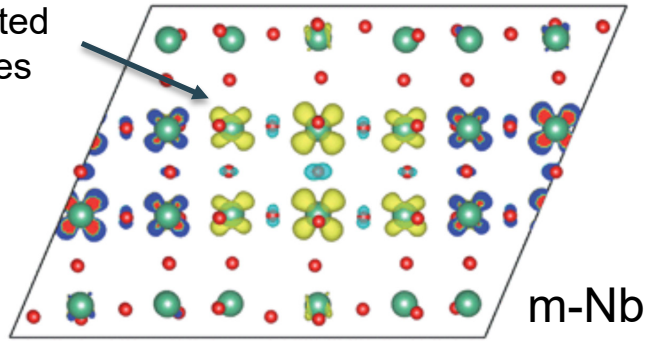


Electronic Structure Origin

- $Nb_{12}O_{29}$ exhibits two forms with different symmetries, monoclinic (m) and orthorhombic (o)
- M-$Nb_{12}O_{29}$ is an unusual metallic antiferromagnetic below 12 K
- Stoner-like instability but with delocalized moments across multiple Nb sites



Moments hosted on Nb t_{2g} states



m-$Nb_{12}O_{29}$

Fang, C. M., van Huis, M. A., Xu, Q., Cava, R. J., & Zandbergen, H. W. (2015). Unexpected origin of magnetism in monoclinic $Nb_{12}O_{29}$ from first-principles calculations. *Journal of Materials Chemistry C, 3*(3), 651–657 (2015)

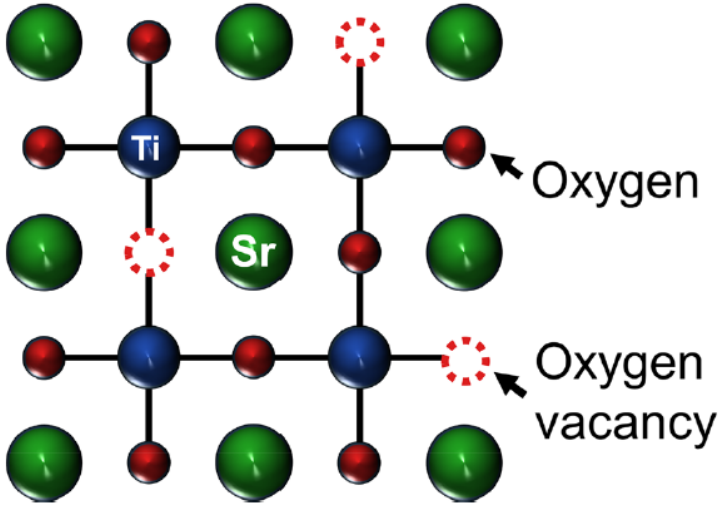
Modeling Nonstoichiometric Crystalline Nb_2O_{5-x} with Oxygen Defects

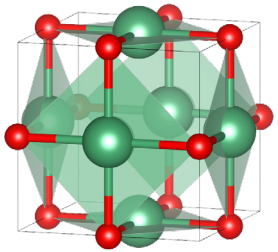
Oxygen vacancies

- Donates two electrons (n-type)
- Occupy conduction band (donor states)

Oxygen interstitials

- Donates two holes (p-type)
- Occupy valence band (acceptor states)





NbO ($Pm\bar{3}m$)
Stabilized by π-type interaction between Nb 4d and O 2p orbitals

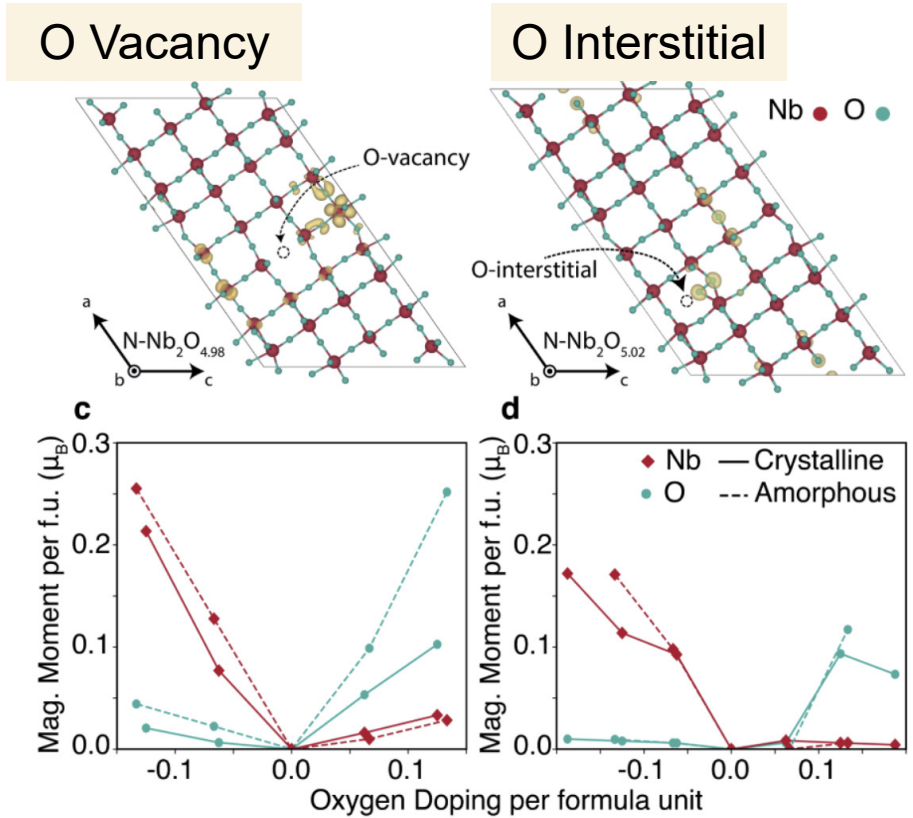
Modeling Nonstoichiometric Crystalline Nb_2O_{5-x} with Oxygen Defects

Rigid band model

- *Pros*: Simple, fast, and qualitatively correct
- *Cons*: Cannot account for localized defect states, structural rearrangements, polarons, etc.

Explicit oxygen vacancies

- Pros: Explicit representation of environment around defects
- Cons: Dilute defects require large simulation cells



Sheridan, E., Harrelson, T. F., Sivonxay, E., Persson, K. A., Altoé, M. V. P., Siddiqi, I., Ogletree, D. F., Santiago, D. I., & Griffin, S. M. (2021). *Microscopic Theory of Magnetic Disorder-Induced Decoherence in Superconducting Nb Films*. https://arxiv.org/abs/2111.11684

Proposed Link: Magnetic induced Losses

- Dilute magnetic moment in superconductors can lead to ‘impurity’ band development in SC density of states
  - SCs have gap at the Fermi level
    - Cooper pair states below fermi level
    - Broken cooper pairs (e-) above fermi level
    - Scattering of e- leads to resistive losses
  - For large gap, thermal occupation of states above fermi level is small
  - With impurity band, these states can be more easily thermally occupied

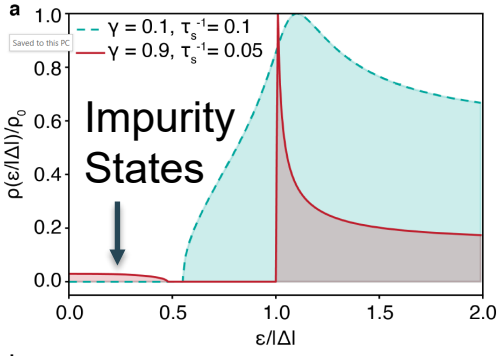


FIG. 4. (a) The normalised superconducting density of states for a Nb film with magnetic impurities in the strong (red) $[\gamma = 0.9, \tau_s^{-1} = 0.05]$ and weak (teal) $[\gamma = 0.1, \tau_s^{-1} = 0.1]$ coupling limits in the vicinity of the Fermi level. (b) The real part of the current dissipation function in the corresponding limits, where the inset shows the region near the Fermi level which participates in the dissipation. For strong coupling, the decoherence is associated to d-channel losses, while for weak coupling it is compatible with p-channel losses.

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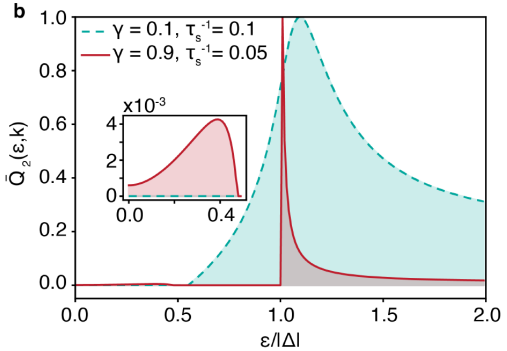
Proposed Link: Magnetic induced Losses

- Dilute magnetic moment in superconductors can lead to ‘impurity’ band development in SC density of states

- Add microscopics to phenomenological theory

Key parameters:
J: magnetic coupling strength (from DFT)
Ts: Scattering time (measured, approximated DFT)
Δ: Energy gap (measured, DFT)

Current Dissipation Function



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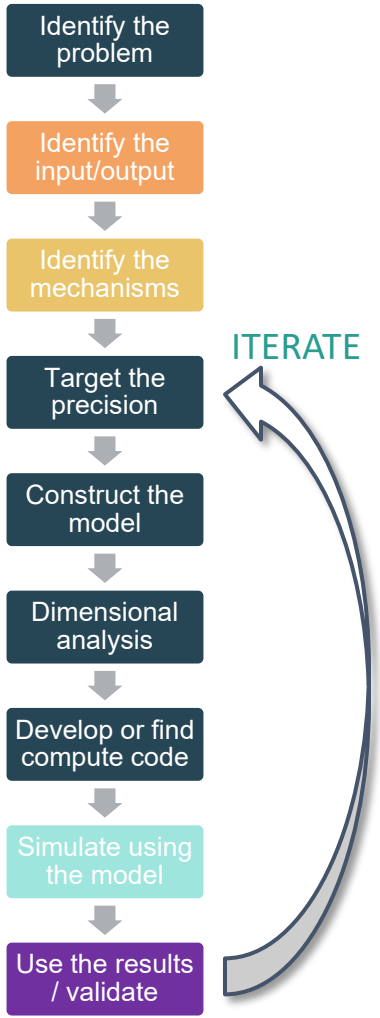
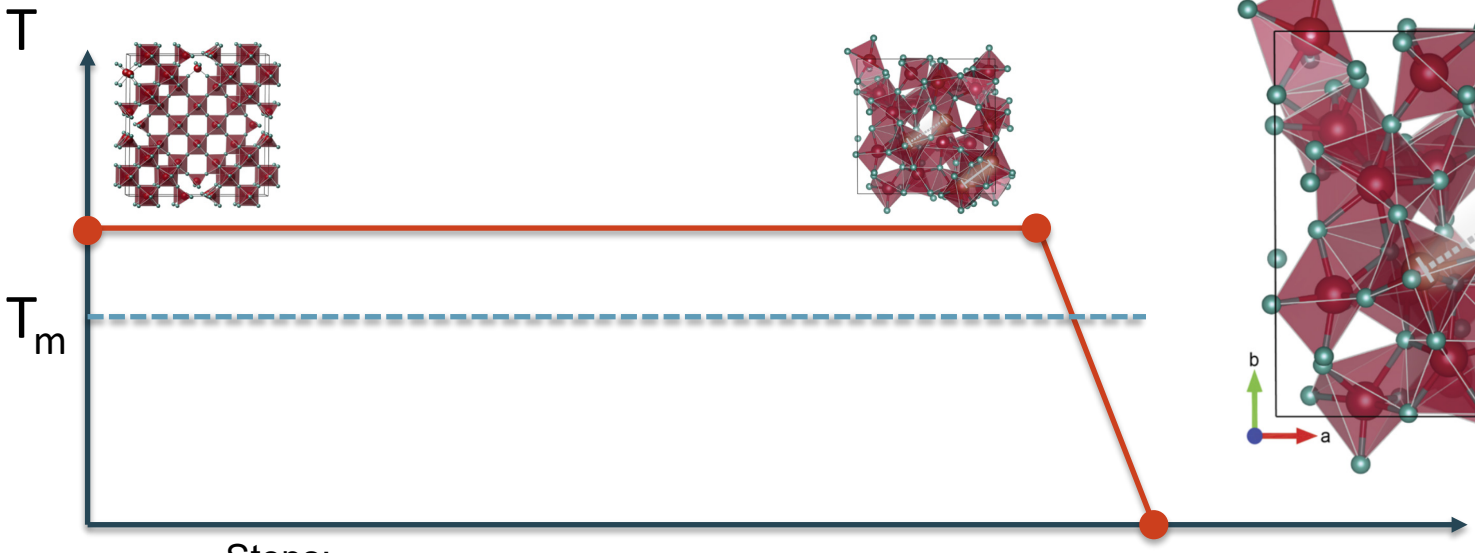
- Various NbO_x structures
  - Bulk Crystalline
  - Bulk Amorphous

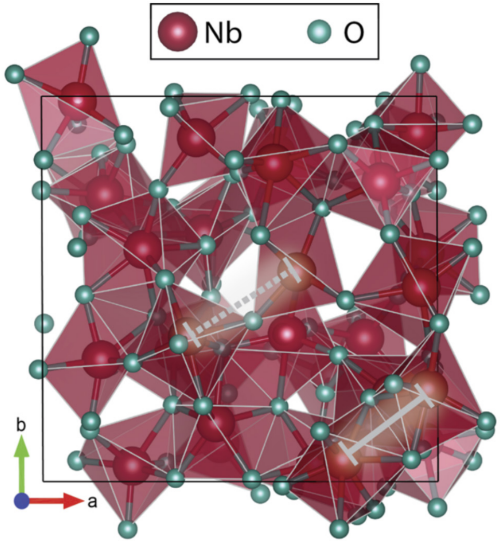
- Electronic structure



Simulating Amorphous Nb_2O_5 with DFT

- Combine simulated-annealing process with ab initio molecular dynamics (AIMD)





Steps:

1. Increase T to >3000K with expanded cell (15% expansion) (*NVE*)
2. Decrease temperature to 500 K (*NVE*)
3. AIMD at 500 K for 1-2ps (*NVT*)

Validation of Model

- Why should we trust simulations?
  - Elucidating the local atomic and electronic structure of amorphous oxidized superconducting niobium films. *Applied Physics Letters*, *119*(24), 244004 (2021)

- Good match between simulated and experimental amorphous XAS absorption spectra

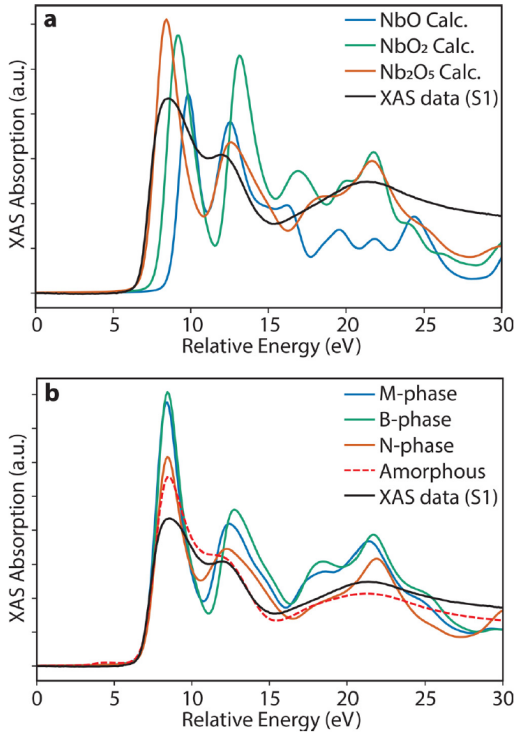


FIG. 3. (a) Calculated XAS spectra for crystalline NbO, NbO_2, and Nb_2O_5 (averaged over all three calculated phases) and XAS measurements of the O K edge of sample 1. (b) Calculated XAS spectra for crystalline Nb_2O_5 in the M-, B-, and B-phases, a representative *ab initio* generated amorphous structure, and XAS measurements of sample 1. Experimental data are normalized by rigidly shifting the spectrum to the relative scale, removing the background signal, and normalizing the heights to be comparable to our XAS calculations.

Implications of Magnetic-Induced Losses

- d-band moments (on Nb atoms from oxygen vacancies) lead to impurity band states in the SC DOS
  - There thermal occupation leads to additional dissipation channels (YSR dissipation)

- p-band moments (on O atoms from oxygen interstitials) do not lead to impurity band states

- Mitigation strategies
  - Need to fill oxygen vacancies (annealing, surface passivation, etc.)
  - Remove native oxides completely

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Papers for More Information

Sheridan Nb_2O_5 magnetism and structure

- Sheridan, E., Harrelson, T. F., Sivonxay, E., Persson, K. A., Altoé, M. V. P., Siddiqi, I., Ogletree, D. F., Santiago, D. I., & Griffin, S. M. (2021). *Microscopic Theory of Magnetic Disorder-Induced Decoherence in Superconducting Nb Films*. https://arxiv.org/abs/2111.11684
- Elucidating the local atomic and electronic structure of amorphous oxidized superconducting niobium films. *Applied Physics Letters, 119*(24), 244004 (2021)

Nb_2O_5 Crystalline paramagnetism and electronic structure origin of moments

- Electrical and magnetic properties of $Nb_2O_{5-\delta}$ crystallographic shear structures. *Physical Review B, 44*(13), 6973–6981 (1991)
- Fang, C. M., van Huis, M. A., Xu, Q., Cava, R. J., & Zandbergen, H. W. (2015). Unexpected origin of magnetism in monoclinic $Nb_{12}O_{29}$ from first-principles calculations. *Journal of Materials Chemistry C, 3*(3), 651–657 (2015)

Nb_2O_5 structure in resonators

- Localization and Mitigation of Loss in Niobium Superconducting Circuits, PRX Quantum 3, 020312 (2022)

Lambda Ta_2O_5

- Hidden Structural Order in Orthorhombic Ta_2O_5, Phys. Rev. Lett. 110, 235502 (2013)

Stephenson Roth Phase

- Structural systematics in the binary system $Ta2O_5$-WO_3, Acta Cryst. B27, 1037-1044 (1971)

Agenda

- SC Qubit Materials and Systems Charts – Introduction

- Modeling Materials
  - Model Formulation
  - Electronic Structure Models
  - Atomistic Models
  - From Phenomenological to Microscopic

- Use Cases
  - Nb and its hydrides
  - Nb and its oxides

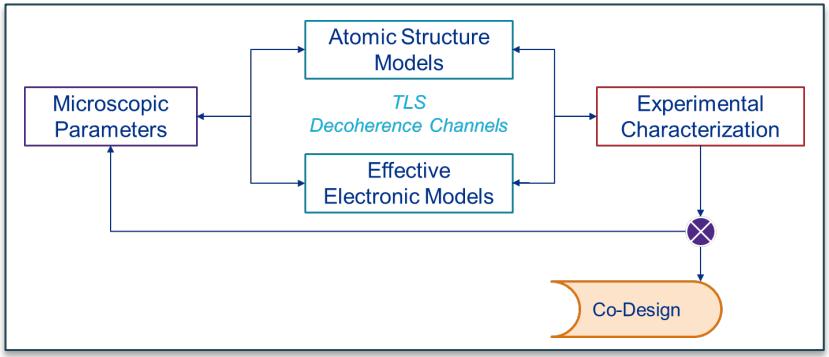
- Co-Design and Integration with Experimentation – Summary

Integrated theoretical, computational & experimental approaches

- Advance novel experimental methods guided by systems design charts

PROCESSING → STRUCTURE → PROPERTIES → PERFORMANCE ← ARCHITECTURE

- Fuse simulations at multiple length scales with phenomenological models
- Computationally assess mitigation strategies for identified decoherence mechanisms and ensure industry compatible
- Streamline data acquisition and analysis for rapid model assessments



Identify Key Components and Materials → Structure and Property Characterization → Performance Tests / Models → Evaluate Coherence

Thank you!

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Learn more about our work