Stress-induced structural changes in Nb thin film

Fermi National Accelerator Laboratory

Jaeyel Lee, Zuhawn Sung, Akshay Murthy, Grigory V. Eremeev, Anna Grasselino, Alex Romanenko

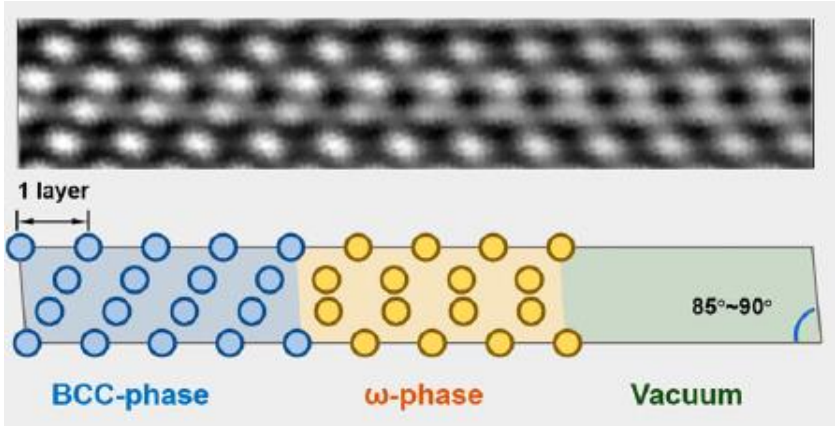
9/22/2022

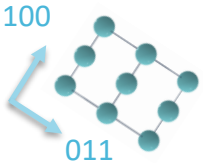
Contents

Structural changes in Nb under stress

- Nb is soft and easily deformed: Yield Strength (20-80 MPa)

- There are recent reports on omega (ω) phase with hexagonal structure in Nb under stress





MATERIALS RESEARCH LETTERS
2021, VOL. 9, NO. 12, 523-530
https://doi.org/10.1080/21663831.2021.1992523

Taylor & Francis
Taylor & Francis Group

Open access

Shear band mediated ω phase transformation in Nb single crystals deformed at 77 K

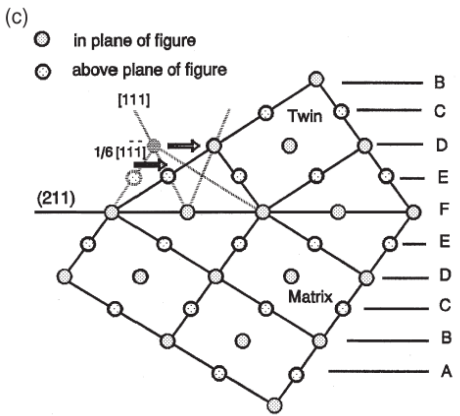
Xiyao Li[a,*], Qingkun Zhao[b,*], Qiannan Wang[c], Yanzhong Tian[d], Haofei Zhou[b], and Jiangwei Wang[a,e]

[a] Center of Electron Microscopy and State Key Laboratory of Silicon Materials, School of Materials Science and Engineering, Zhejiang University, Hangzhou, People's Republic of China [b] Center for X-Mechanics, Department of Engineering Mechanics, Zhejiang University, Hangzhou, People's Republic of China [c] Laboratory for Shock Wave and Detonation Physics, Institute of Fluid Physics, China Academy of Engineering Physics, Mianyang, People's Republic of China [d] Key Laboratory for Anisotropy and Texture of Materials, Ministry of Education, School of Materials Science and Engineering, Northeastern University, Shenyang, People's Republic of China [e] Wenzhou Key Laboratory of Novel Optoelectronic and Nano Materials, Institute of Wenzhou, Zhejiang University, Wenzhou, People's Republic of China

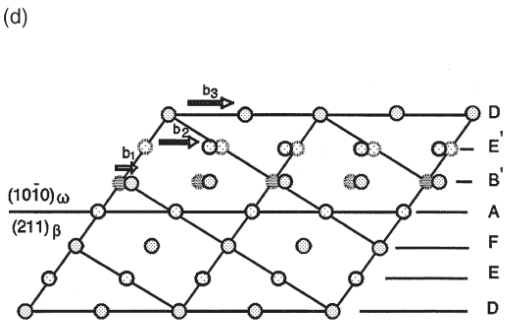
X Li et al, Mater Res Lett (2021)

Fermilab SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

Omega phase (ω) transition in other alloys: Ta, Ti alloys etc



Twinning in bcc metal



Phase transformation from bcc to ω phase

LM Hsiung et al, Acta Mater (2000)

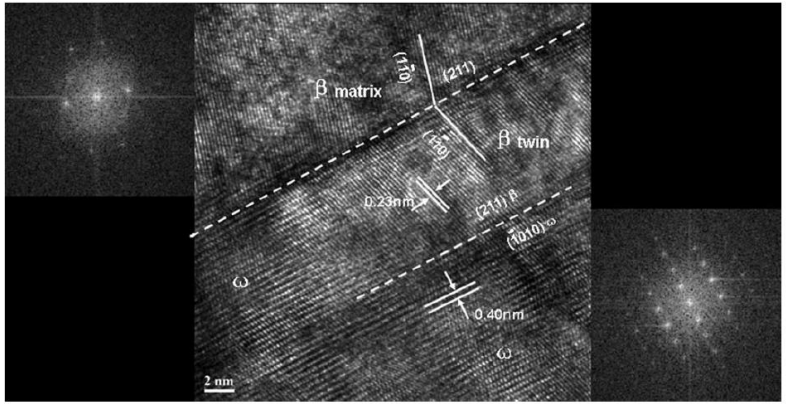


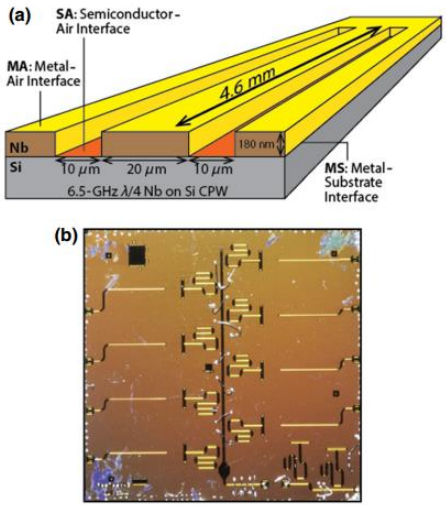
FIG. 2. HRTEM image taken along [11$\bar{3}$] showing mechanical twin lamella and associated stress-induced ω phase.

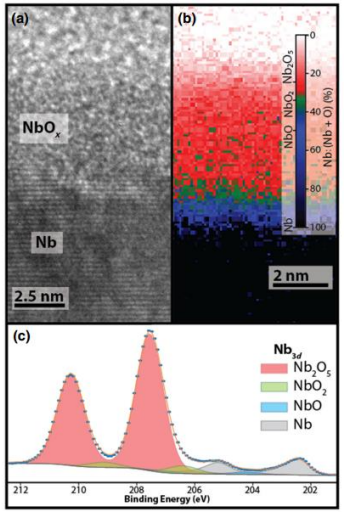
H Xing et al, APL (2008)

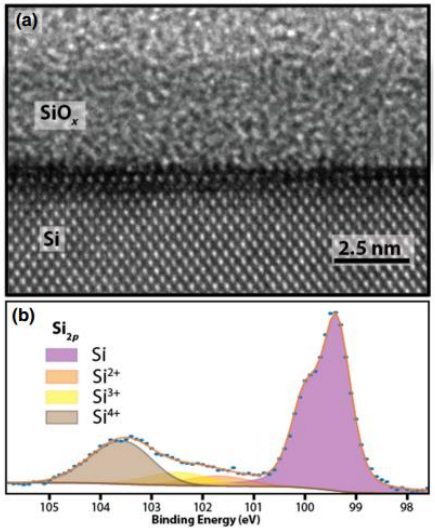
Nb thin film resonators for superconducting qubits

- Nb thin film 2D resonator shows ~10^6 of Q-factor significantly lower than 3D-resonator

- Understanding materials origins for the degradation of quality factor of Nb thin film resonators for superconducting qubits.



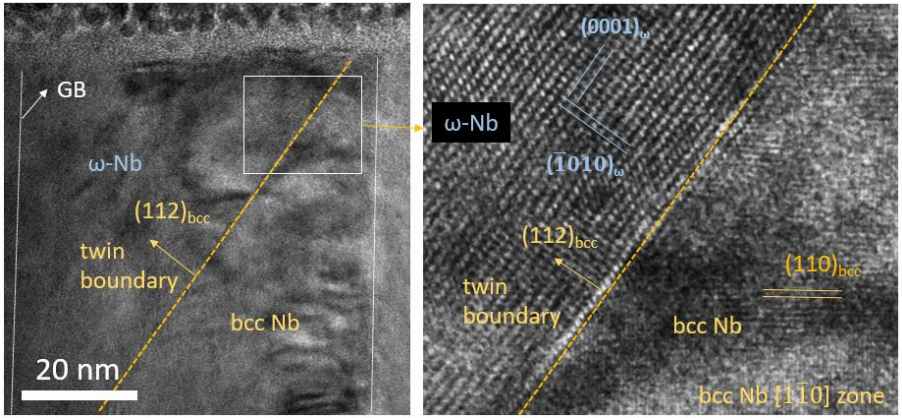




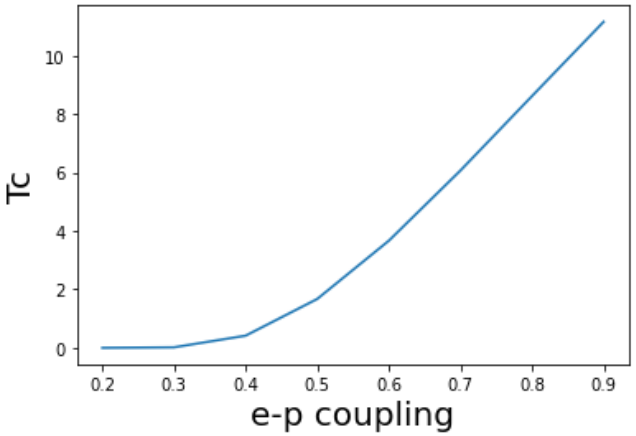
MVP Altoe et al., PRX Quantum (2022)

Structural changes in Nb under stress

- Interestingly, omega (ω) phases are seen in Nb thin films deposited by HiPIMS or Sputtering
- Superconducting properties of the omega phase and their possible effects on Nb thin film SRF cavities is unknown



J. Lee et al., arXiv (2022)



Possible roles of the omega (ω) phases in Nb thin film SRF cavities is open question

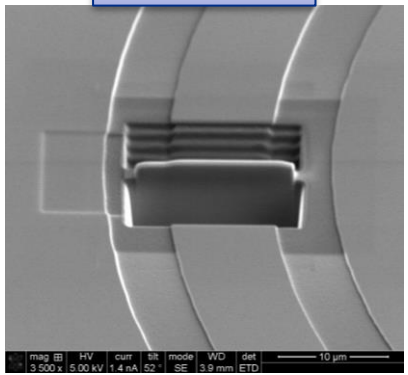
Nb thin film resonators for superconducting qubits

- Nb thin film is deposited by high-power impulse magnetron sputtering (HiPIMS) at Rigetti computing

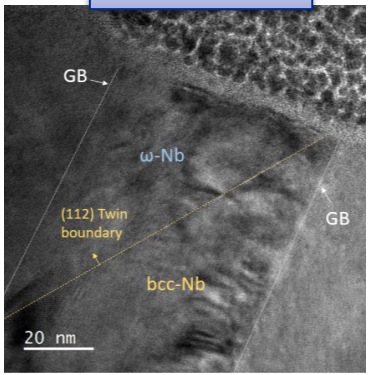
- TEM sample is prepared by Focused Ion Beam (FIB) and analyzed in TEM.

- Because of the challenges to measure the superconducting properties of the omega phase in Nb thin films, we used Density-Functional Theory (DFT) to investigate them.

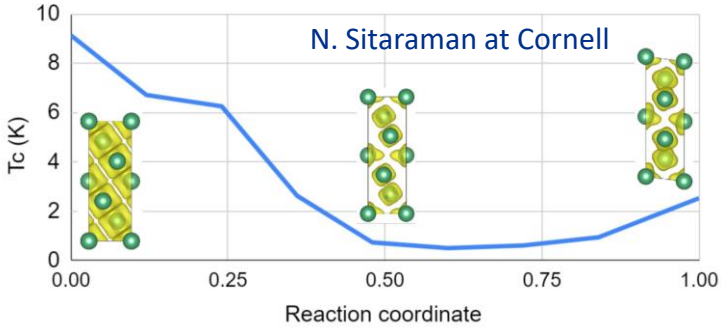
FIB lift-out



TEM

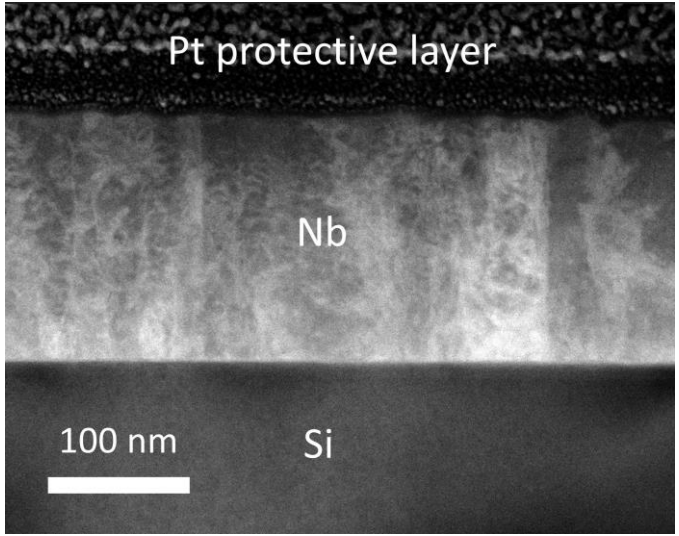


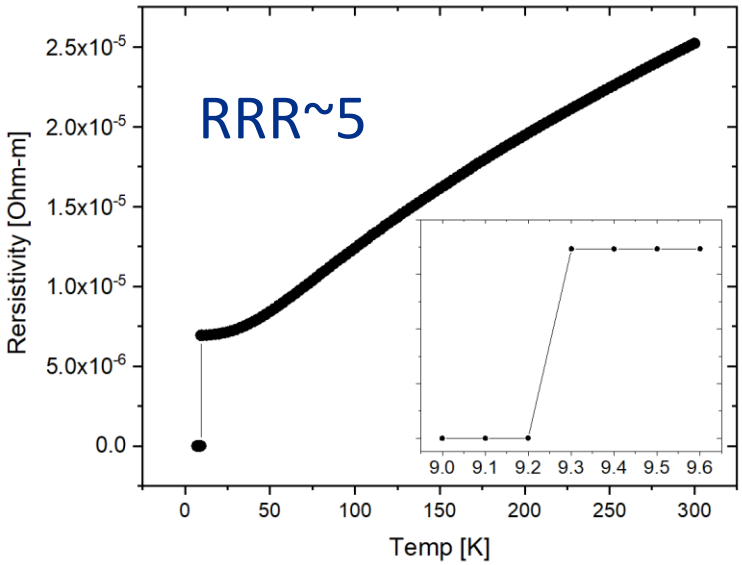
DFT calculations



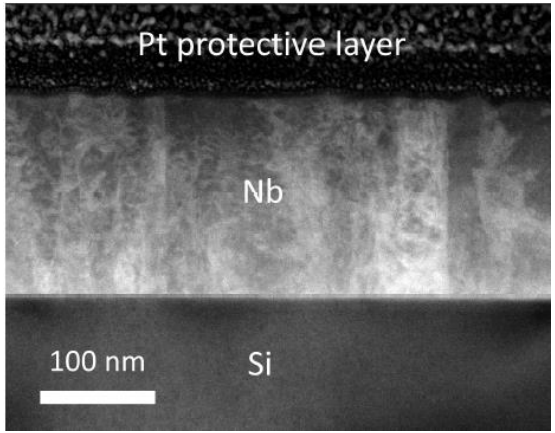
Nb thin film resonators for superconducting qubits

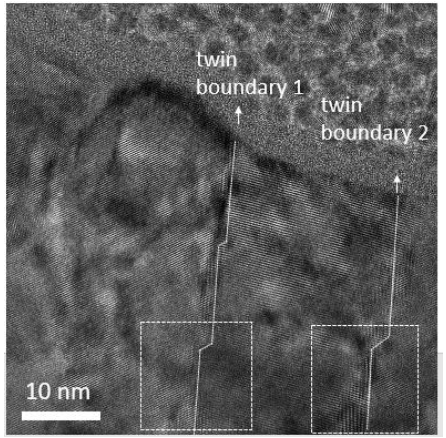
~170 nm Nb thin film is deposited by HiPIMS on Si [100] substrates at Rigetti computing

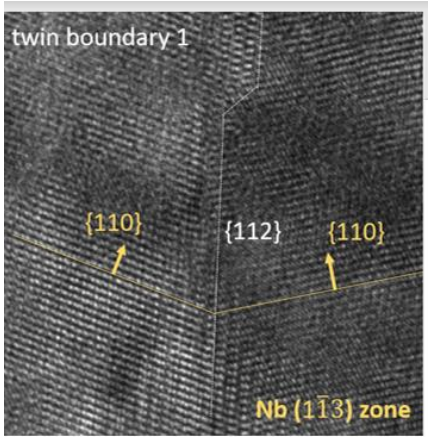


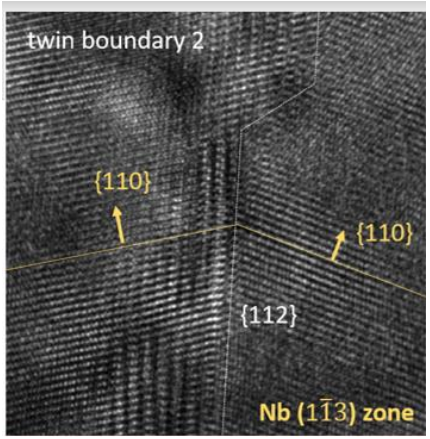


Deformative twins in Nb thin films



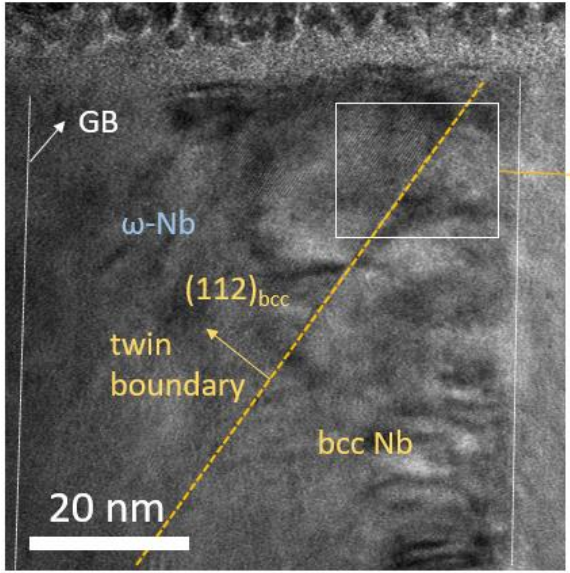


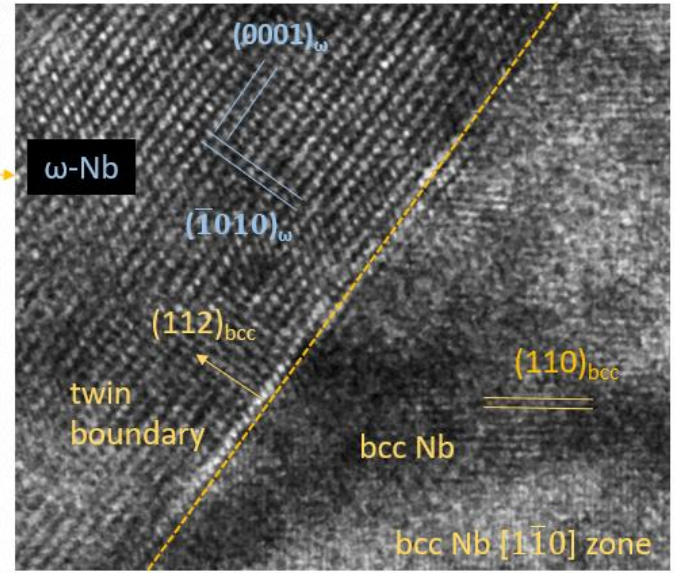


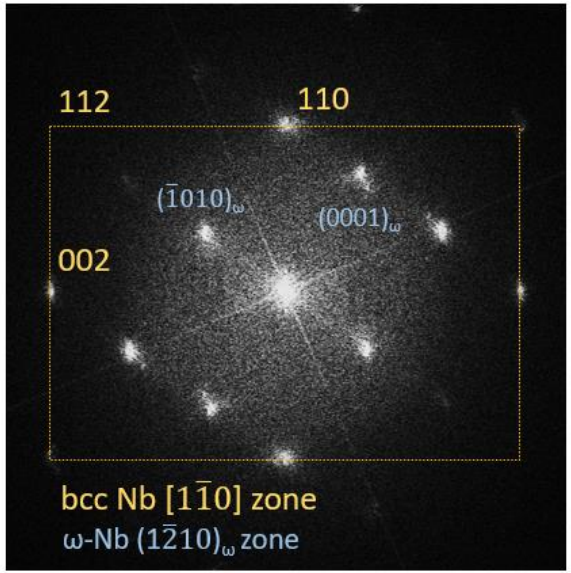


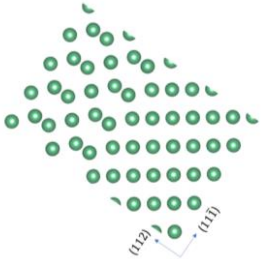
- Deformative twins on the surface of Nb thin film indicates that Nb film is prone to deformation due to the low yield strength (20-80 MPa).
- XRD analysis at NU shows that Nb thin film on Si is under compressive stress up to 900 MPa.

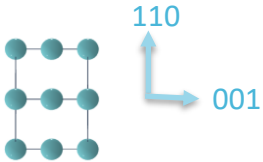
Omega (ω) phase transition at the twin boundaries



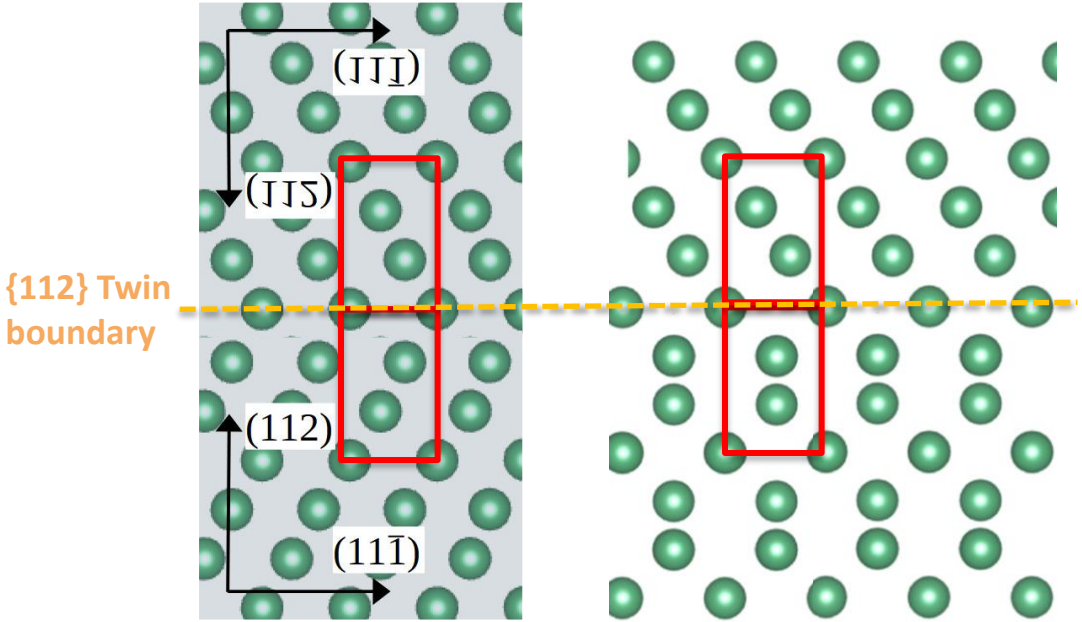


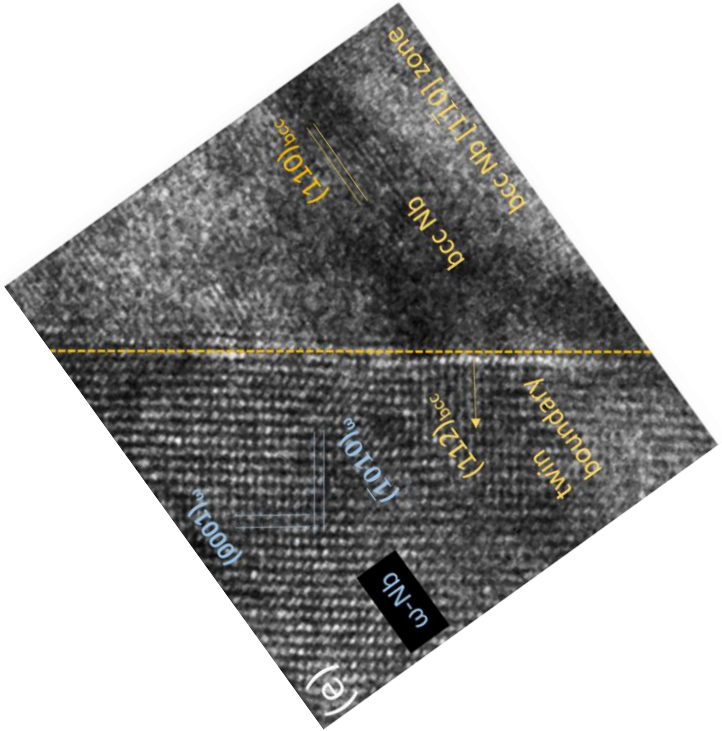


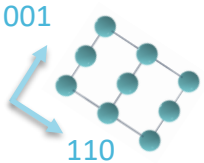




Atomic structure of omega (ω) phase in Nb thin films

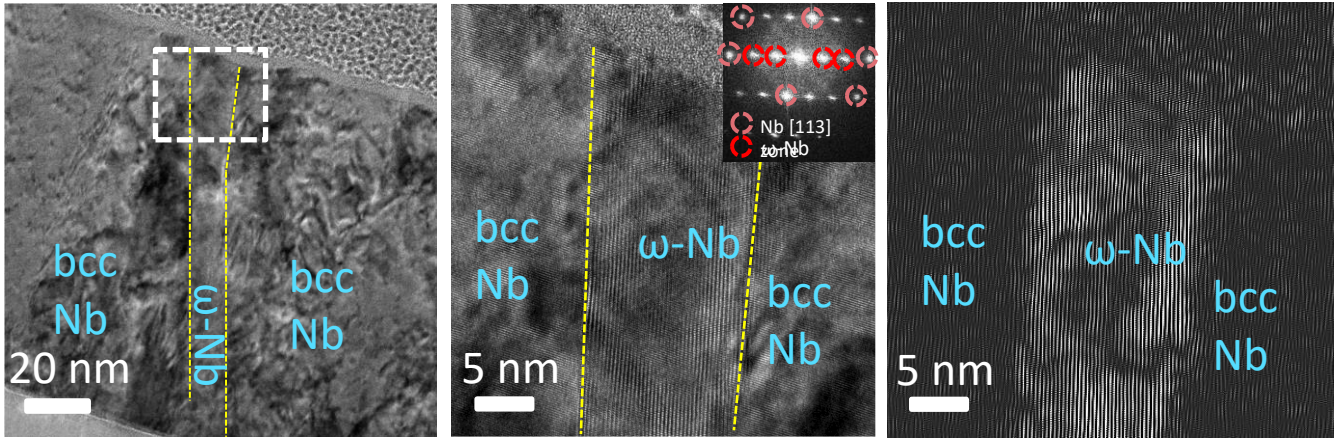






Fermilab SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

Results: Overview of omega (ω) phase in Nb thin films

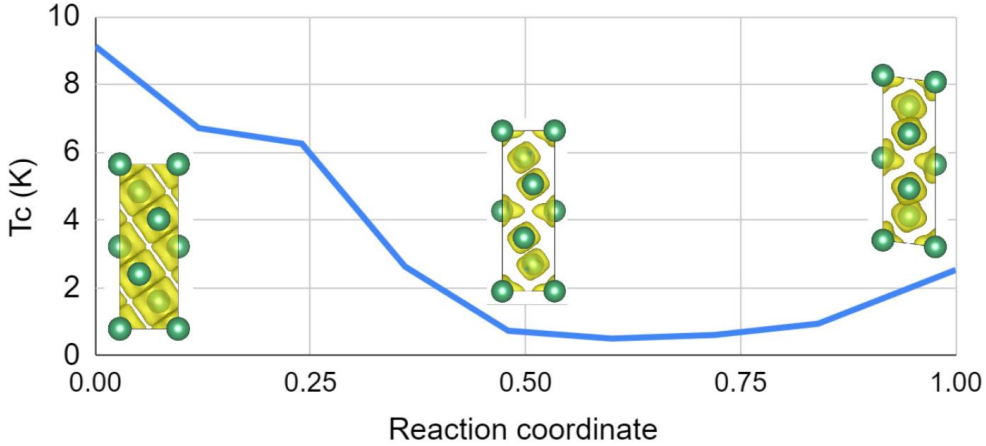


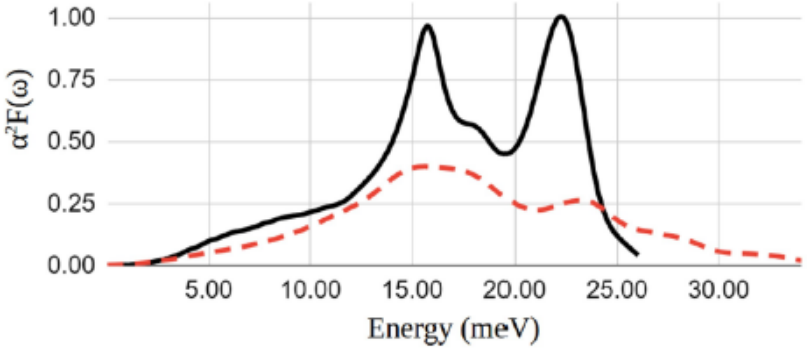
- Size of omega phases is comparable to the coherence length of Nb (~40 nm): 10~100 nm
- Volume fraction: ~1 vol.%

Some of the omega phase in Nb thin film extend along the whole thickness of Nb thin film

Estimating superconducting properties of omega phase Nb

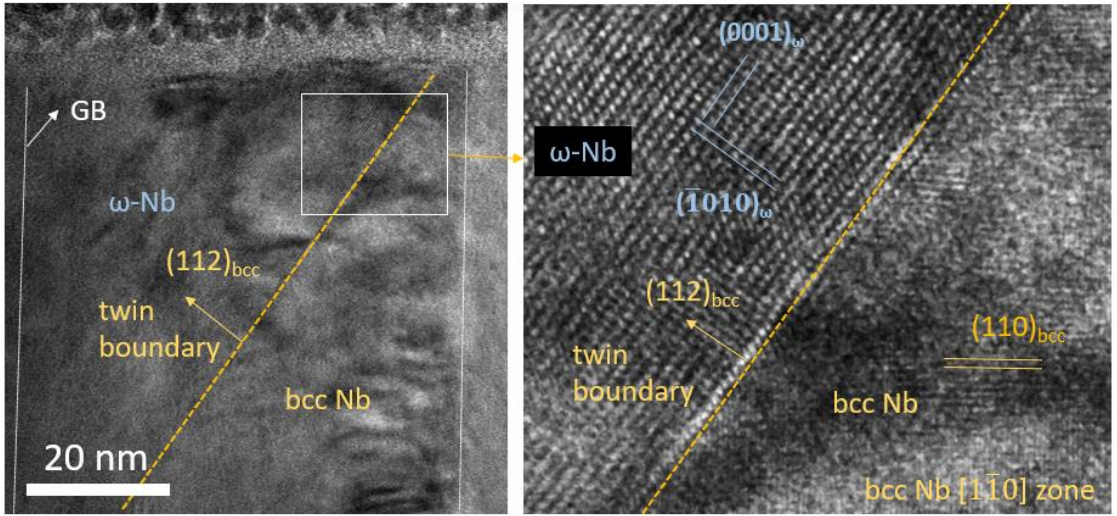
Collaboration with Nathan S. Sitaraman
from Tomas Arias group at Cornell



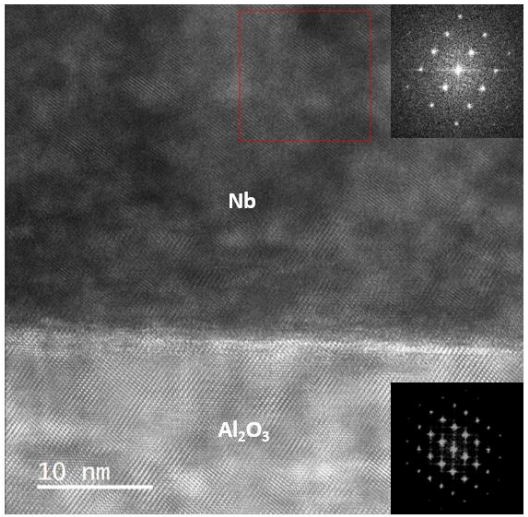


- Deviation from bcc to omega decrease the electron density of state at Fermi level, N(0).
- In turn, it may imply that the critical temperature of Nb may reduce in omega phase.

Role of grain boundaries on the deformative twins and omega (ω) phase in Nb thin films



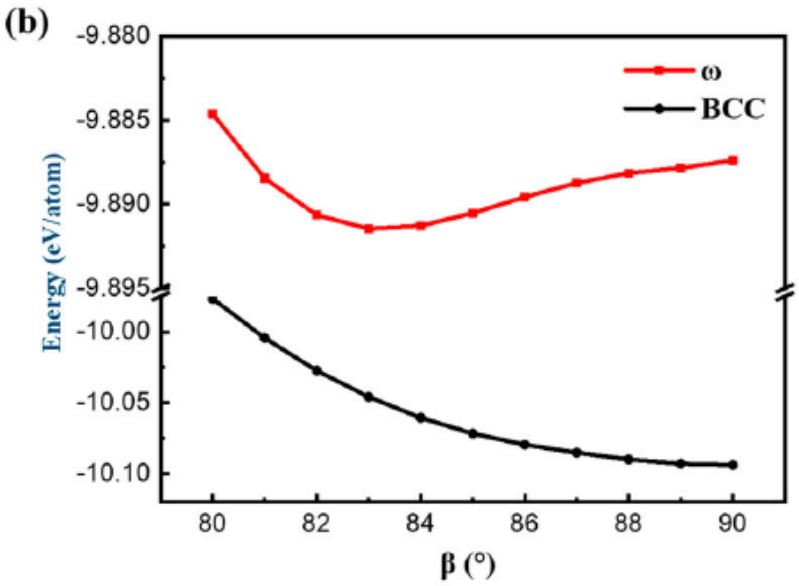
Polycrystalline Nb film on Si



Epitaxial Nb film on sapphire

Possible role of grain boundaries on deformative twins and omega (ω) phase transition

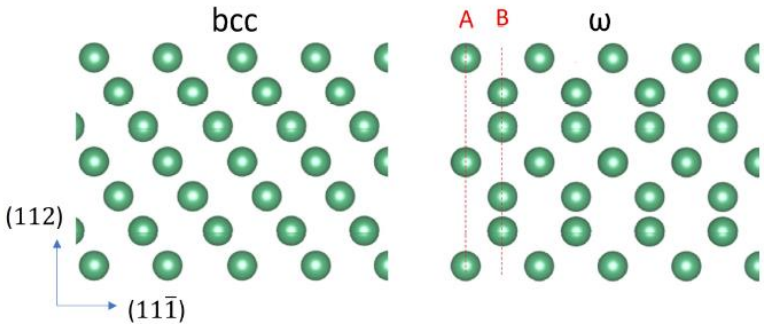
How is the omega (ω) phase stabilized?



X Li et al, Mater Res Lett (2021)

TABLE I. Vacancy formation energies in Nb

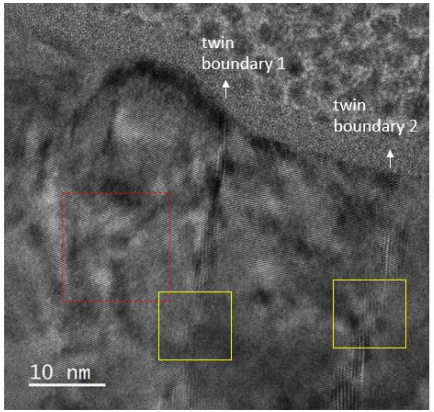
Phase	Sites	Formation energy (eV)
bcc		2.77
ω	{111} plane A	1.22
ω	{111} plane B	-0.52

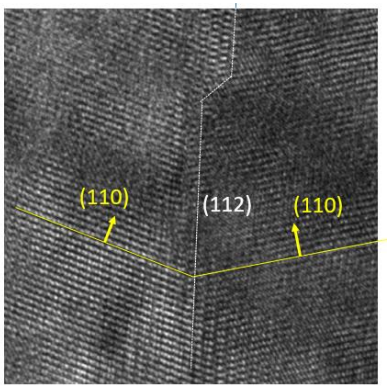


Vacancies or dislocations may play important roles in omega phase (ω) transition.

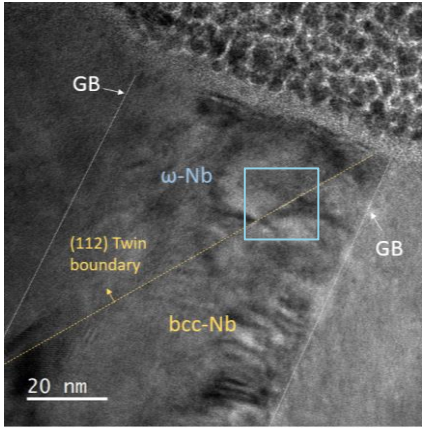
ω-Nb : bcc to hexagonal transition

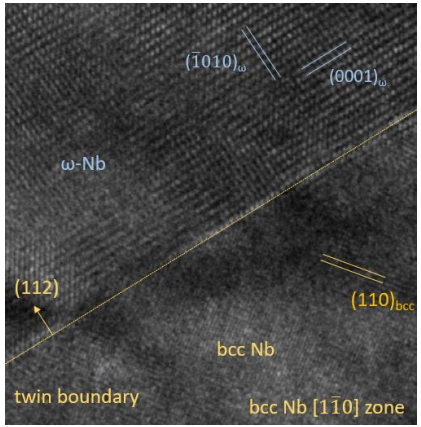
Twinning





ω-Nb





Why do they form? (i) Nb is soft. Internal stress in Nb thin film possibly matter.
(ii) Grain boundaries provide dislocations

Superconducting properties? DFT calculations imply that omega phase may have degraded Tc etc.

How to control? Controlling stress and grain size of Nb (substrate or heat treatment, etc)

Nb thin film resonators for accelerators

- Why Nb thin film SRF cavities quench earlier around ~20 MV/m?

  - Nb/Cu interface?
  - Heat dissipation?

  - Possibility of flux penetration via poor superconducting omega phase?

Nb thin film/Cu samples?

Acknowledgement

Fermilab: Zuhwan Sung, Akshay Murthy, Grigory V. Eremeev, Sam Posen, Alex Romanenko, Anna Grassellino

Northwestern University: Xiaobing Hu (TEM)

Cornell University: Nathan Sitaraman, Tomas Arias

Rigetti: Nb thin films deposited using HiPIMS

Funded by the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Superconducting Quantum Materials and Systems Center (SQMS) under the contract No. DE-AC02-07CH11359

Fermilab SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

supplementary

Summary

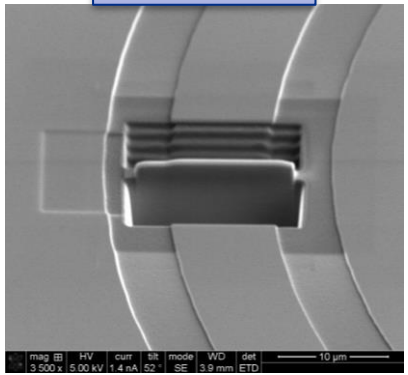
1. Nb is prone to internal stresses in the Nb thin films.

2. Nb thin films show ~1 vol.%

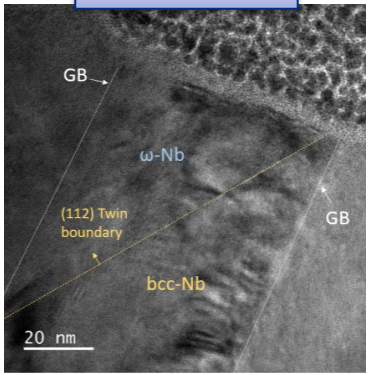
3. DFT calculations imply that they may have degraded superconducting properties.

4. It may need some attention to understand the superconducting properties of omega Nb phase and their possible roles in the Nb thin film SRF cavities.

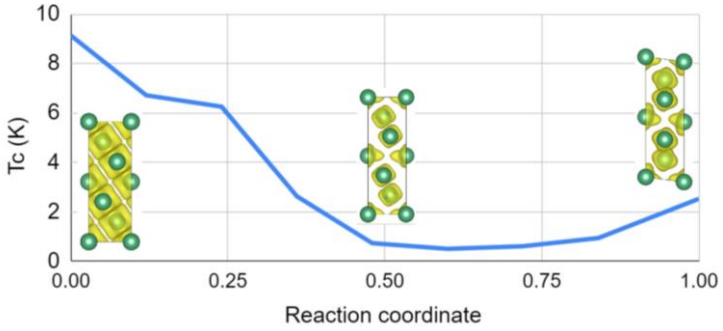
FIB lift-out



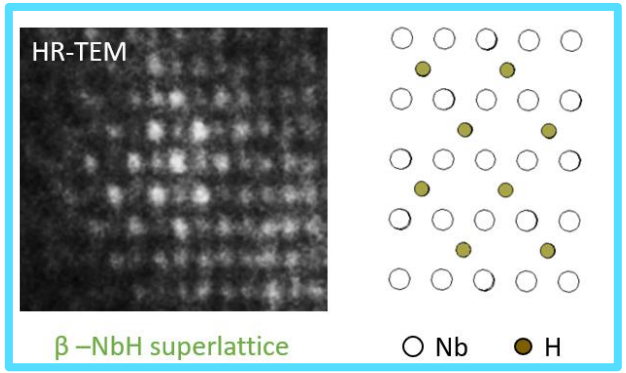
TEM



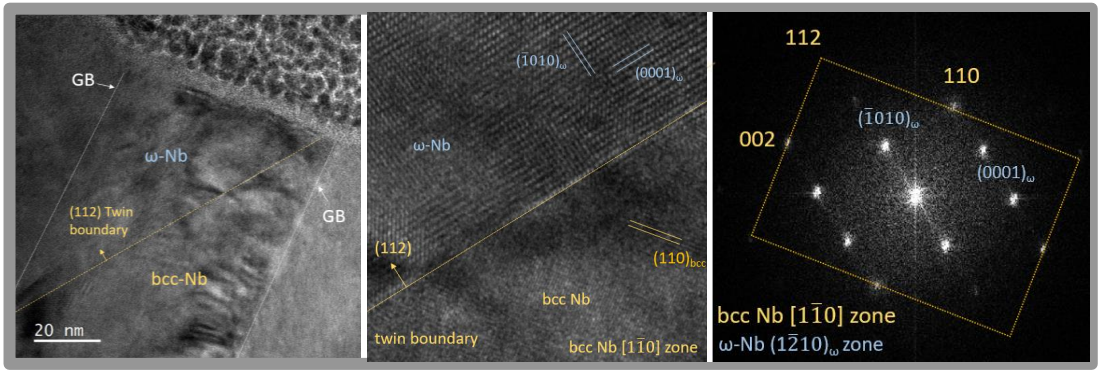
DFT calculations



Secondary phases in Nb thin films qubits



Nb hydride precipitates

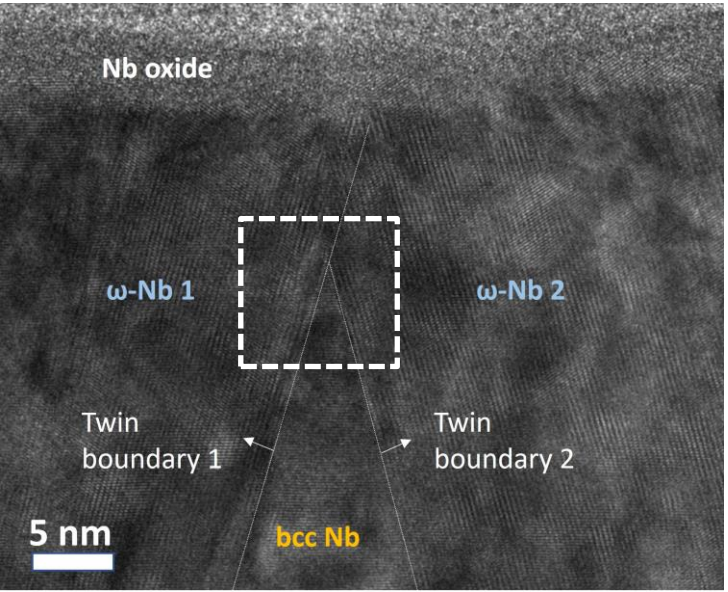


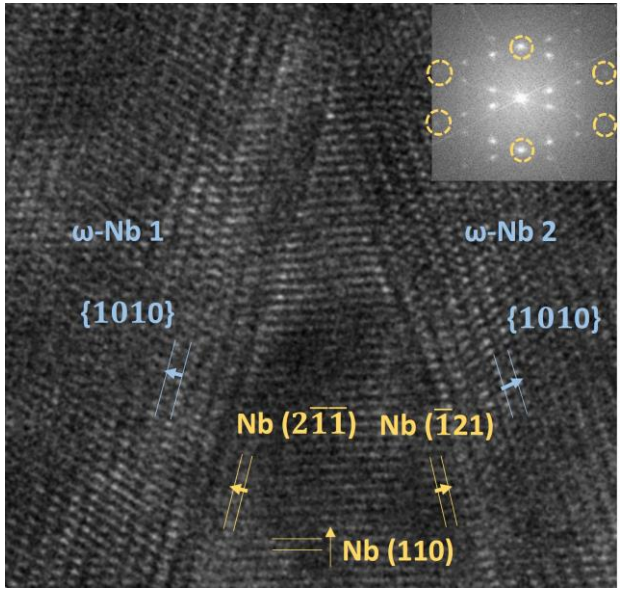
ω-Nb

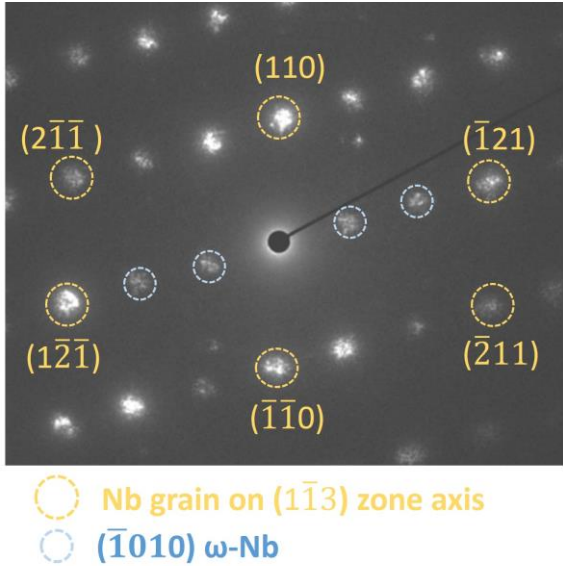
	NbH_x precipitates	ω-Nb
T_c	1.5 K or less	unknown
Size or shape	irregular	10-100 nm
Volume fraction	~0.1 %	~1 %

- Hydride precipitates are observed in Nb thin film during cooling and warming up
- Nb thin film in qubits may need caution to prevent hydride formation during growth and fabrication.
- Hydrides are distributed in Nb in nanoscale with irregular shapes. Possible source of decoherence due to pair breaking.
- Another secondary phase is omega Nb phase.

Results: Nucleation of omega phase at the deformative twins in Nb thin films

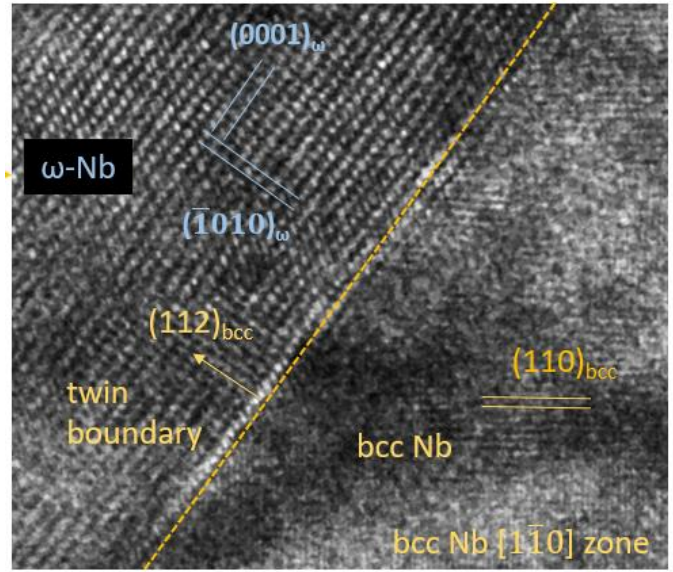


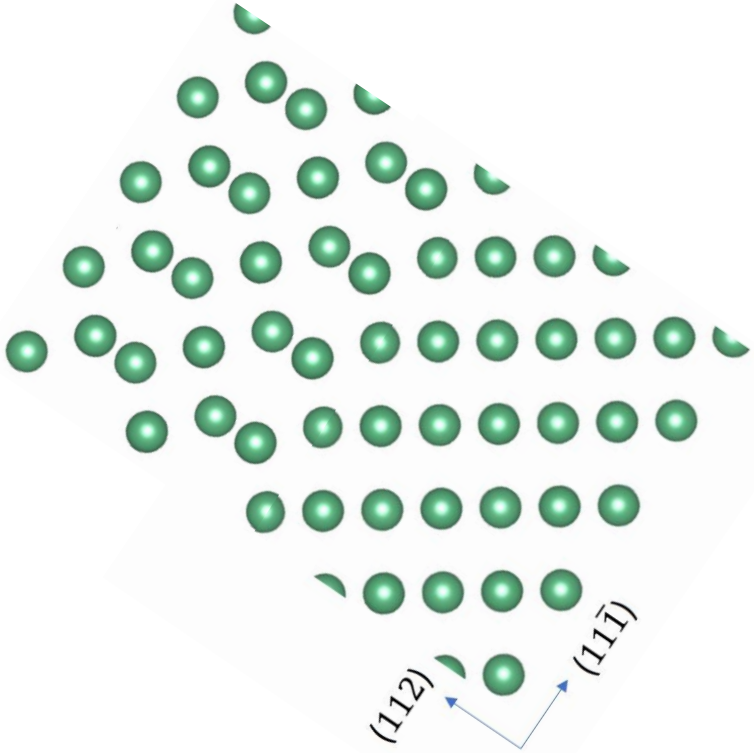




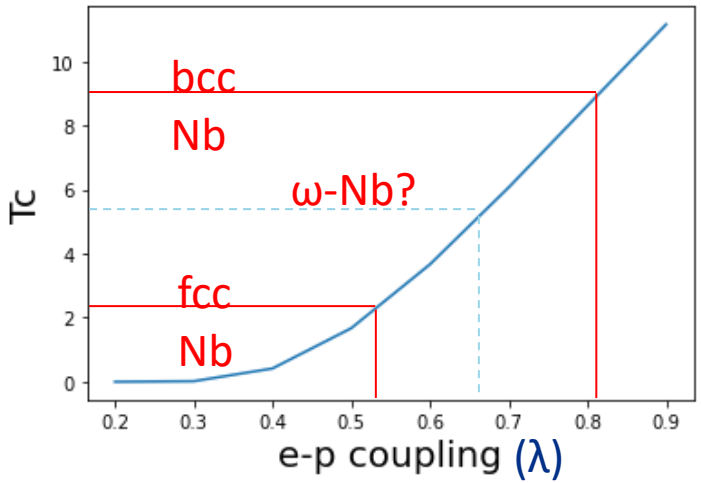
Q. How about superconducting properties?

Structural changes in Nb thin films





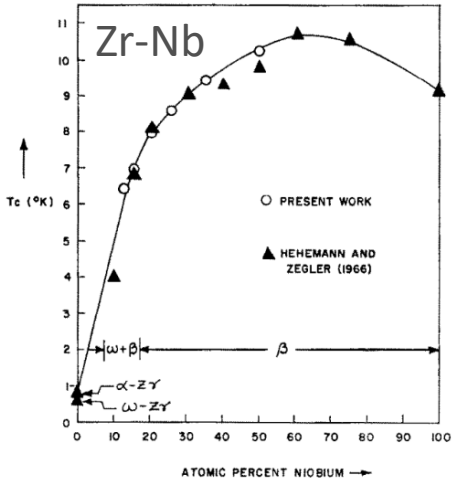
T_c of Nb



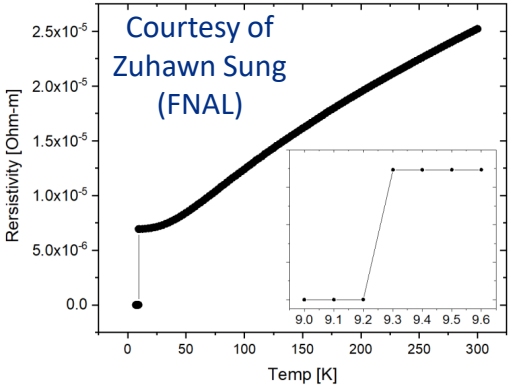
$$T_c = \frac{\theta_D}{1.45}\exp\left\{-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right\}$$

	bcc Nb	fcc Nb	ω-Nb
T_c (K)	9.3	2.3	?
Electron-phonon coupling (λ)	0.83	0.53	?
Electron-electron coupling (μ_*)	0.13		
Debye temperature (θ_D)	275		

M. Sasaki et al, Thin solid films (1998)



S Narasimhan et al., Journal of Nuclear Materials (1972)

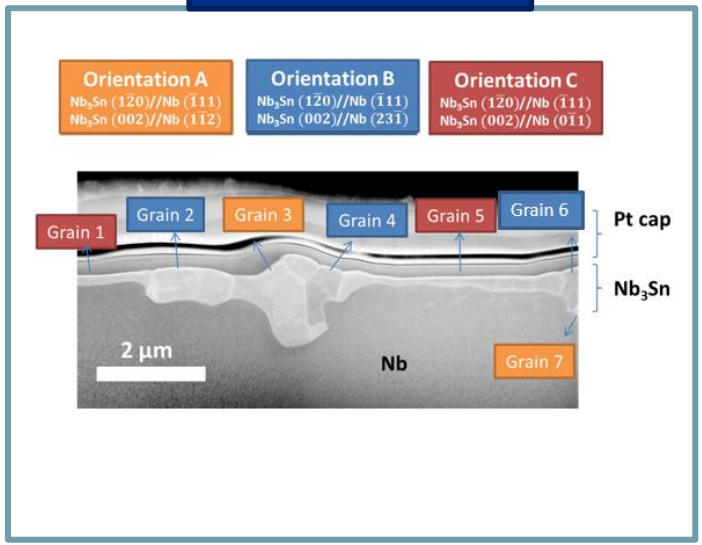


Fermilab SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

Thin film SRF cavities

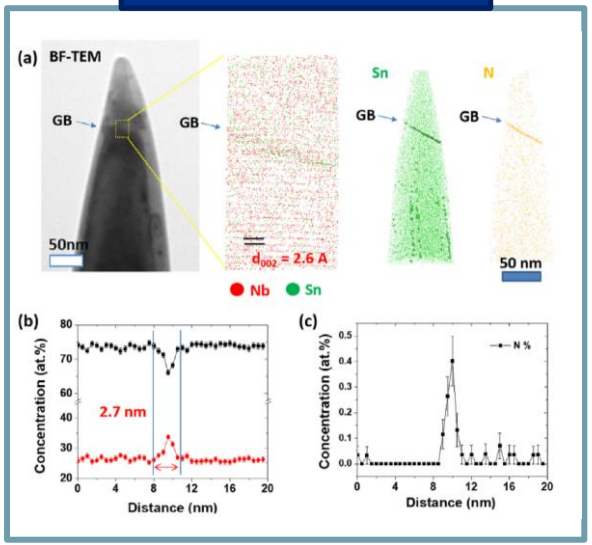
Previous studies on Nb_3Sn with Sam Posen

Poor coating



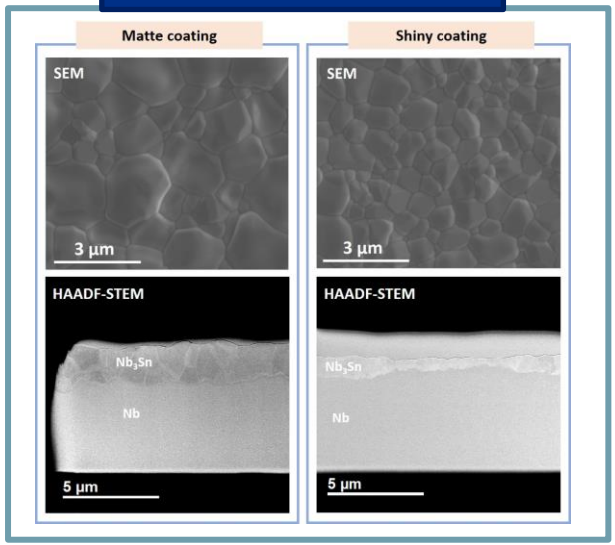
SUST 2019

Grain boundaries



Acta Mater 2020

Surface roughness

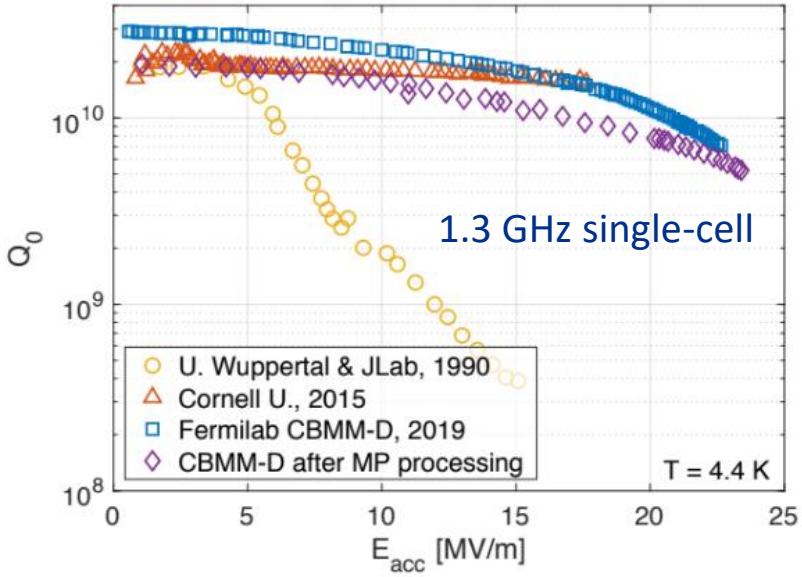


SUST 2021

Fermilab SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

Thin film SRF cavities

Previous studies on Nb_3Sn with Sam Posen



S. Posen et al, SUST (2021)

Omega (ω) phase transition in Nb

MATERIALS RESEARCH LETTERS
2021, VOL. 9, NO. 12, 523-530
https://doi.org/10.1080/21663831.2021.1992523

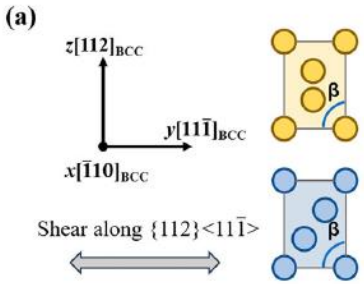
Taylor & Francis
Taylor & Francis Group

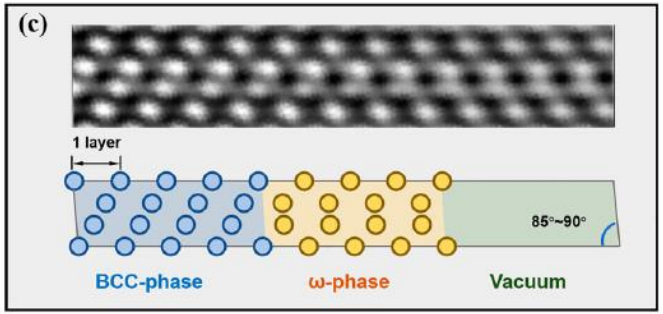
Open access

Shear band mediated ω phase transformation in Nb single crystals deformed at 77 K

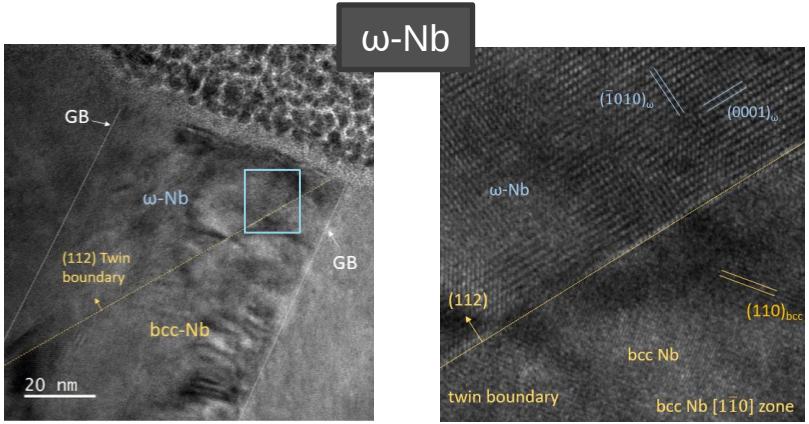
Xiyao Li[a,*], Qingkun Zhao[b,*], Qiannan Wang[c], Yanzhong Tian[d], Haofei Zhou[b], and Jiangwei Wang[a,e]

[a] Center of Electron Microscopy and State Key Laboratory of Silicon Materials, School of Materials Science and Engineering, Zhejiang University, Hangzhou, People's Republic of China [b] Center for X-Mechanics, Department of Engineering Mechanics, Zhejiang University, Hangzhou, People's Republic of China [c] Laboratory for Shock Wave and Detonation Physics, Institute of Fluid Physics, China Academy of Engineering Physics, Mianyang, People's Republic of China [d] Key Laboratory for Anisotropy and Texture of Materials, Ministry of Education, School of Materials Science and Engineering, Northeastern University, Shenyang, People's Republic of China [e] Wenzhou Key Laboratory of Novel Optoelectronic and Nano Materials, Institute of Wenzhou, Zhejiang University, Wenzhou, People's Republic of China





X Li et al, Mater Res Lett (2021)



Rigetti blanket Nb on Si [100]

Why do they form? stress

Superconducting properties?

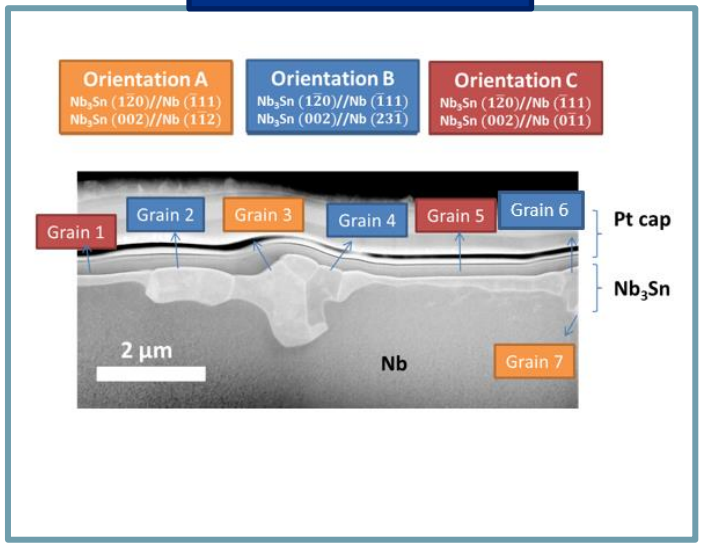
electron-phonon interaction

Fermilab SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

Thin film SRF cavities

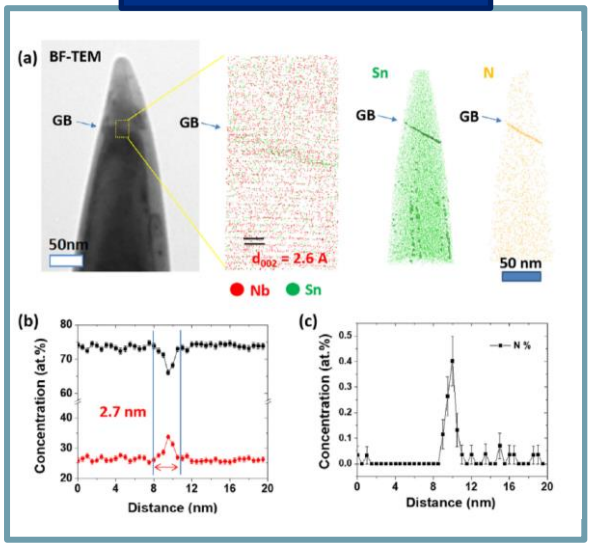
Previous studies on Nb_3Sn with Sam Posen

Poor coating



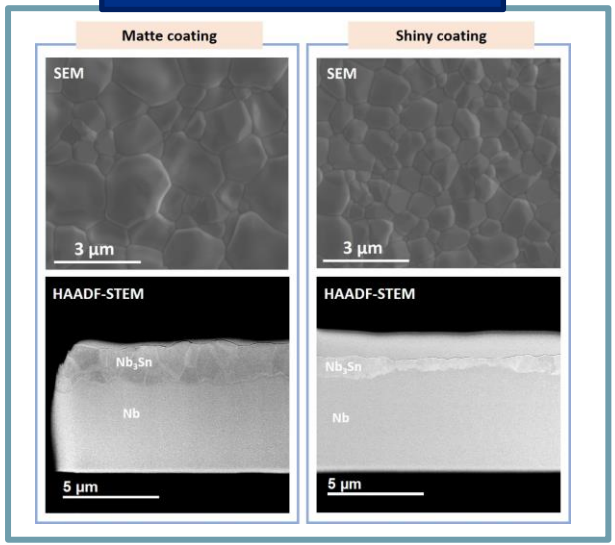
SUST 2019

Grain boundaries



Acta Mater 2020

Surface roughness

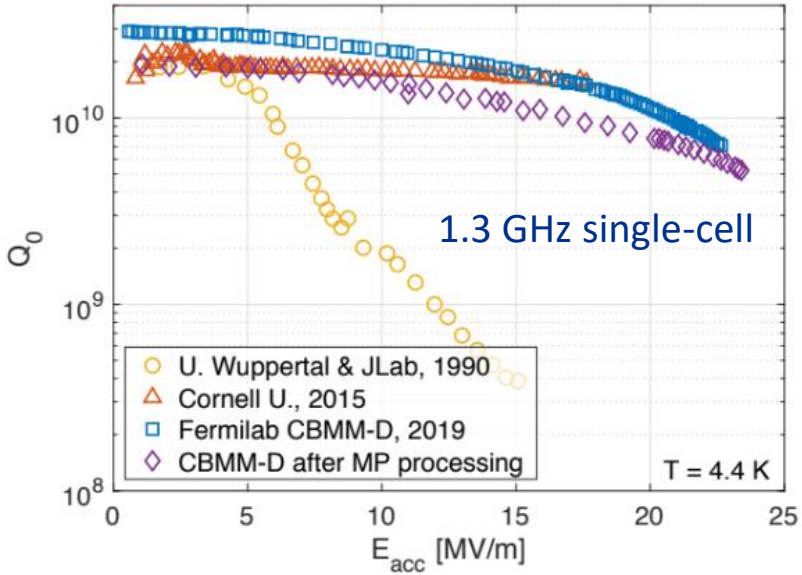


SUST 2021

Fermilab SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

Thin film SRF cavities

Previous studies on Nb_3Sn with Sam Posen



S. Posen et al, SUST (2021)

Contents

1. Thin film SRF cavities: previous experiences in Nb_3Sn
2. Structural changes in Nb thin films for superconducting qubits
3. Possible link to Nb thin film SRF cavities?