The Center for
BRIGHT BEAMS
A National Science Foundation Science & Technology Center

NSF

First principles study on the impact of grain boundaries on Nb_3Sn

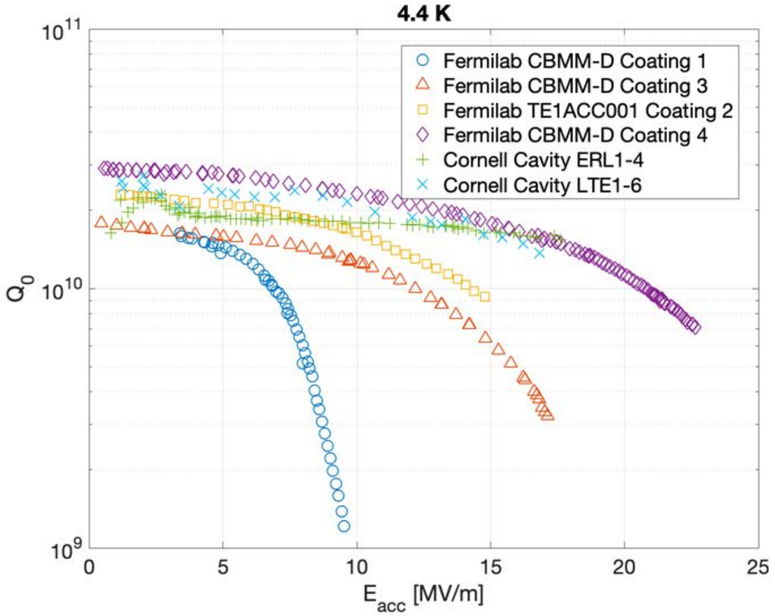
9:30am Tuesday 10 November 2020

Virtual International Workshop on Nb_3Sn SRF Science, Technology & Applications

Michelle Kelley, Nathan Sitaraman and Tomás Arias (Cornell University)

Nb_3Sn grain boundaries & cavity performance

Nb_3Sn SRF cavity studies[1] indicate correlation between cavity performance and grain boundary (GB) composition.



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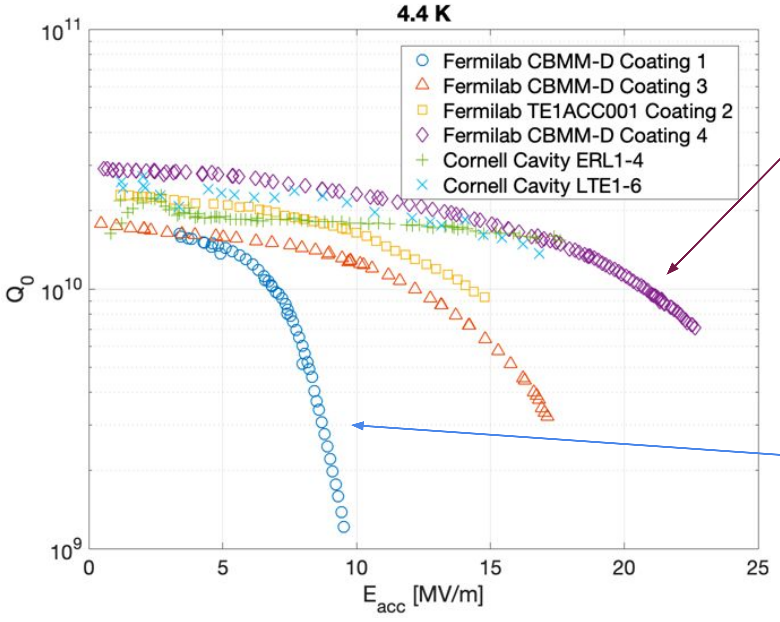

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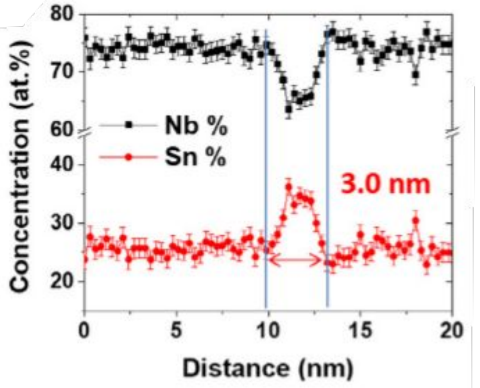
Degraded Q in cavities with **excess tin at GBs!**



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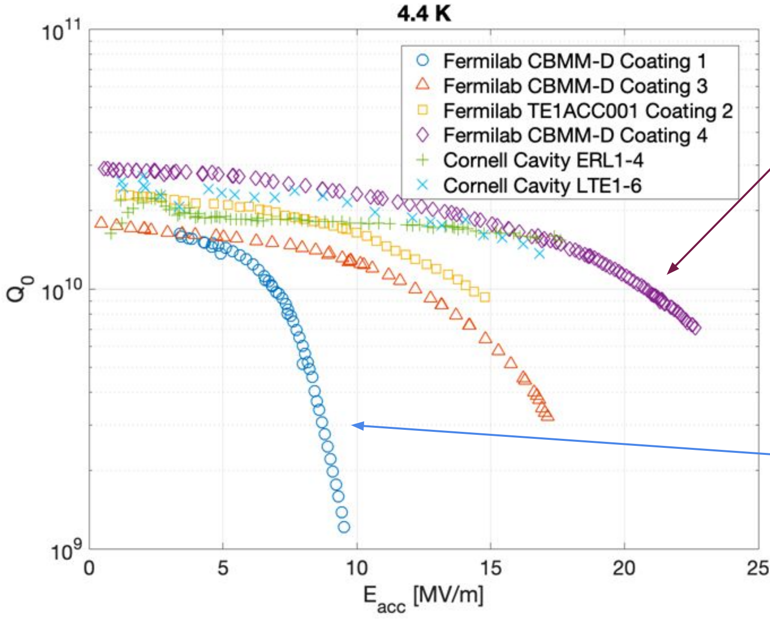

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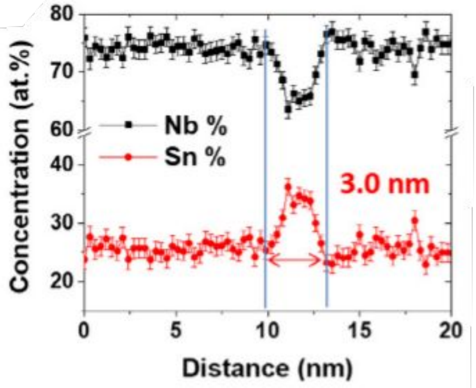

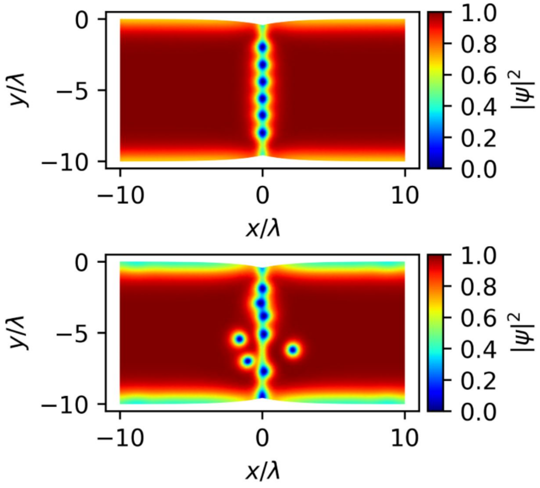

Ginzburg-Landau simulations suggest GBs with degraded properties can lower the flux entry field[2].

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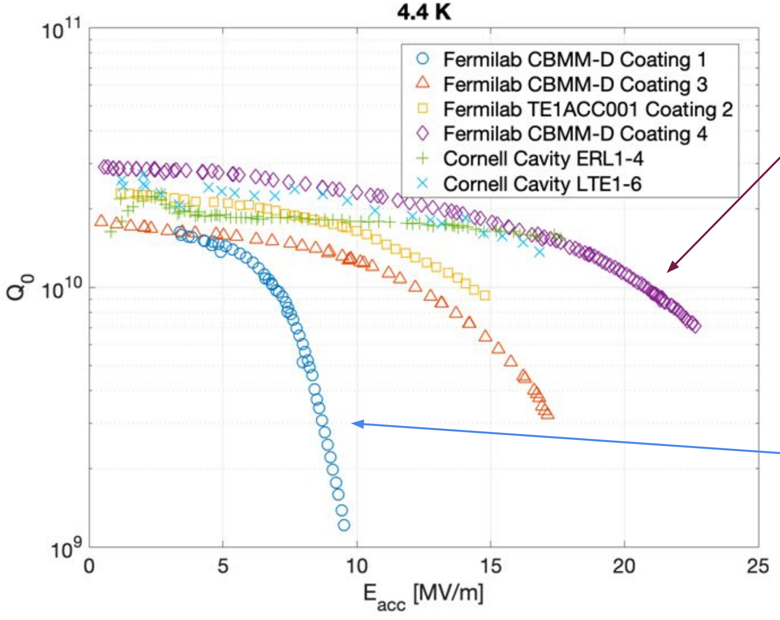

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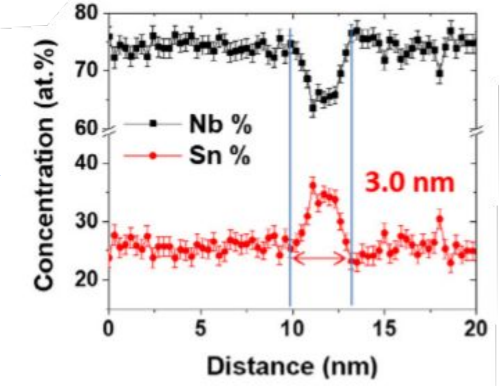

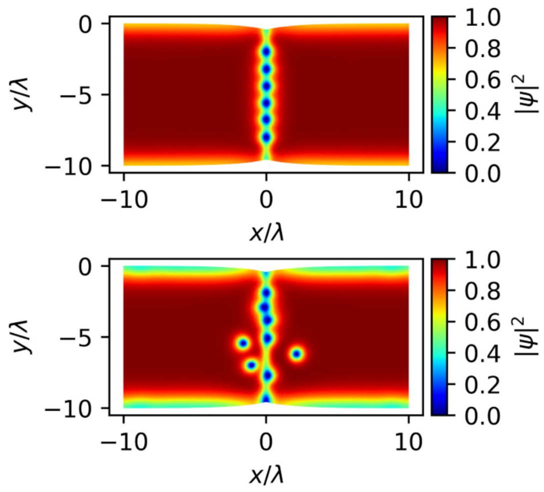

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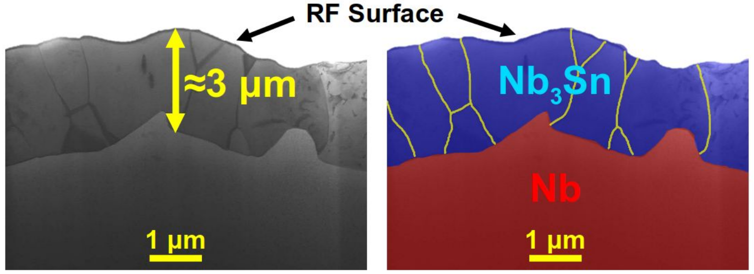

	Tc (K)	ξ (nm)
Nb_3Sn	18	
Nb	9	

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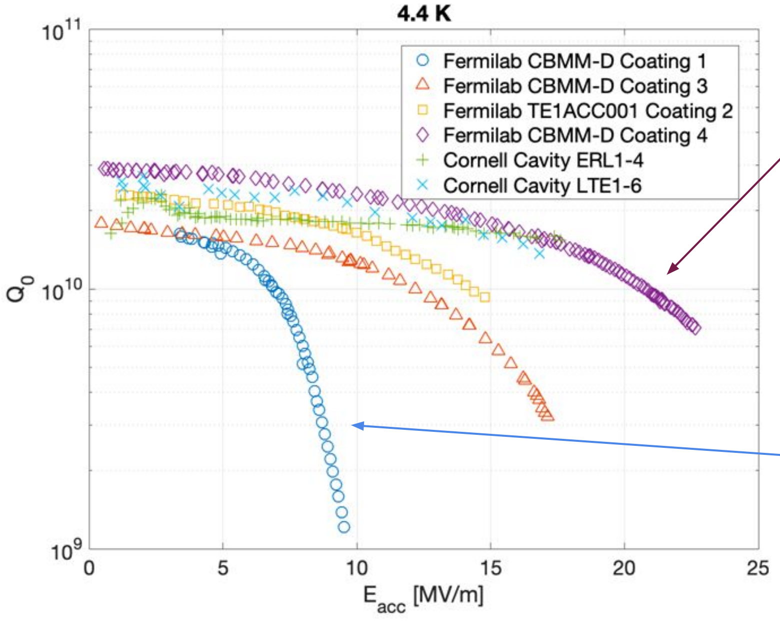

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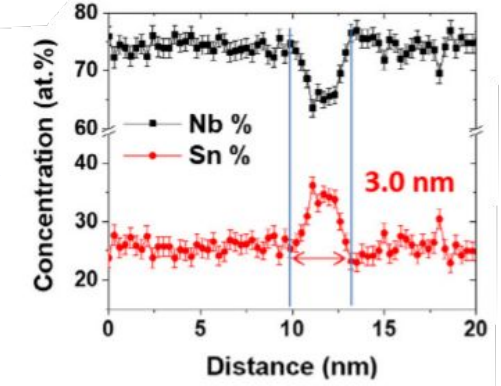

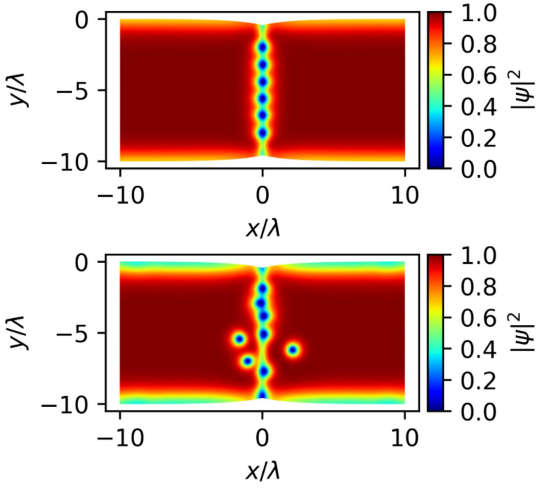

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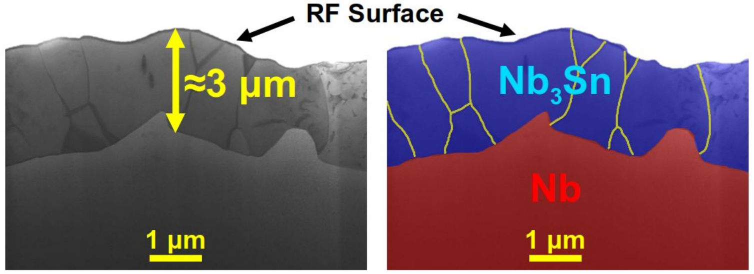

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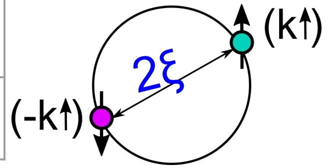

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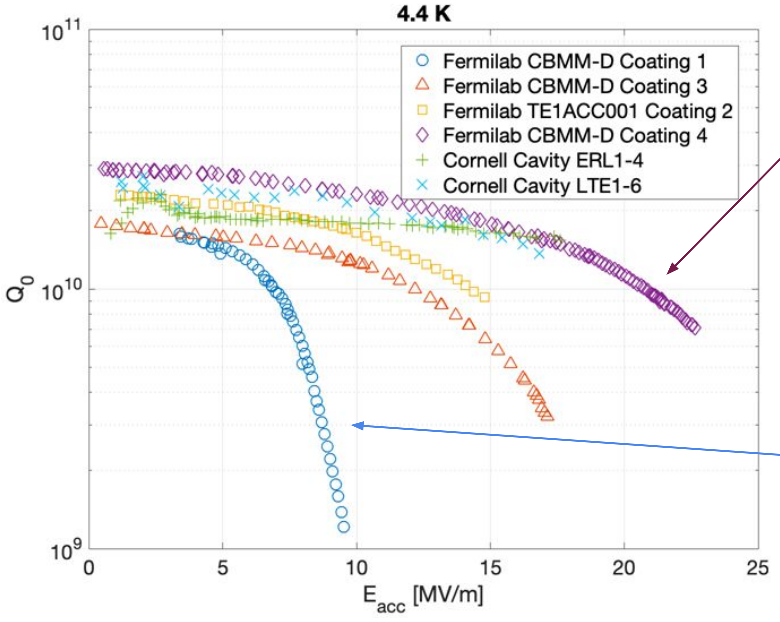

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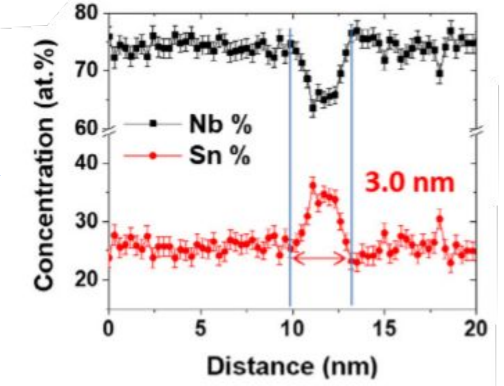

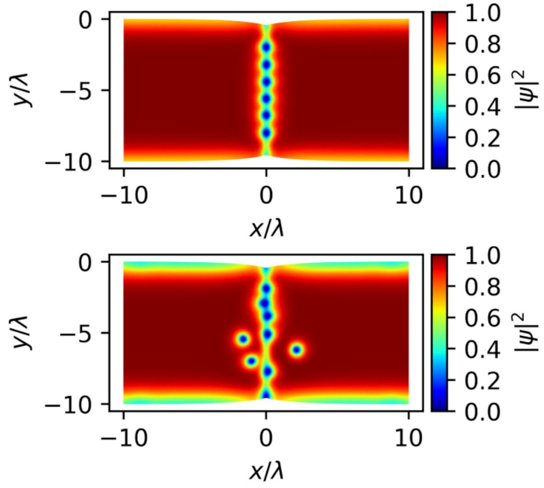

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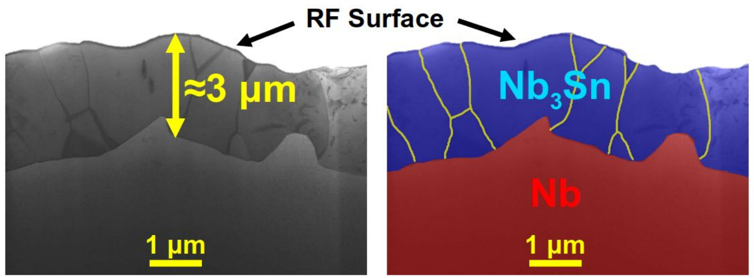

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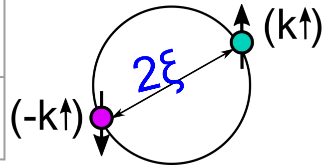

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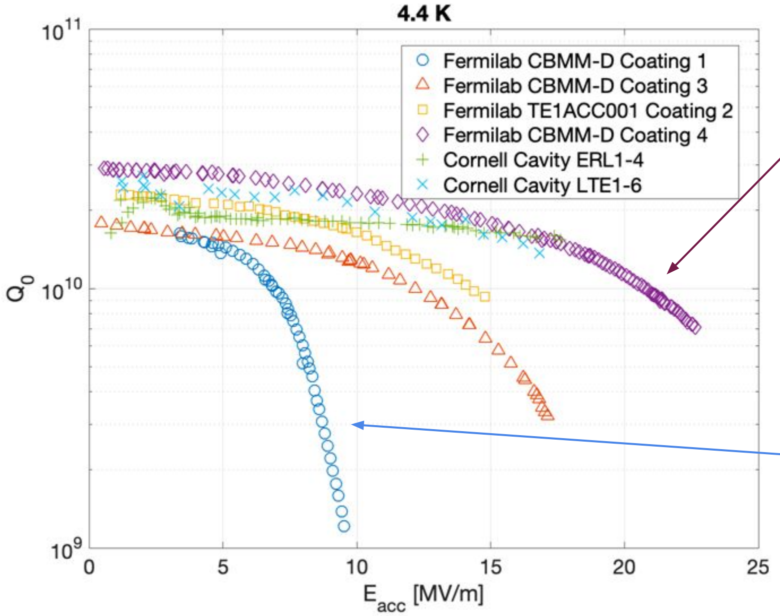

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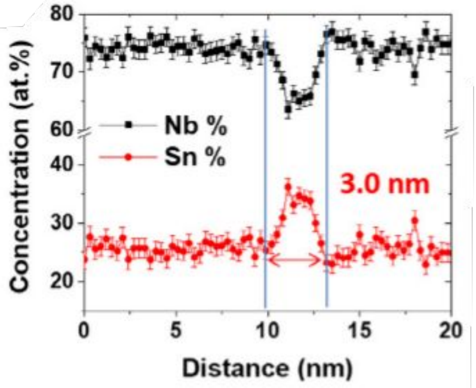

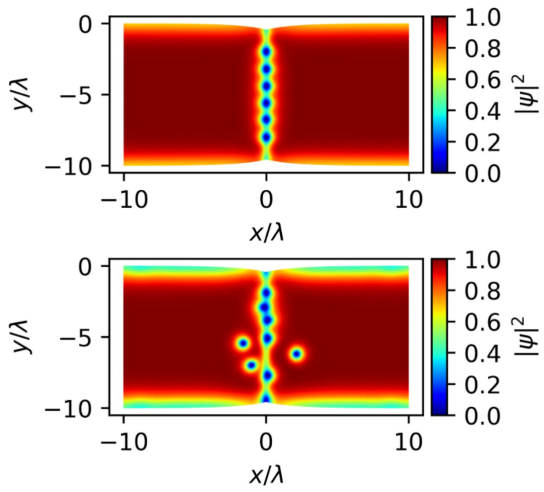

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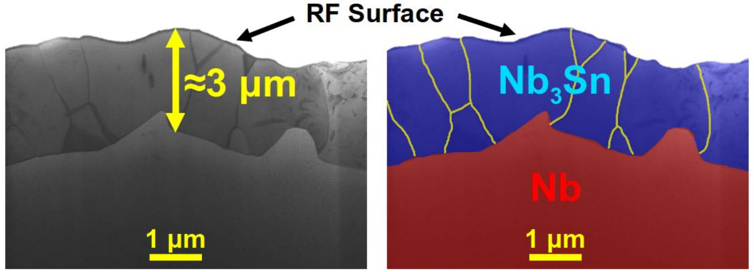

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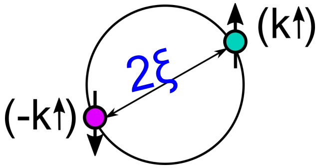

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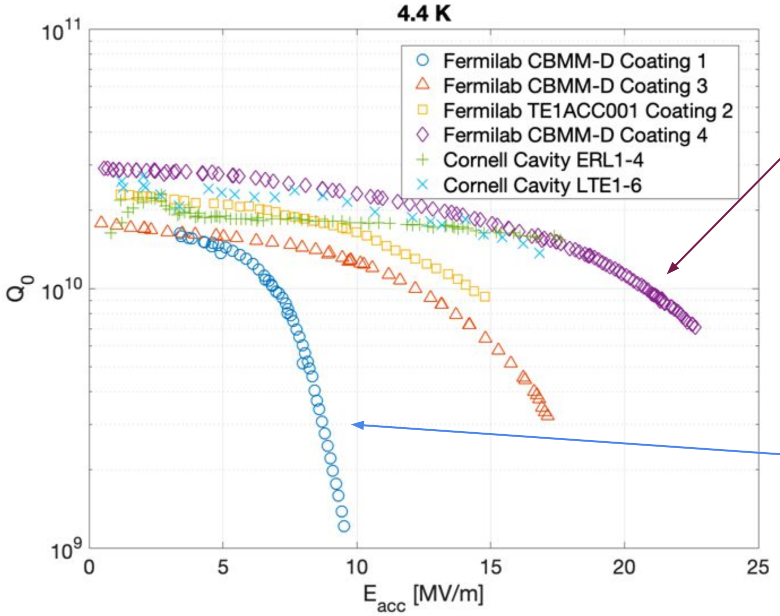

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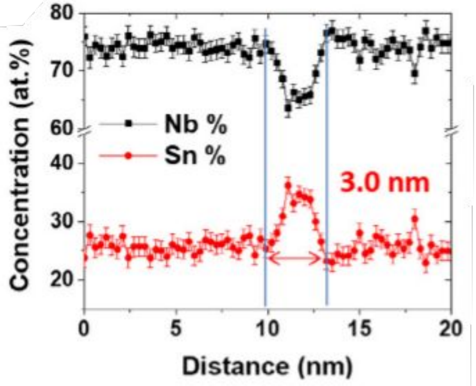

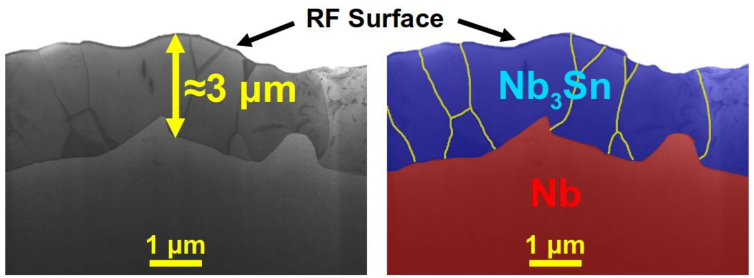

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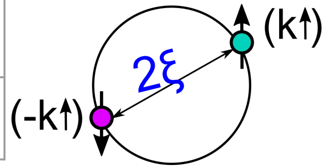

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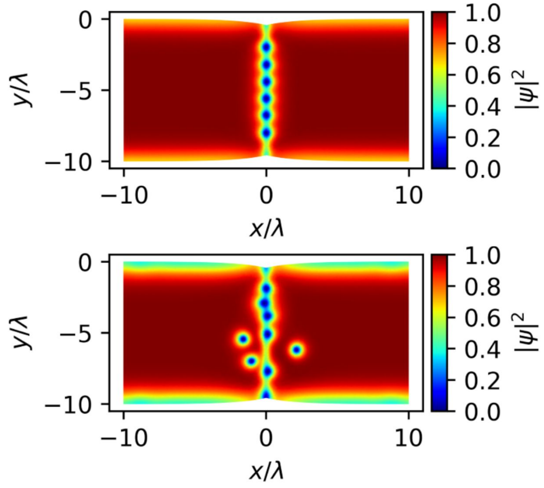

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- have *surprisingly* not been studied in detail using density-functional theory (DFT)

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Superconducting Nb_3Sn (undefected material)

A15 Superconductors:

highest Tc from 1954-1986

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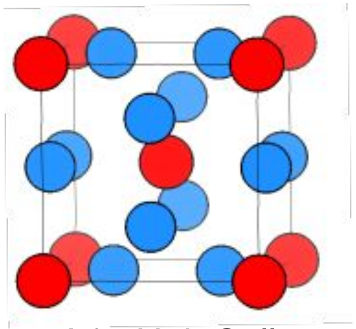

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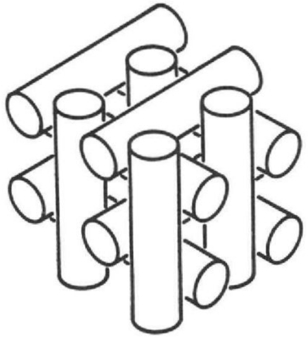

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Debye cut-off energy

Electron-phonon coupling potential

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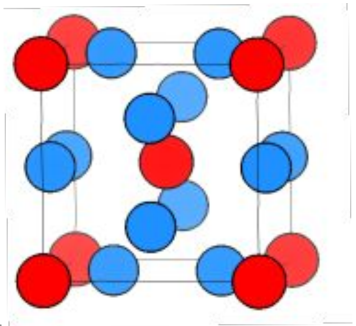
Density of states at Fermi level



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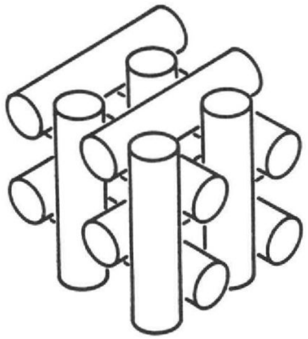

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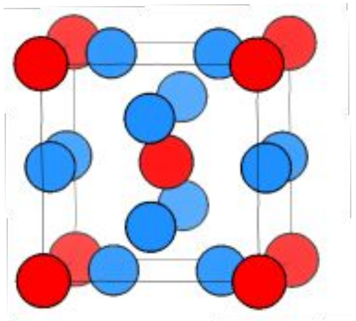

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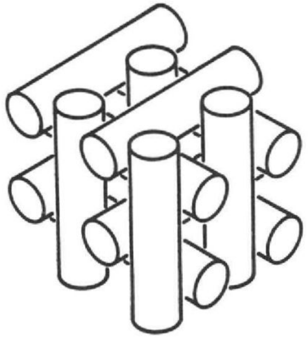

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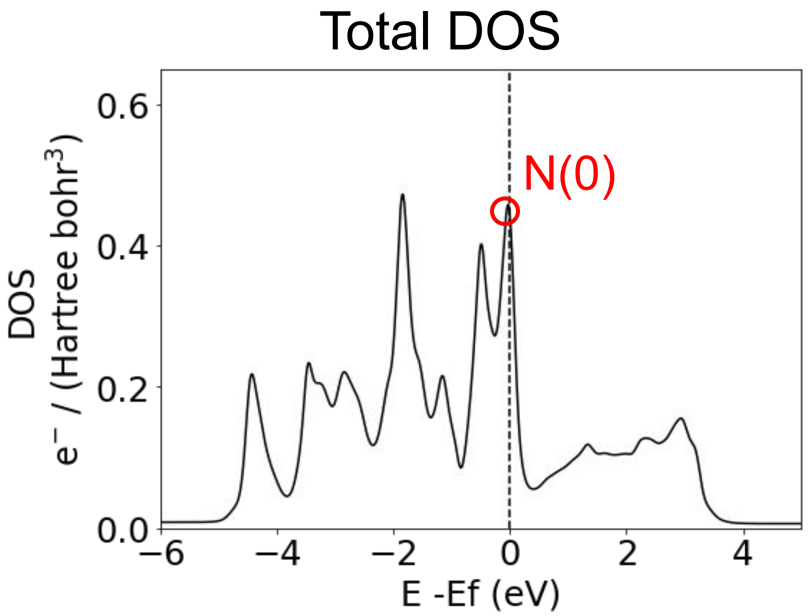

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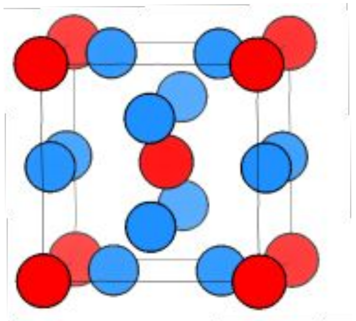

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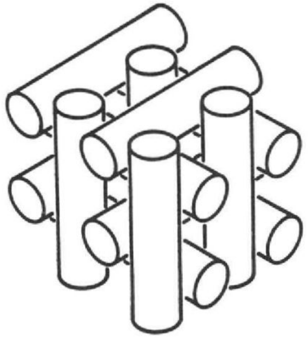

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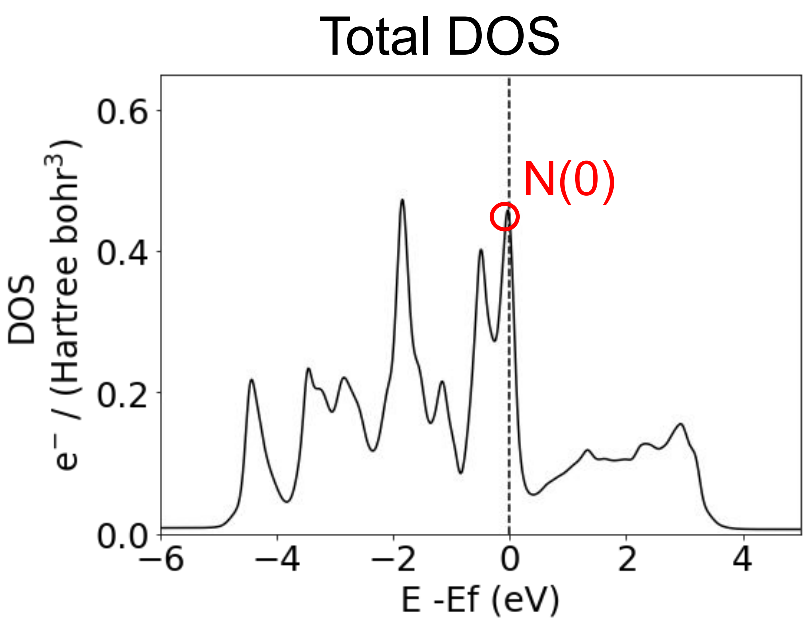
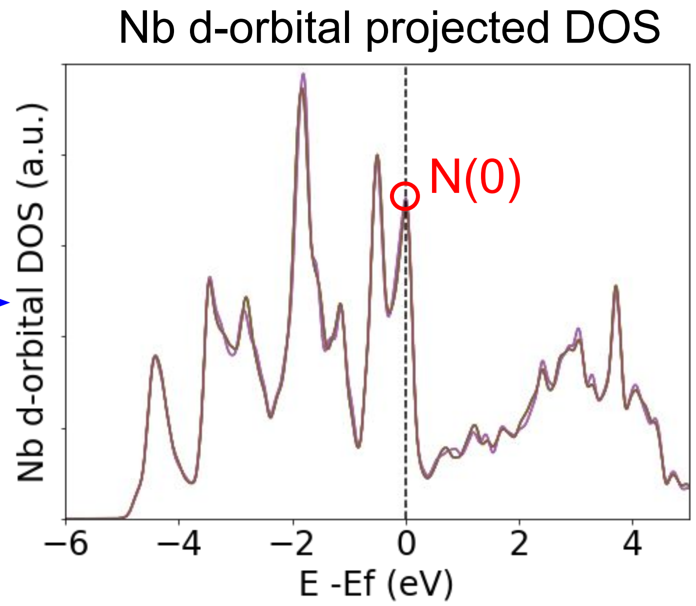


Total DOS projected onto d-orbitals of Nb atoms



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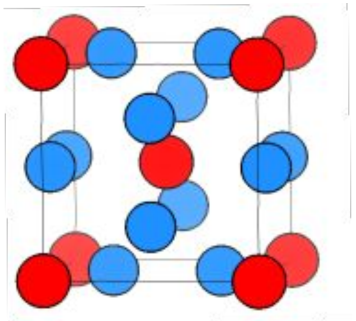

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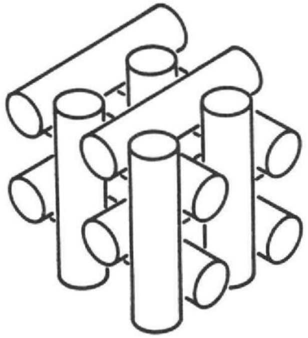

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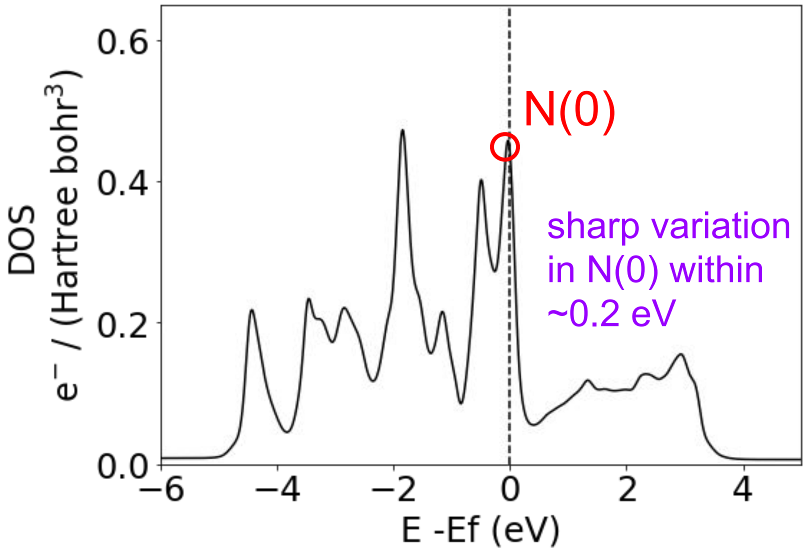

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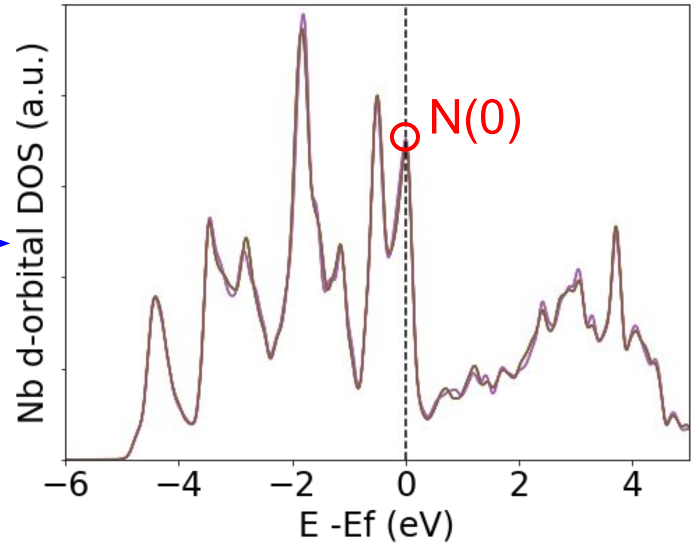
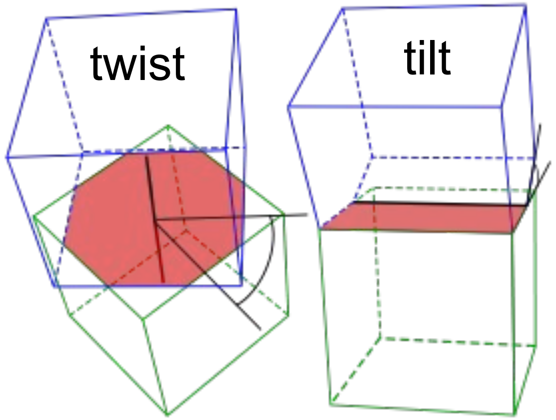
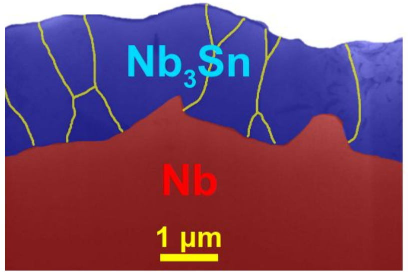
Nb d-orbital projected DOS



Grain boundaries in Nb_3Sn calculated with DFT





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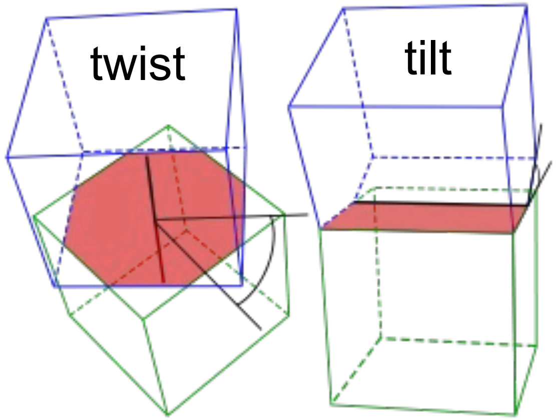

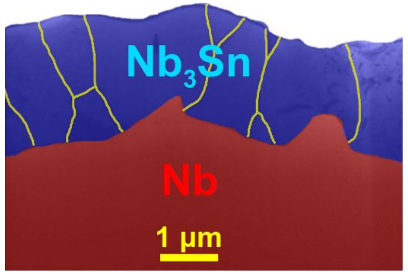

	# atoms	Grain separation (nm)	Grain boundary energy (mJ m^{-2})
(110)-tilt **(c)**	128	2.99	1455
(112)-tilt	192	2.59	840
(100)-twist	78	2.64	650
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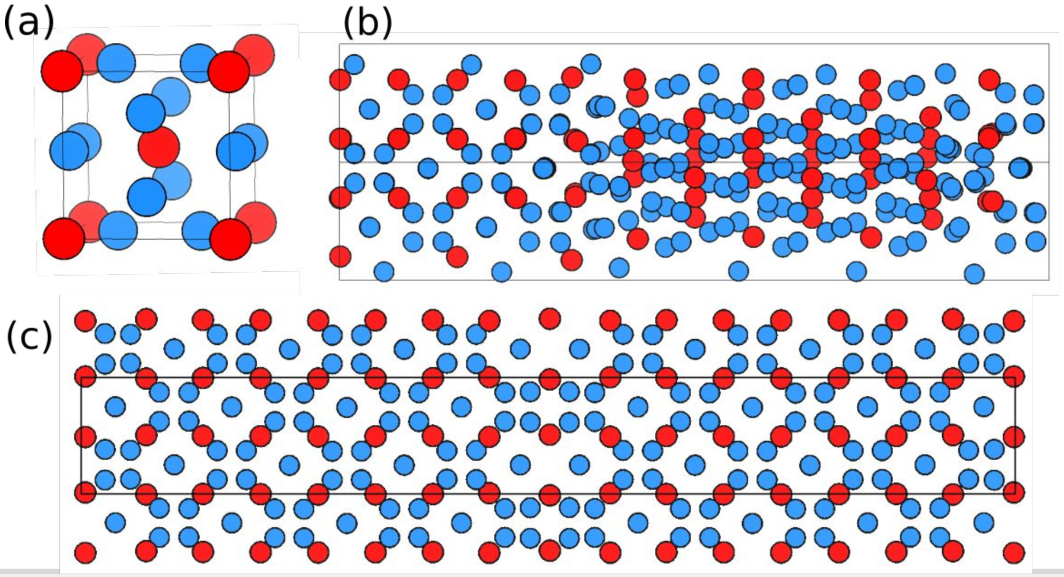

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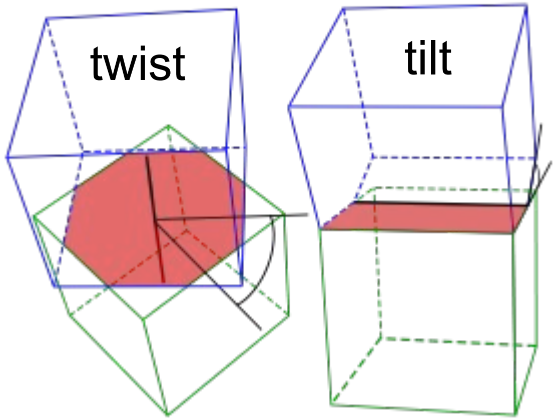

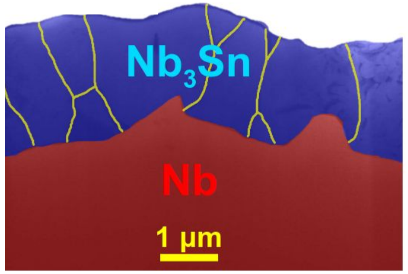

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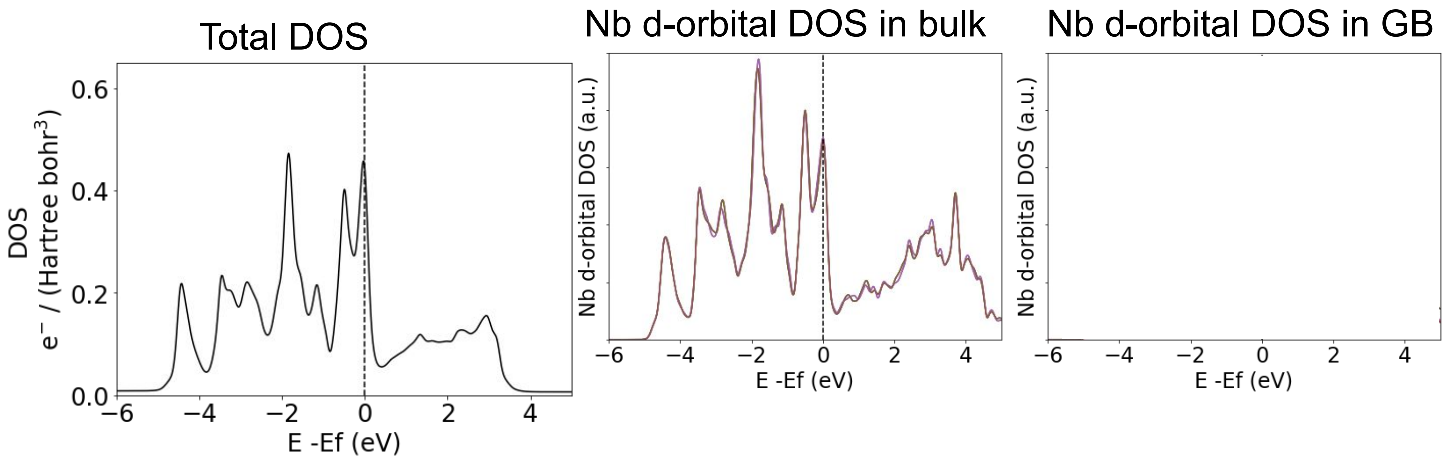

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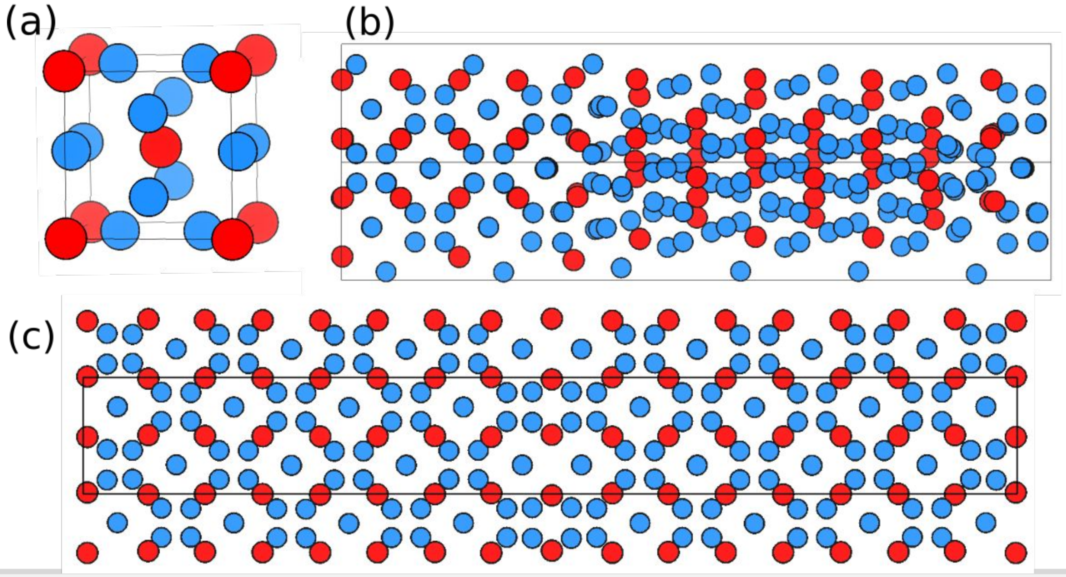

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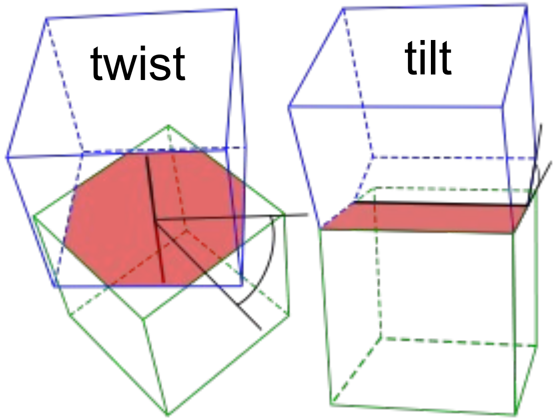
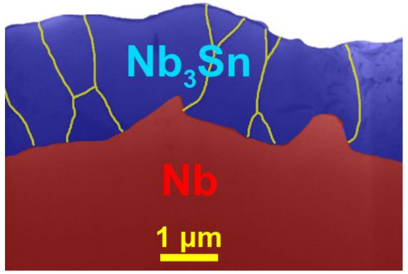
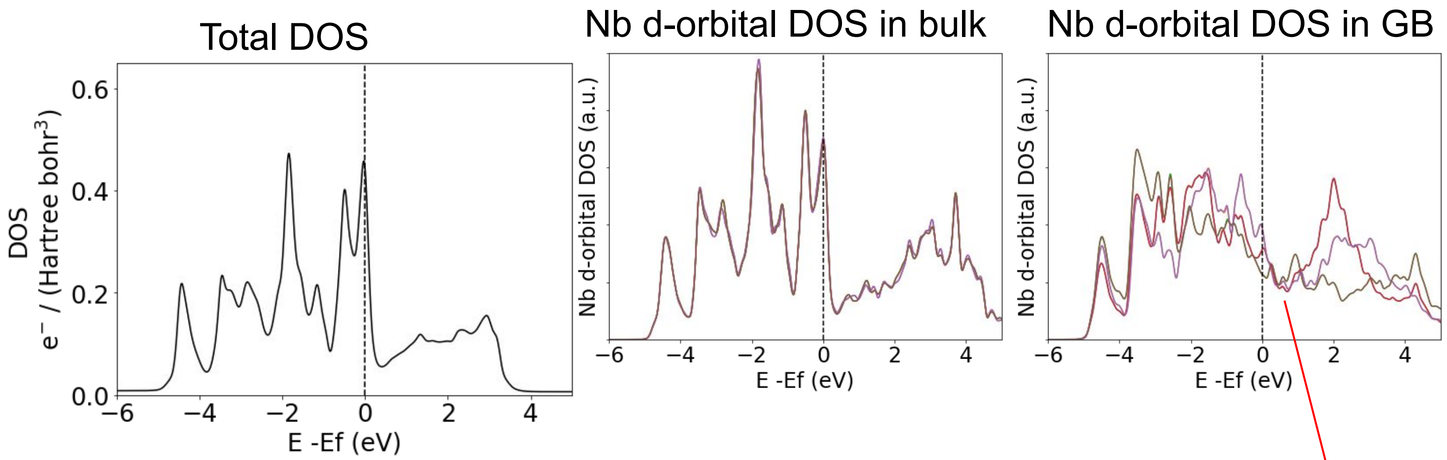
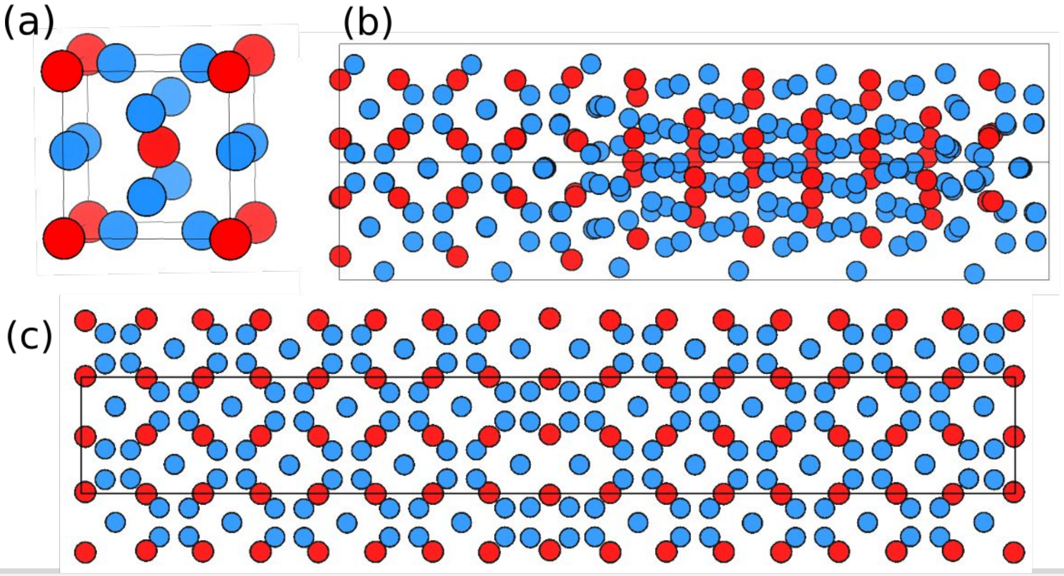




$$k_B T_c = 1.13 E_D \exp\left(-1/\left(N(0)V\right)\right)$$



	# atoms	Grain separation (nm)	Grain boundary energy (mJ m^{-2})
(110)-tilt **(c)**	128	2.99	1455
(112)-tilt	192	2.59	840
(100)-twist	78	2.64	650
(110)-twist **(b)**	288	2.24	1300
(120)-tilt	160	2.36	1440



GBs reduce N(0) by > a factor of 2!

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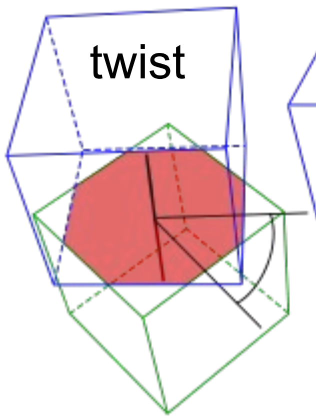

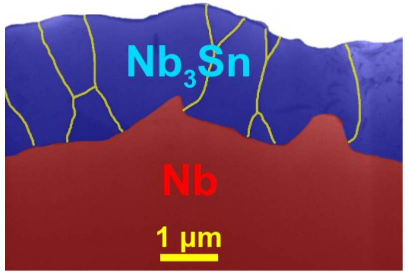

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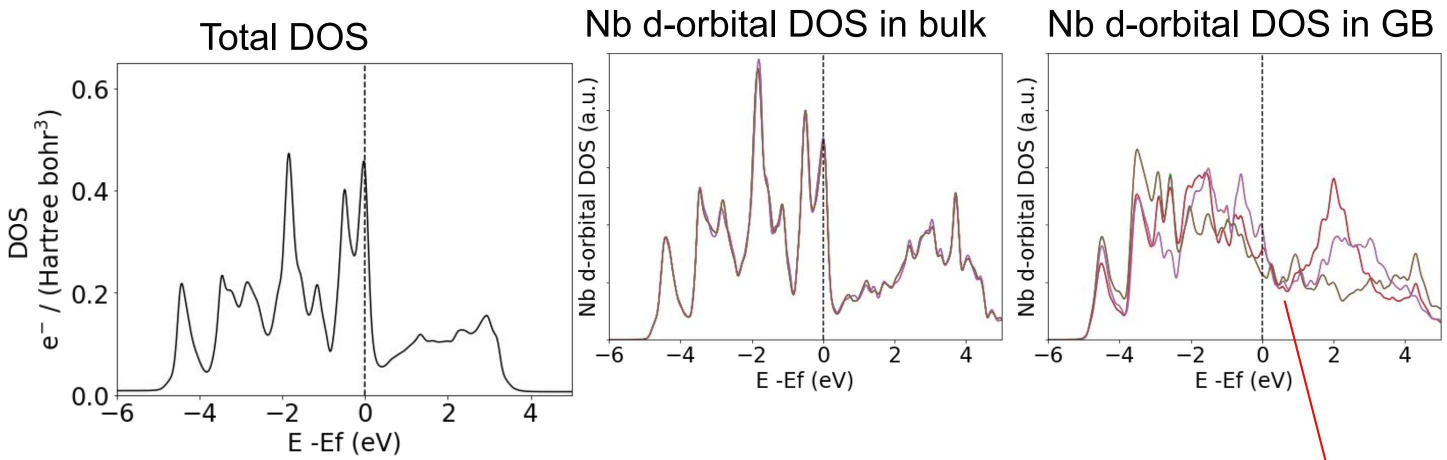

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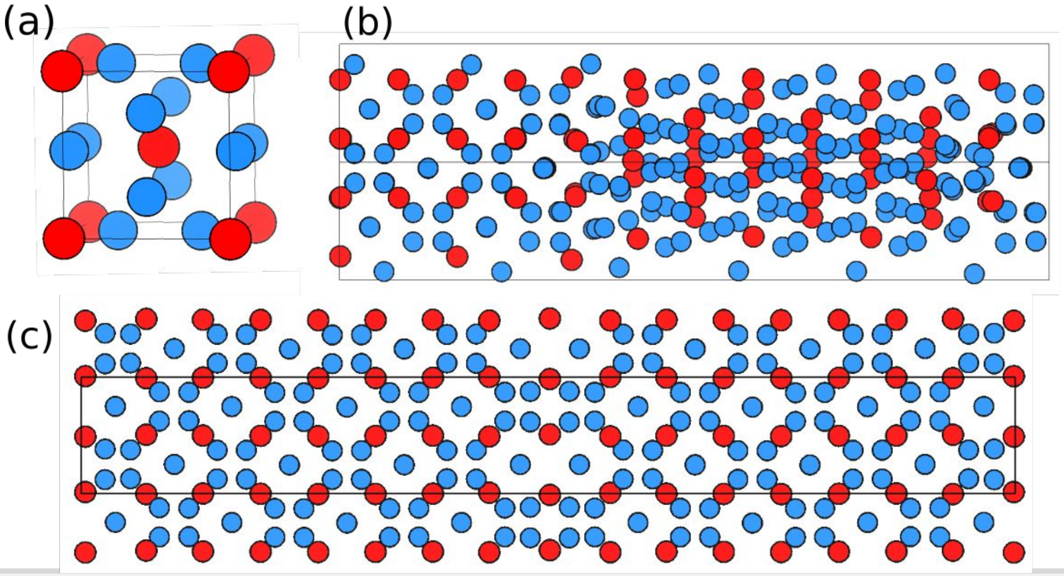


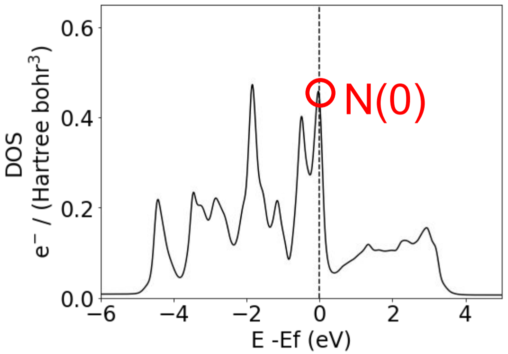
GBs reduce N(0) by > a factor of 2!

Global reduction?
Tc ≈ 18 K
→ Tc <10 K

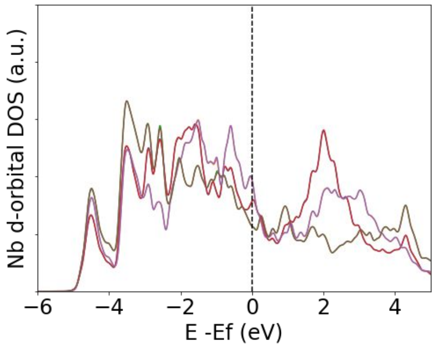
Local DOS vs distance from a “clean” GB

Global reduction in N(0) by > a factor of 2: Tc ≈ 18 K → Tc <10 K $k_B T_c = 1.13 E_D \exp\left(-1/\left(N(0)V\right)\right)$

Total DOS



Nb d-orbital DOS in GB



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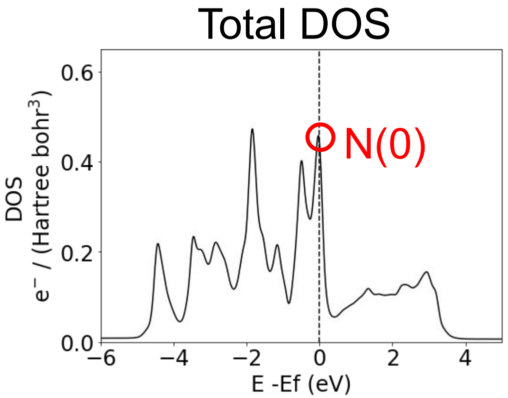

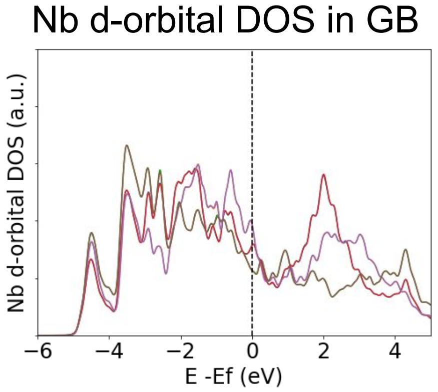

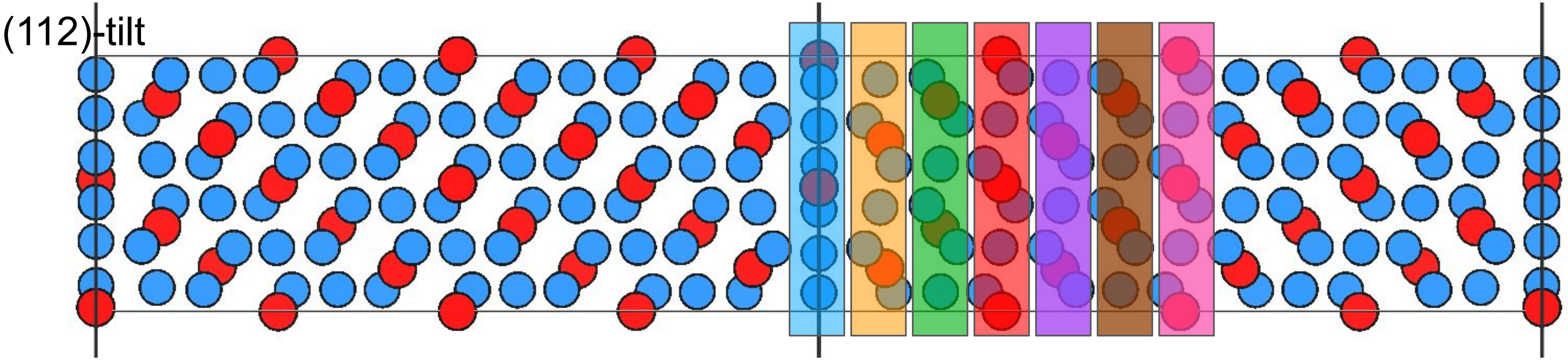

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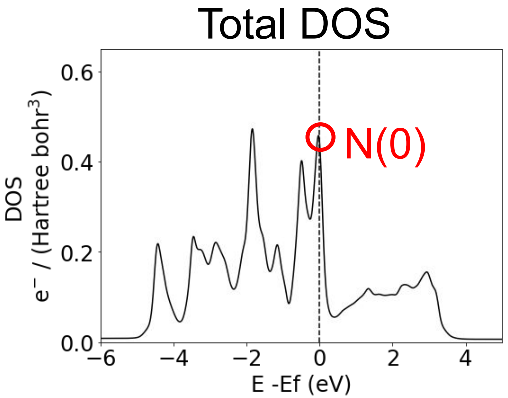

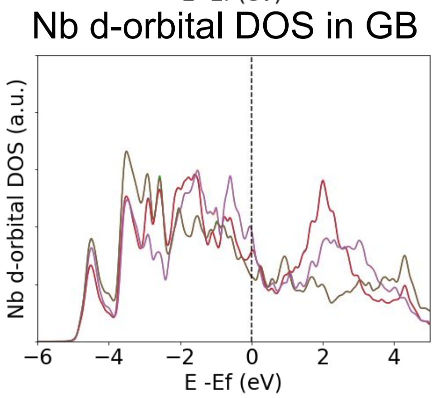

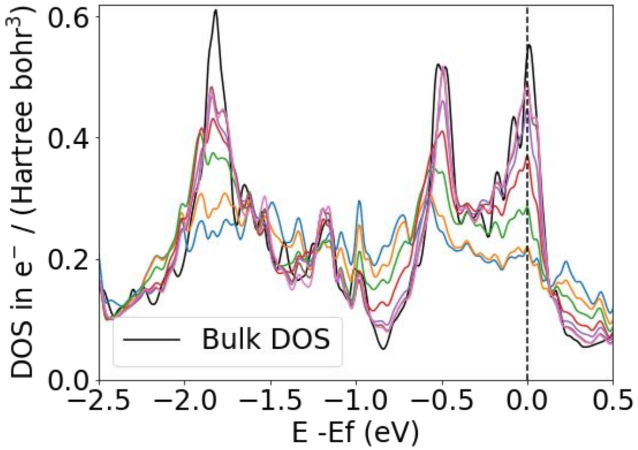

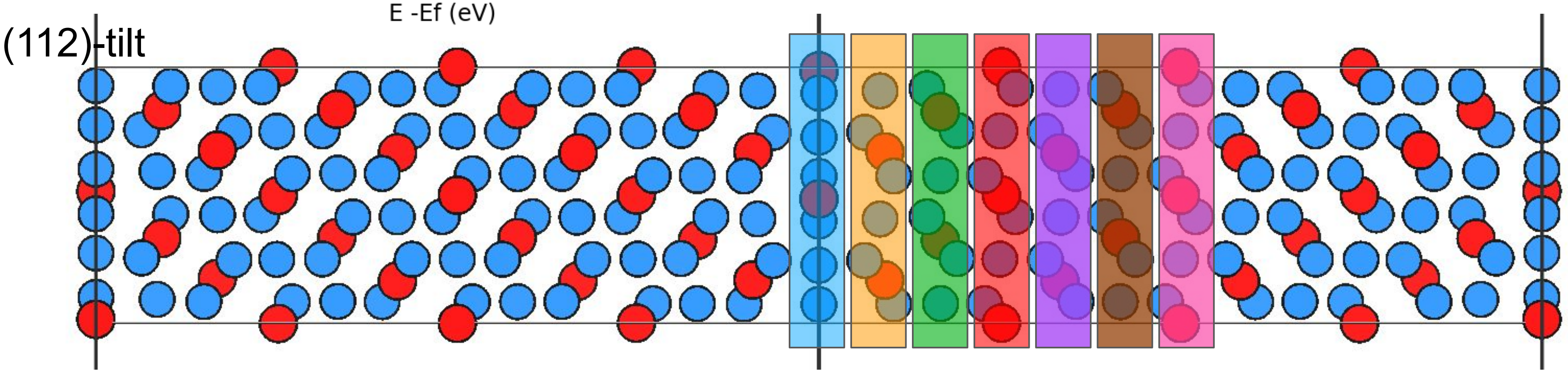

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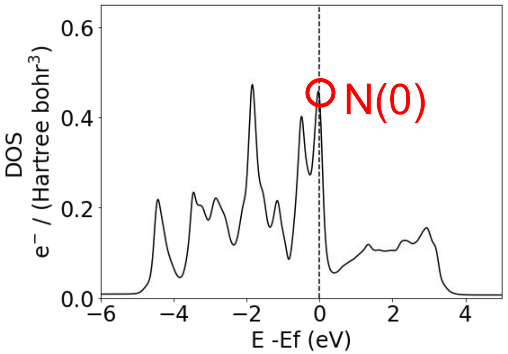

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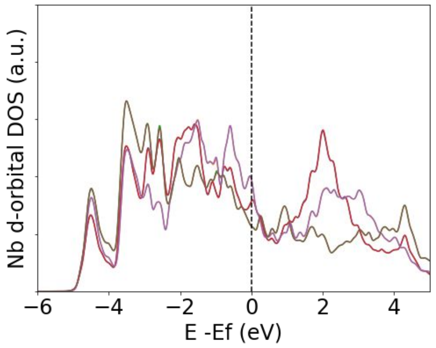
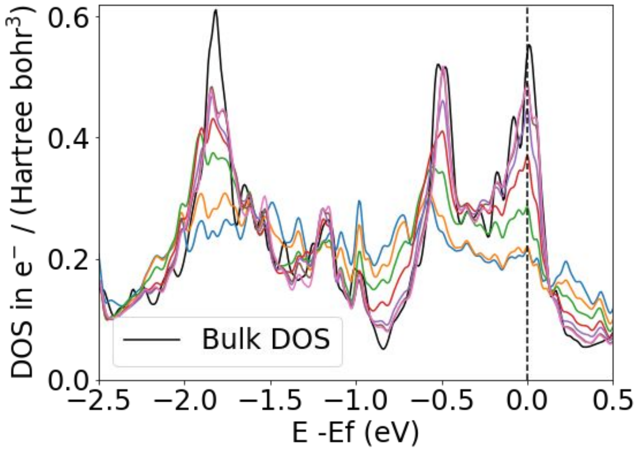
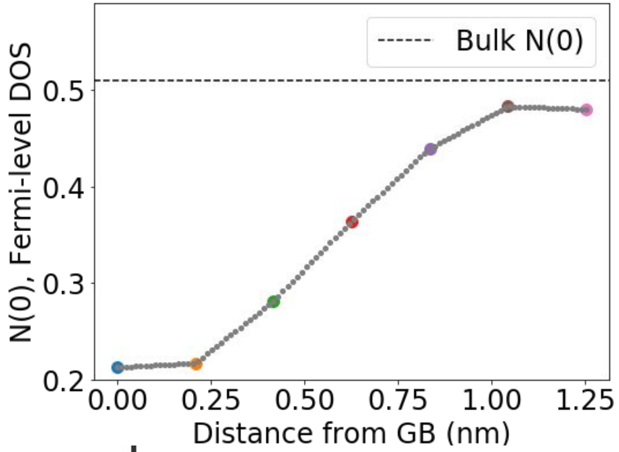
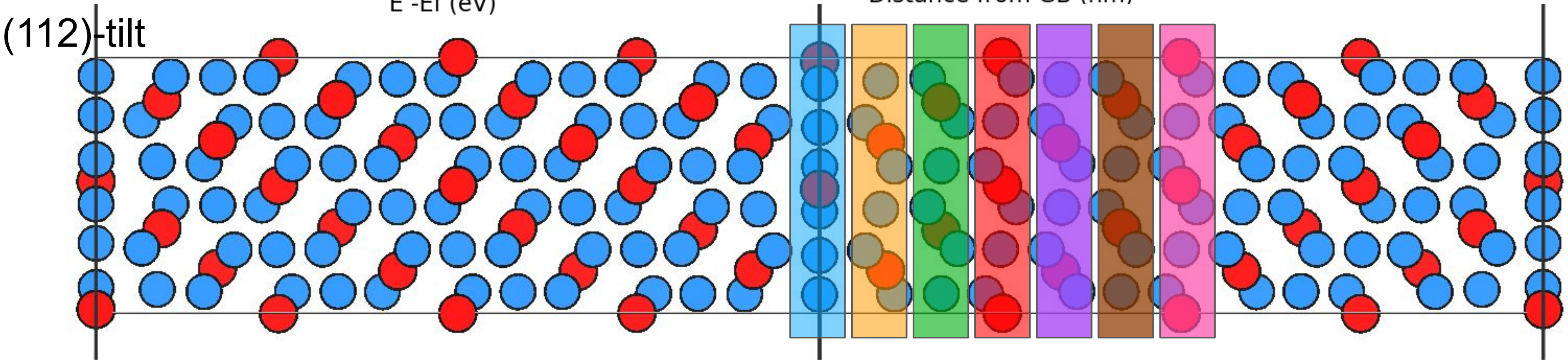






N(0) relaxes back to bulk in ~1-1.5 nm



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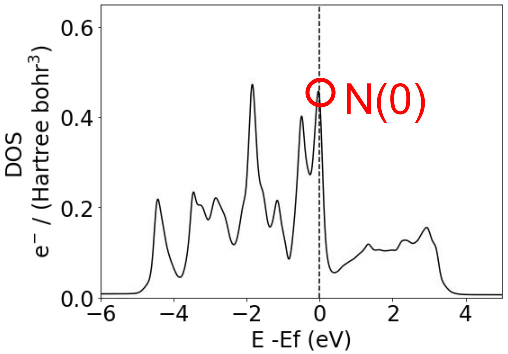

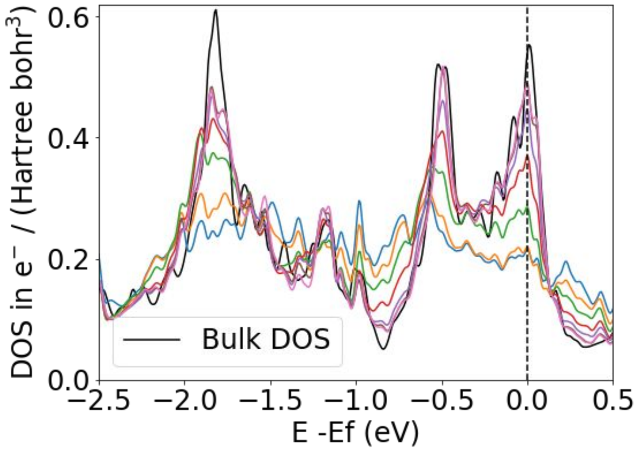

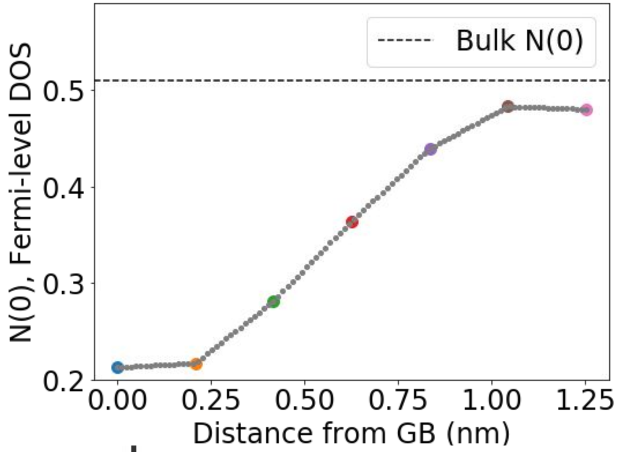

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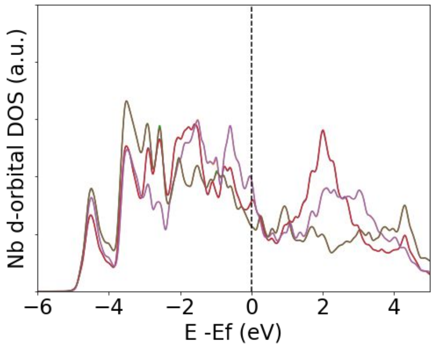
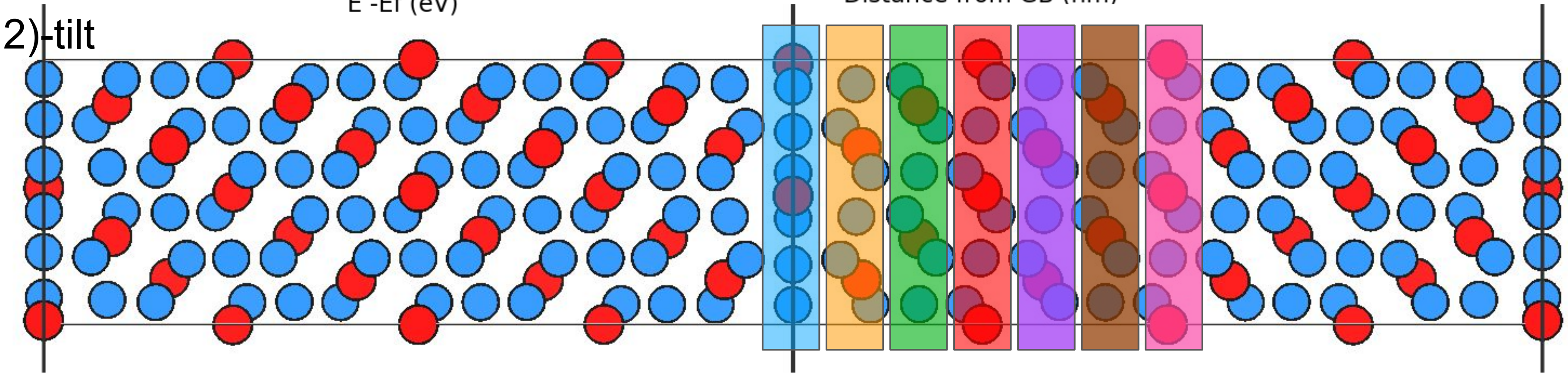
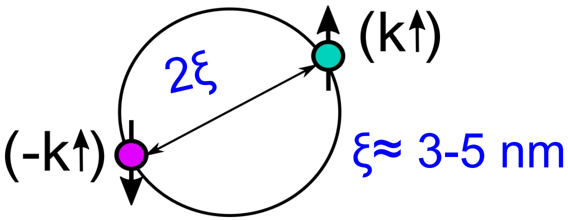


(112)-tilt





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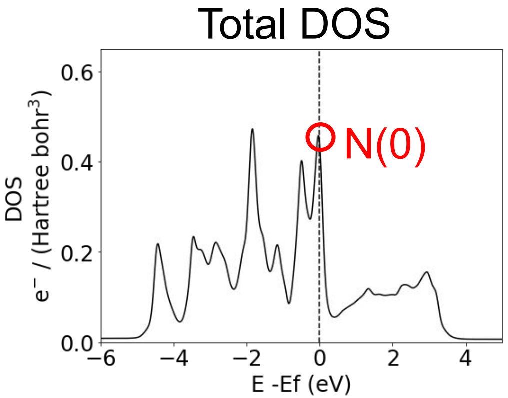

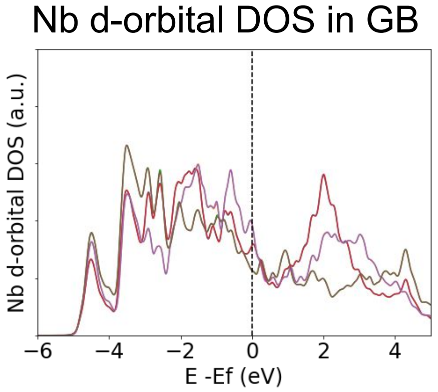

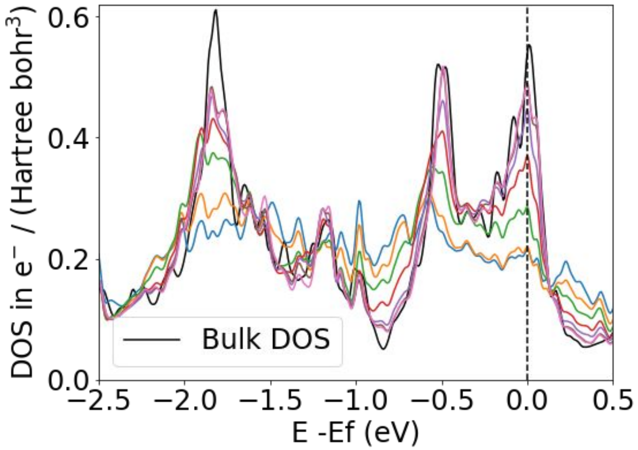

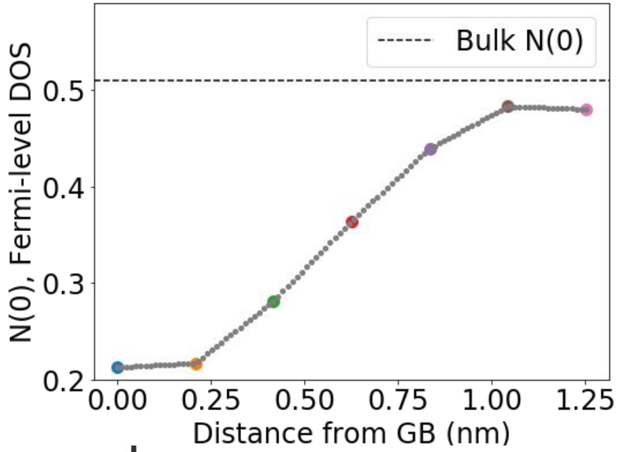

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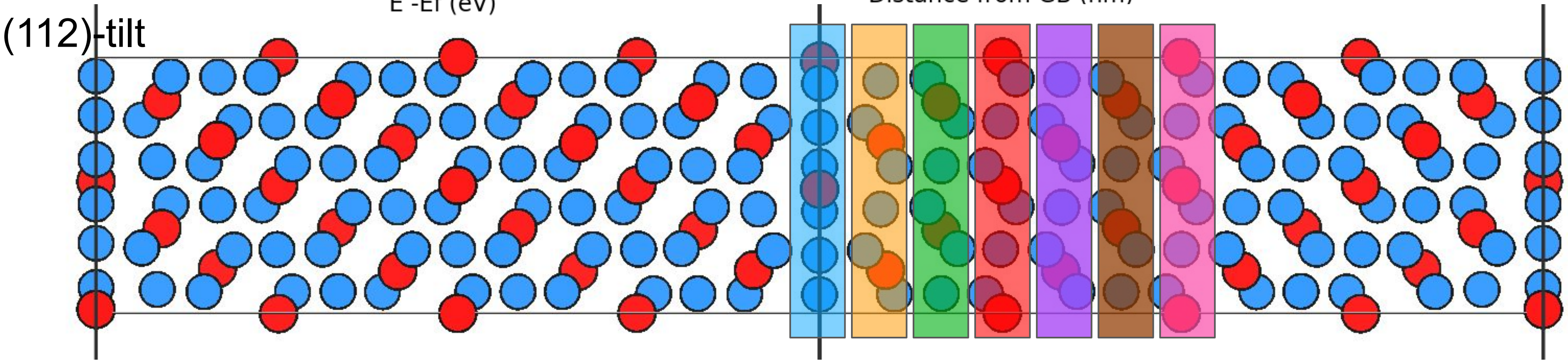
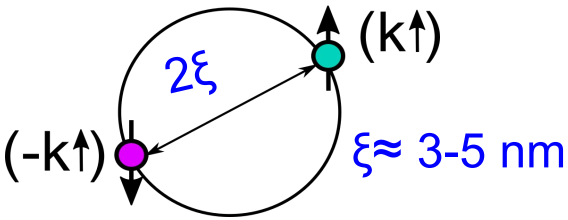
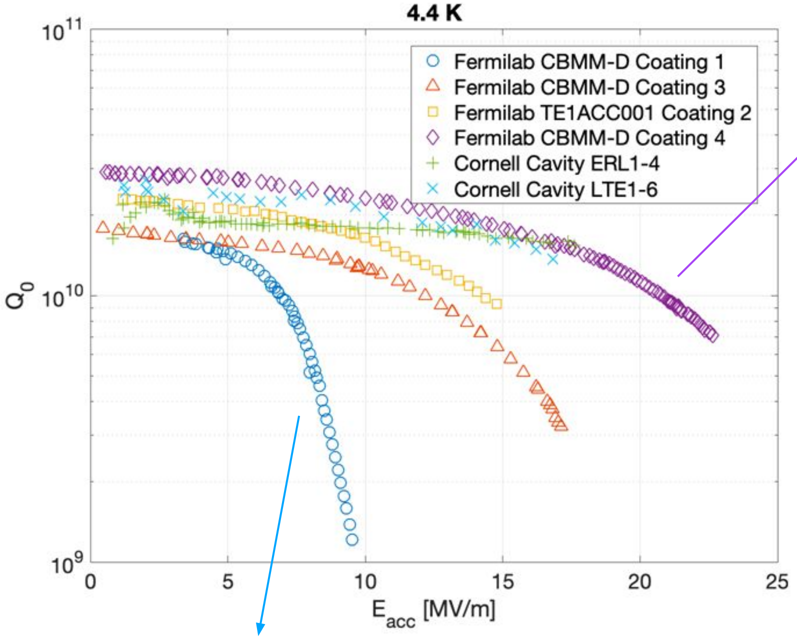




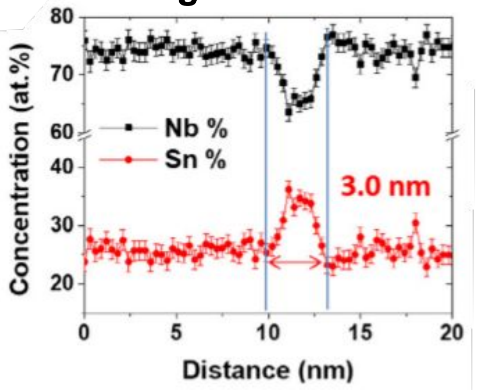
Cannot directly translate local N(0) into a local Tc since ~1-1.5 nm < ~3-5 nm
(Superconductors should not be sensitive to defects < ξ)

Tin antisite defect binding energies to GBs



Stable Q in cavities with **clean grain boundaries**

Degraded Q in cavities with **tin-rich grain boundaries**!



Lee et al. (2020) Acta Mat. 188, 1505

What causes tin to segregate towards GBs?

Tin antisite defect study

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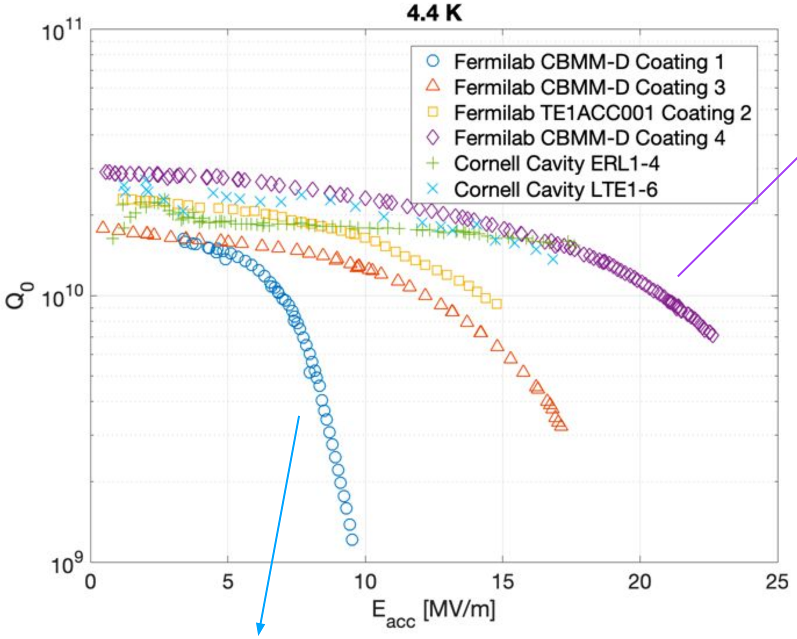

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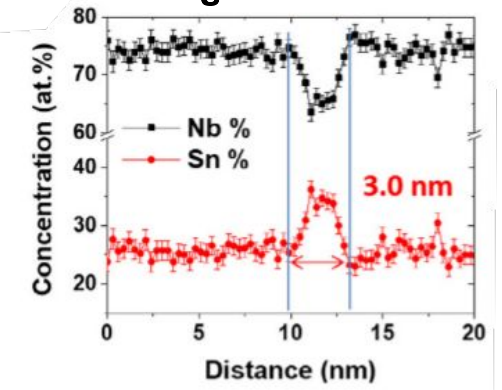

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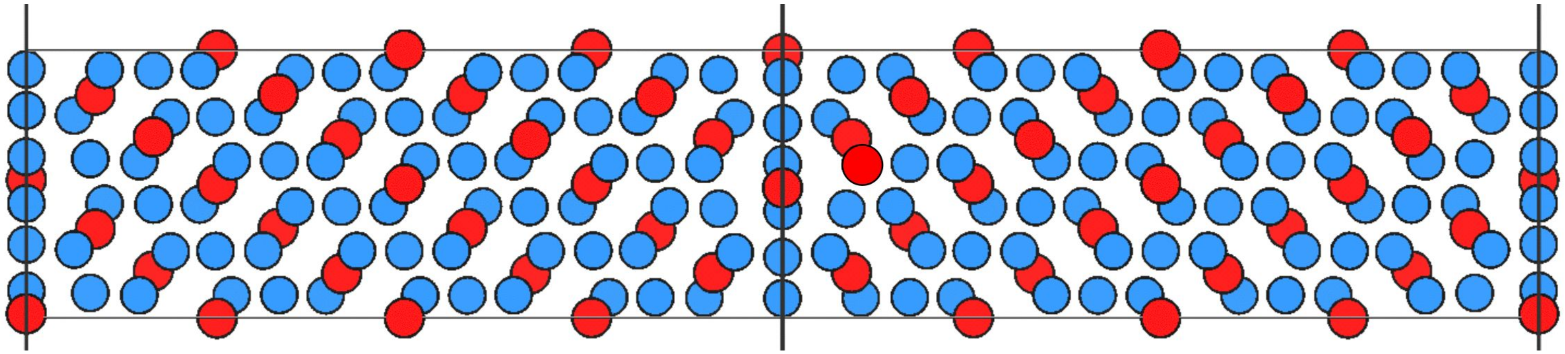
Tin antisite defect study

(112)-tilt



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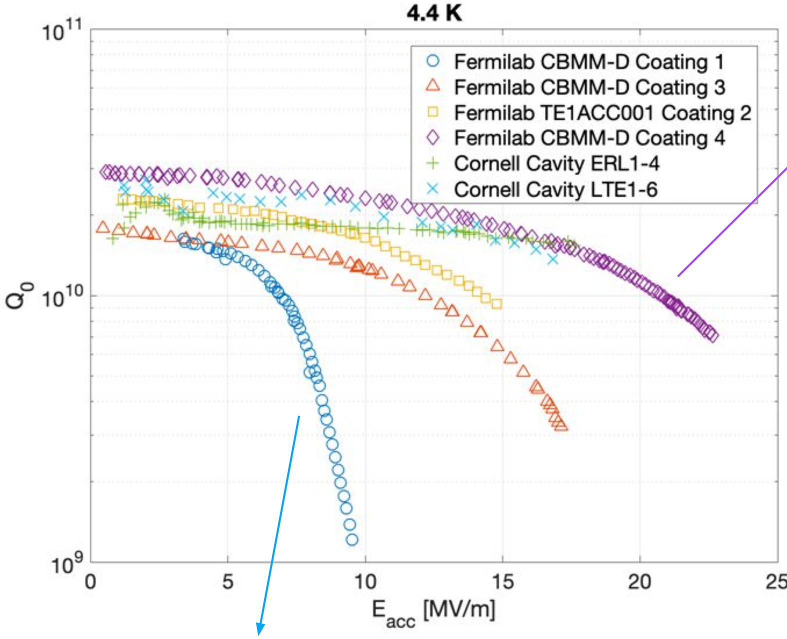

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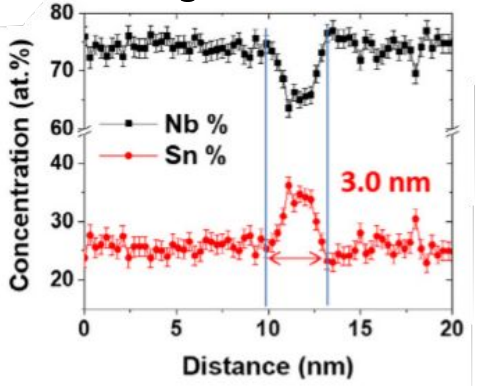

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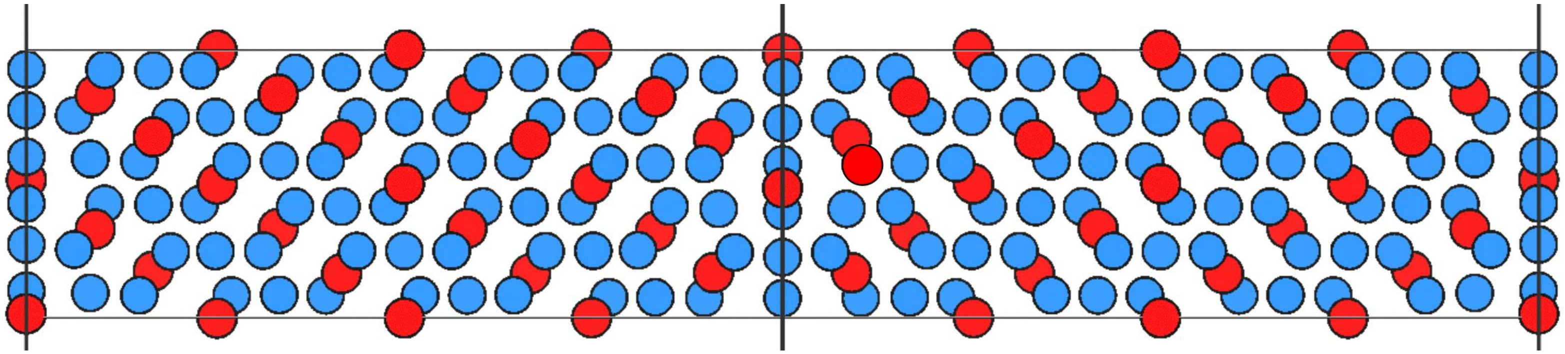

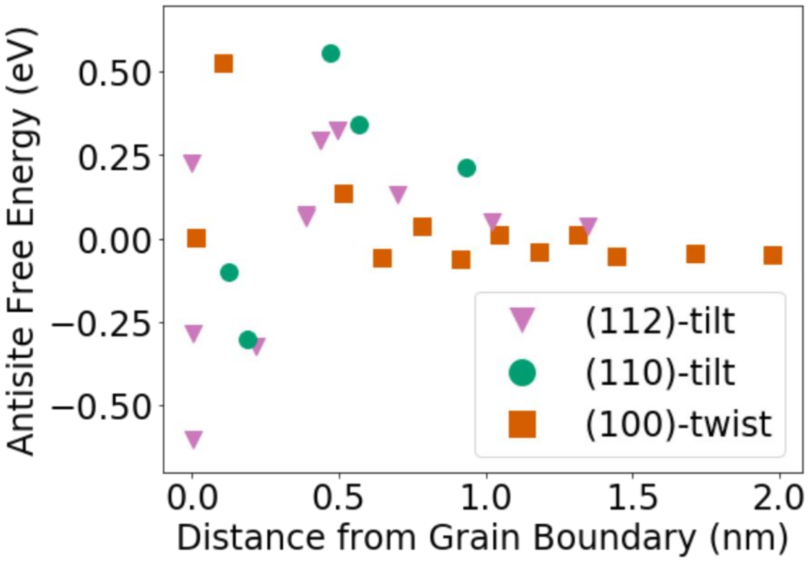

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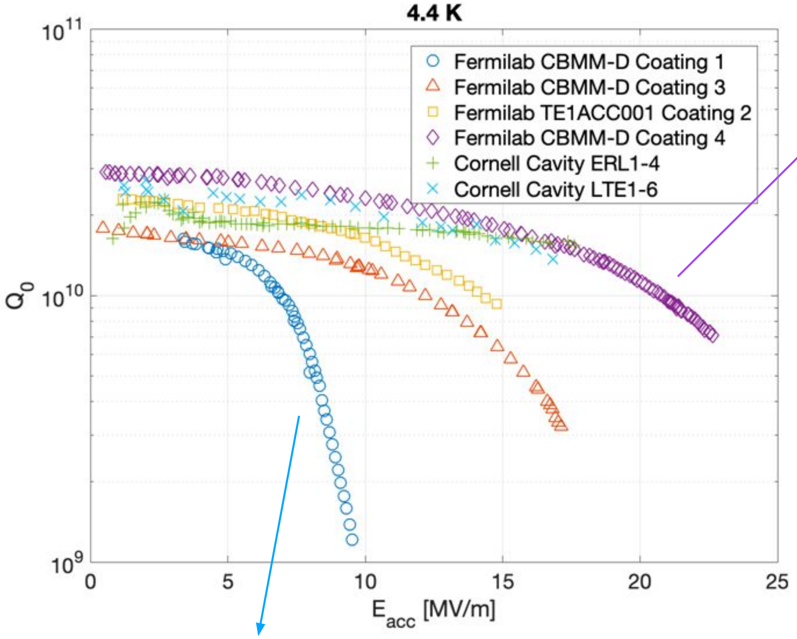

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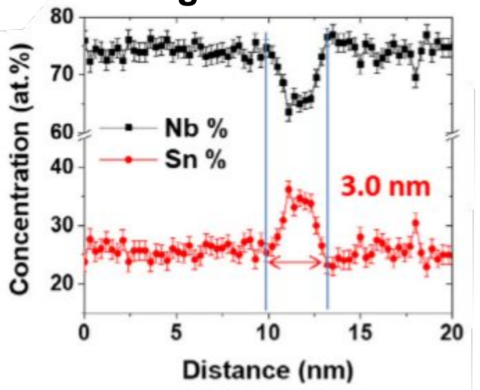

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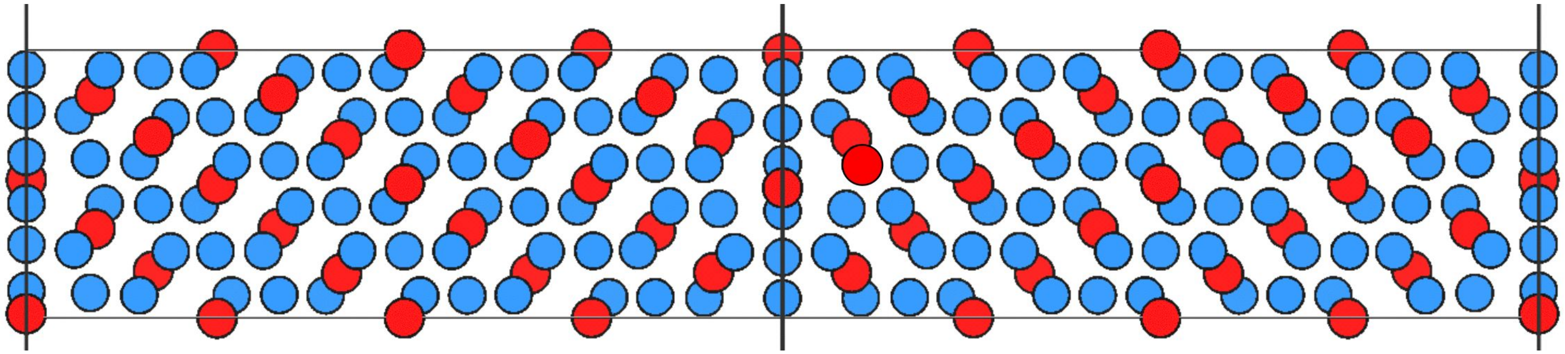
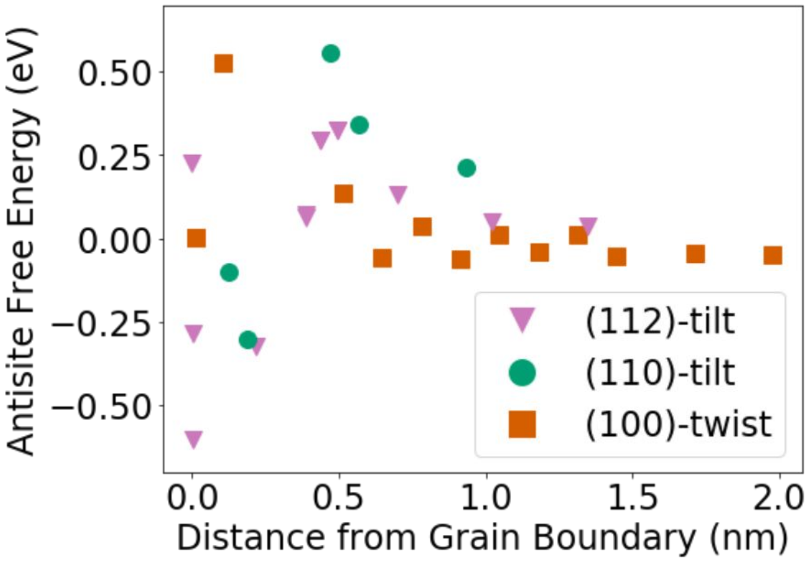
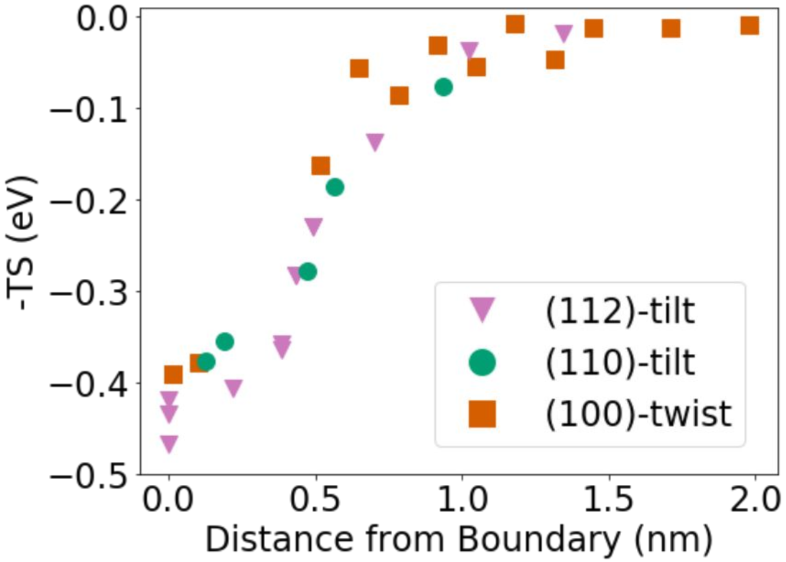
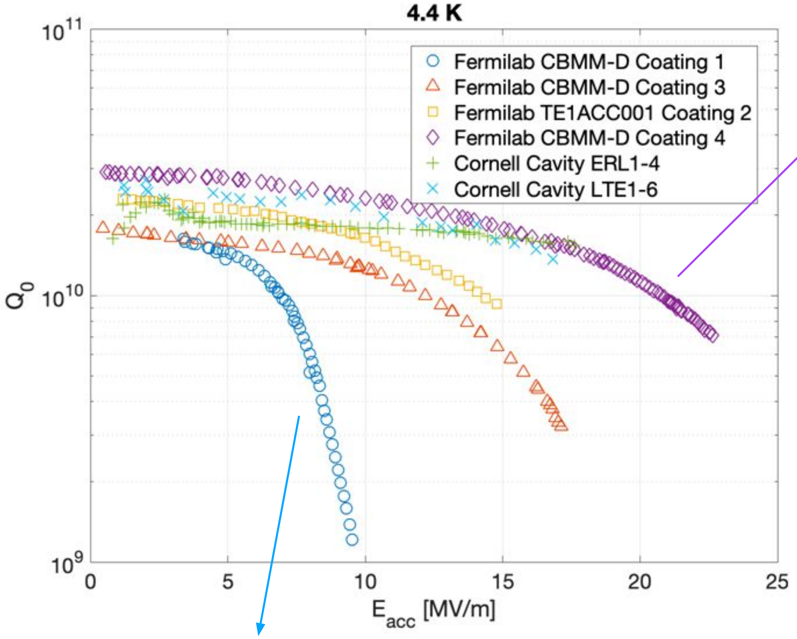






Model for local Tc with GB composition



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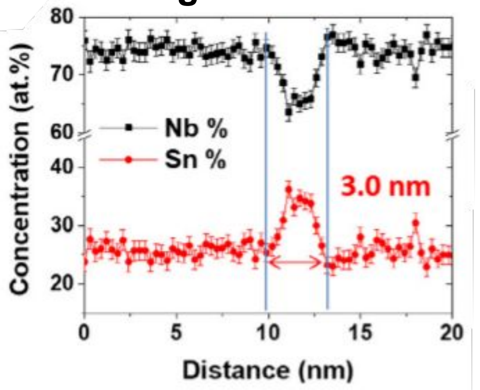

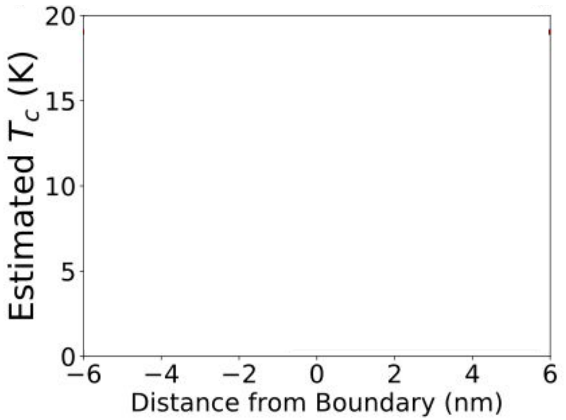

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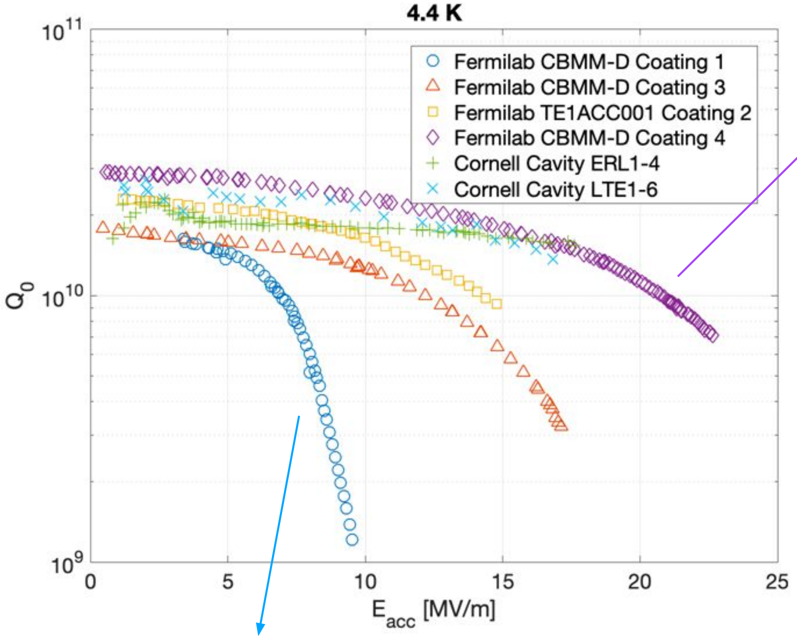

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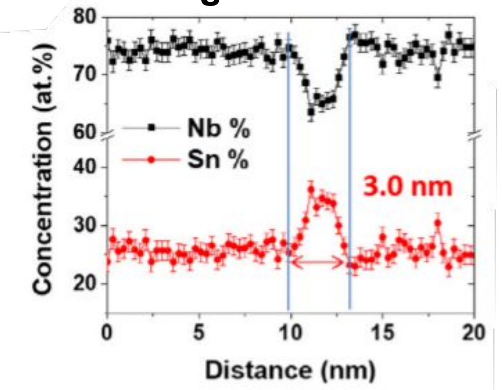
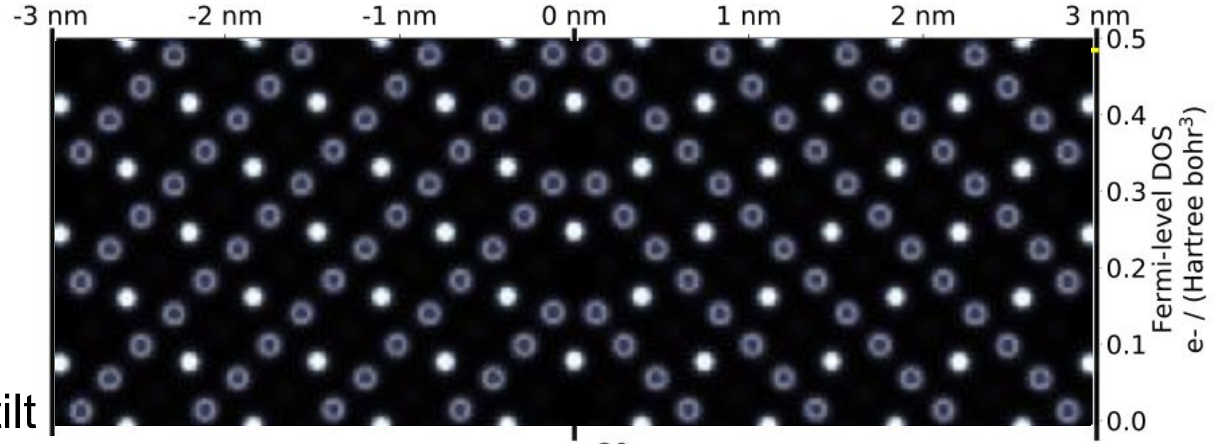
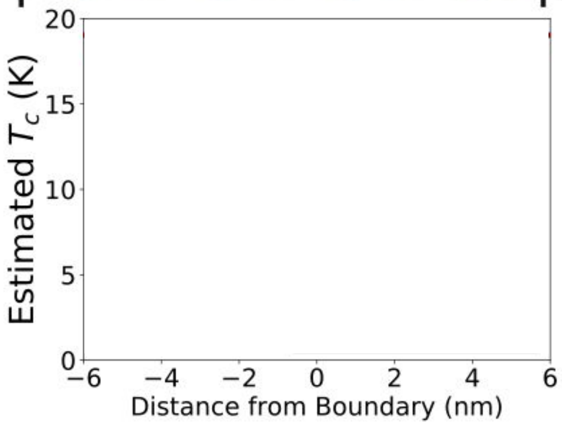


(110)-tilt





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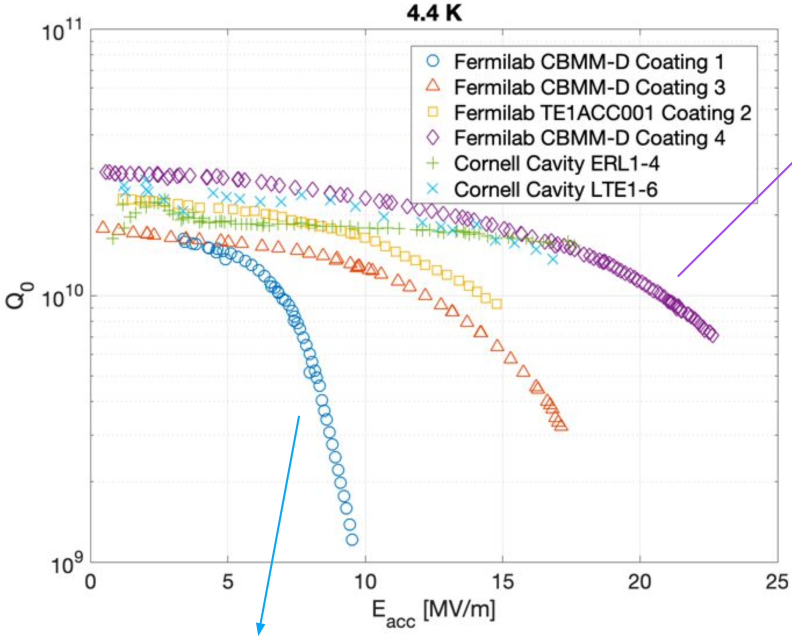

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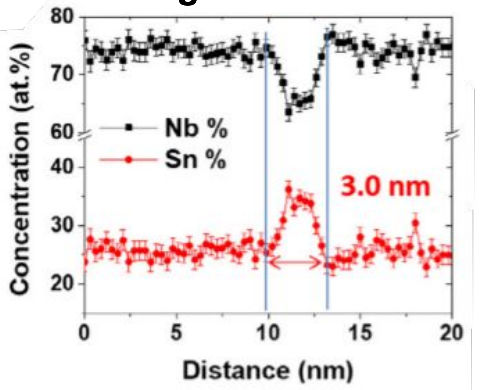

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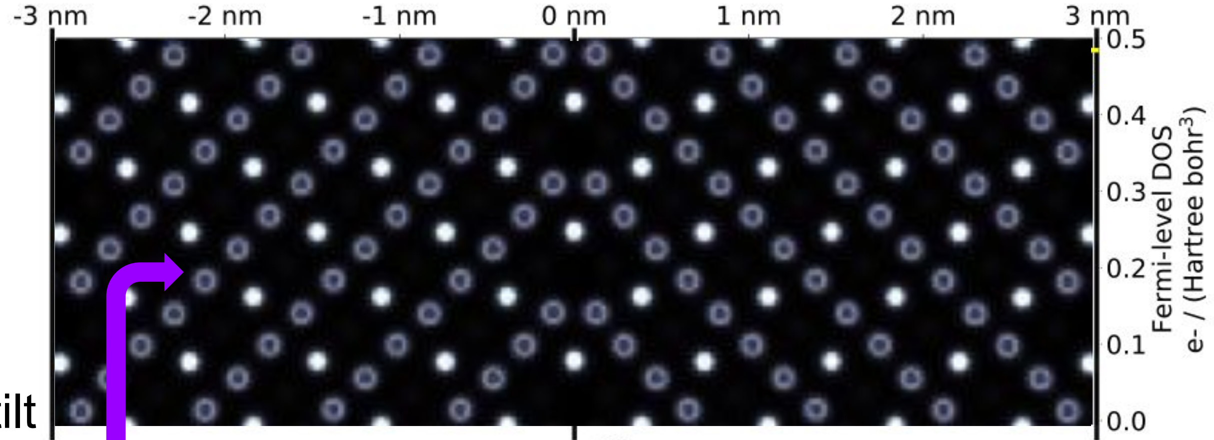

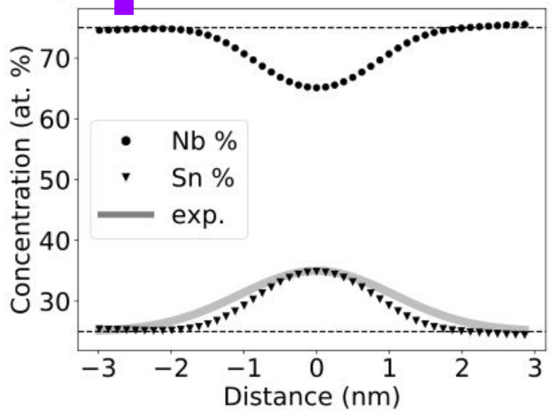

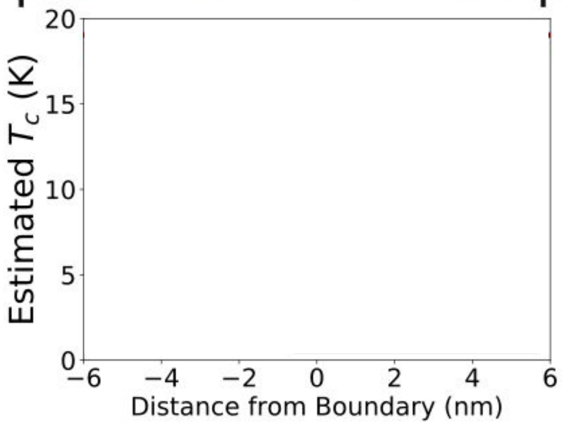

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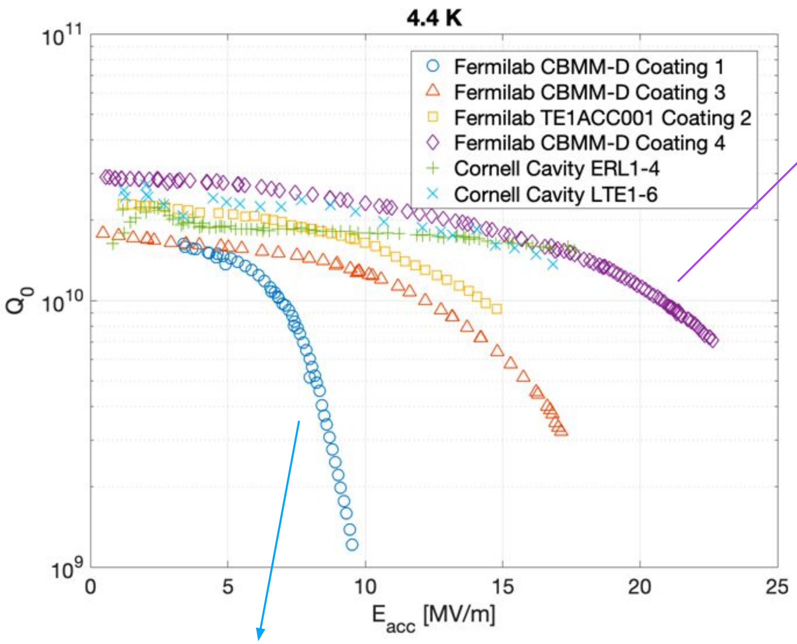

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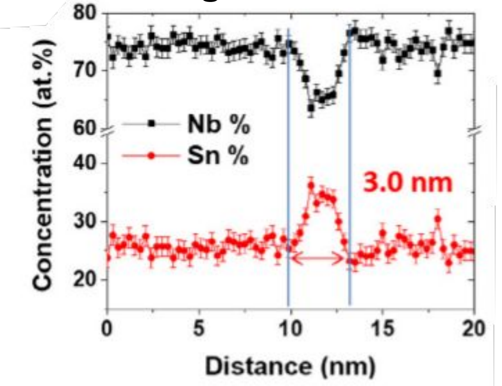

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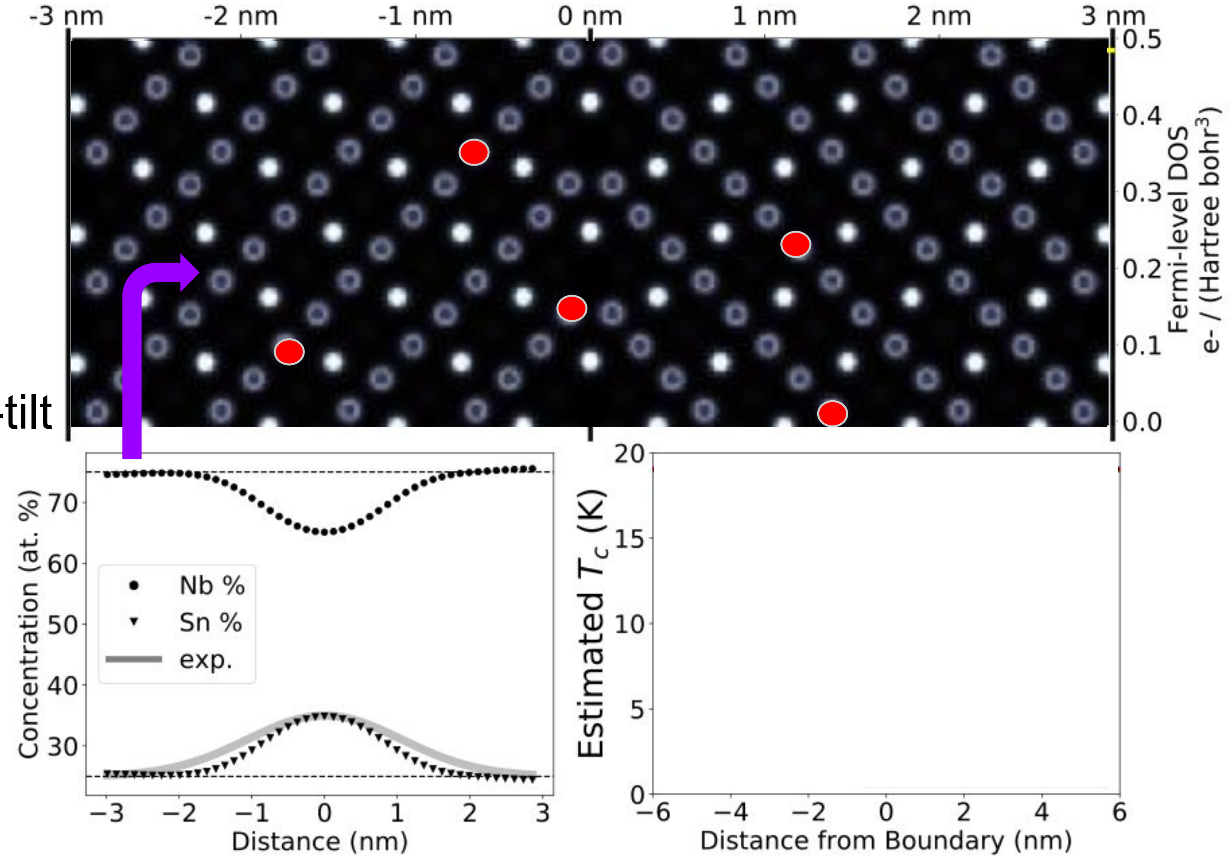

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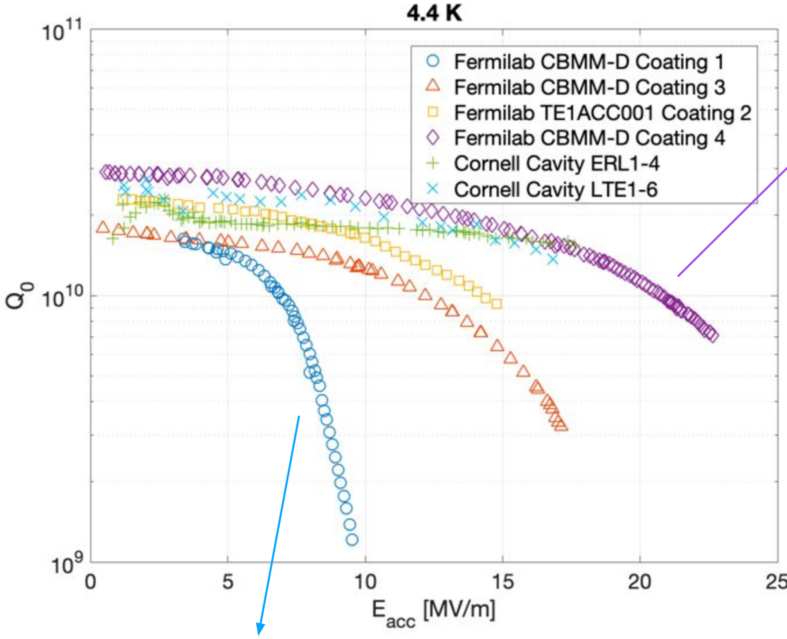
Model for local Tc with GB composition



Stable *Q* in cavities with **clean grain boundaries**

$$k_{\mathrm{B}} T_{\mathrm{c}} = 1.13 E_{\mathrm{D}} \exp\left(-1/\left(N(0)V\right)\right)$$

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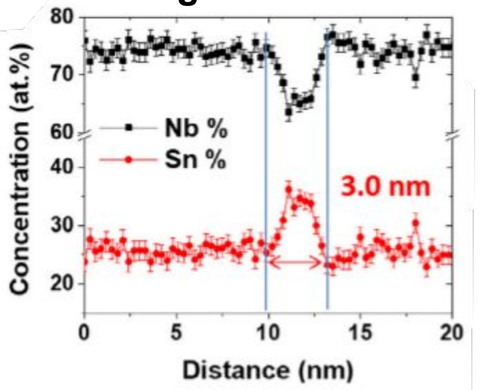

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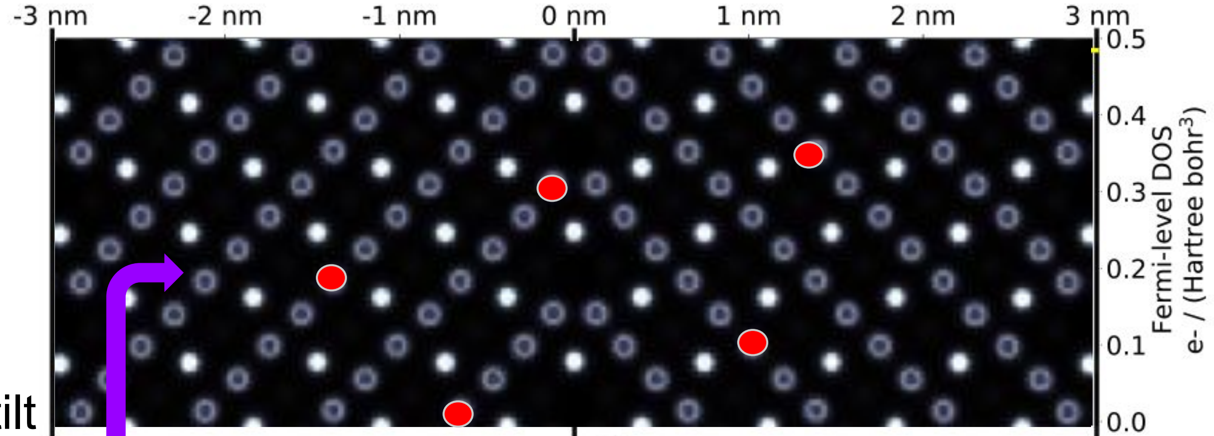

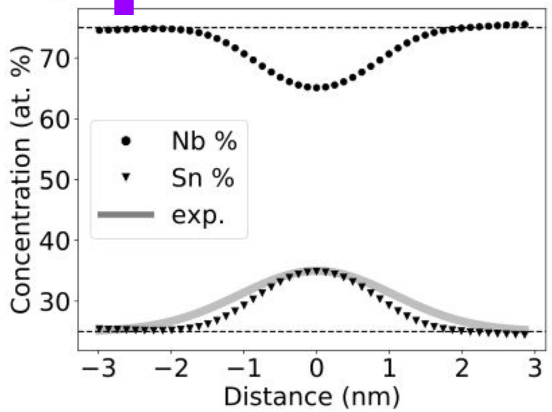

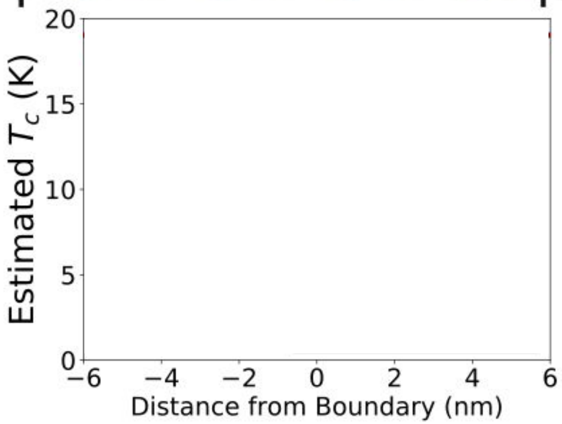

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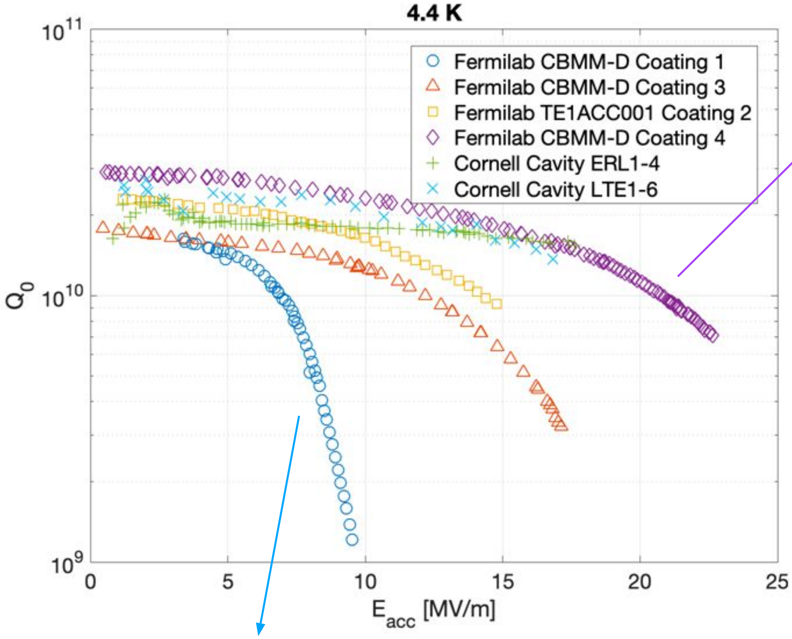

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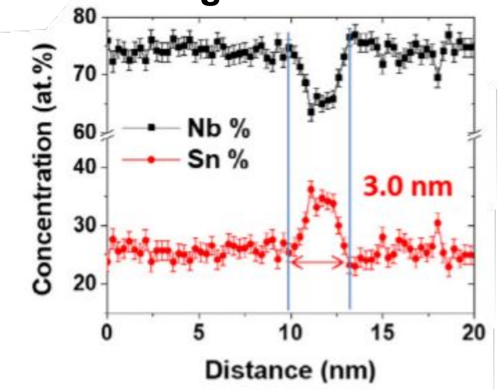

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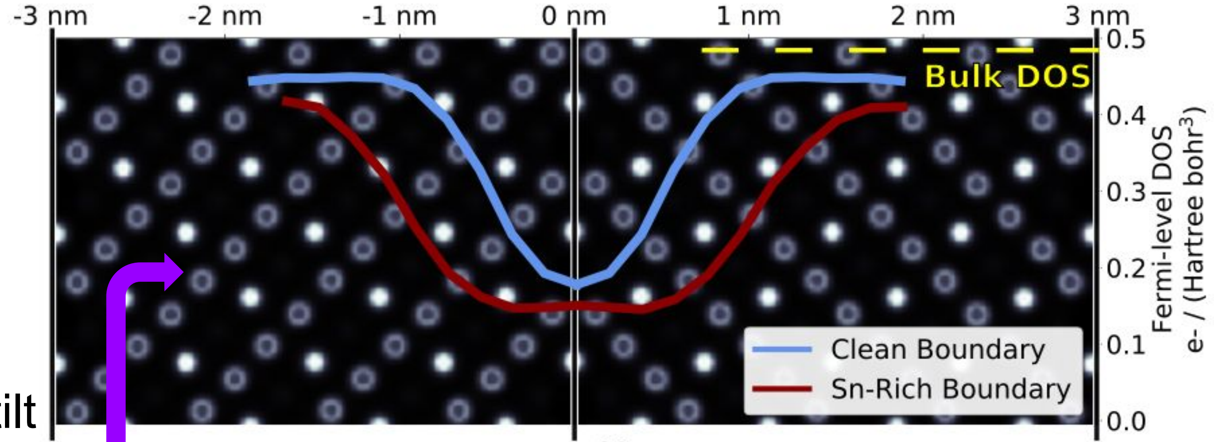

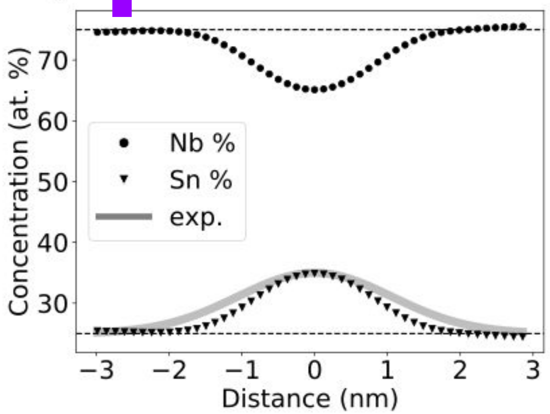

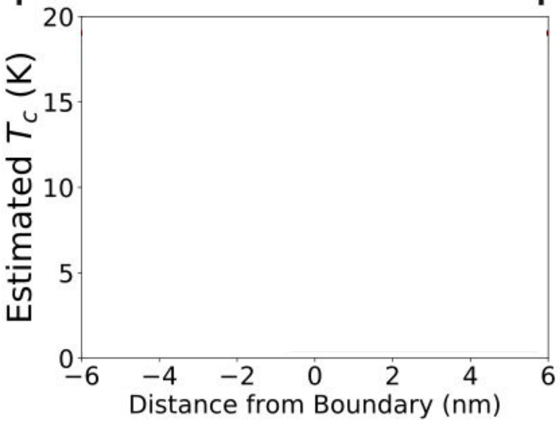

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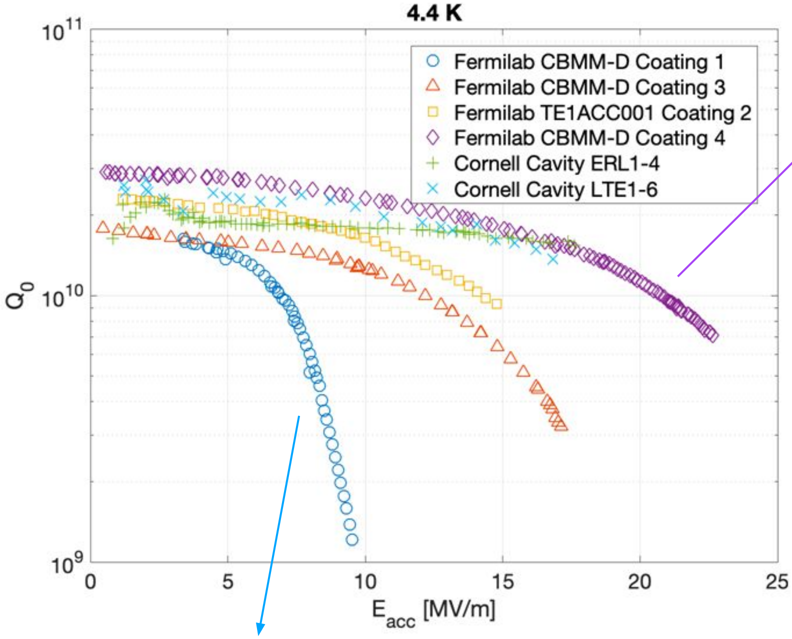

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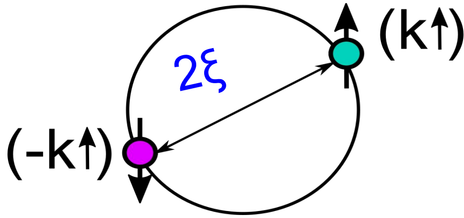
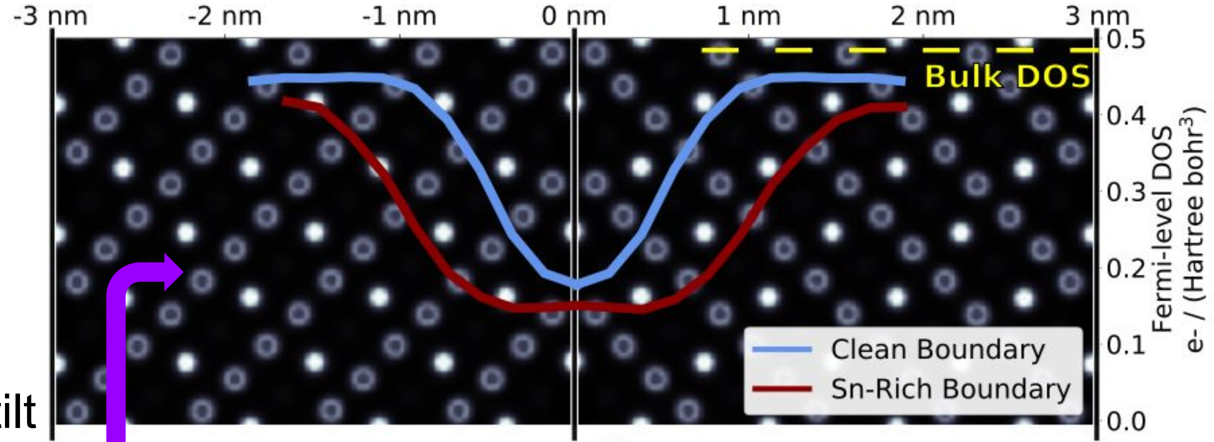


ξ≈ 3-5 nm



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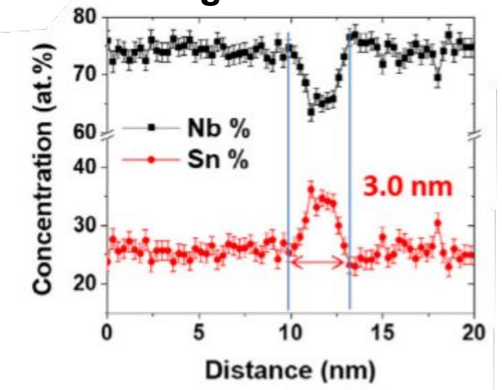

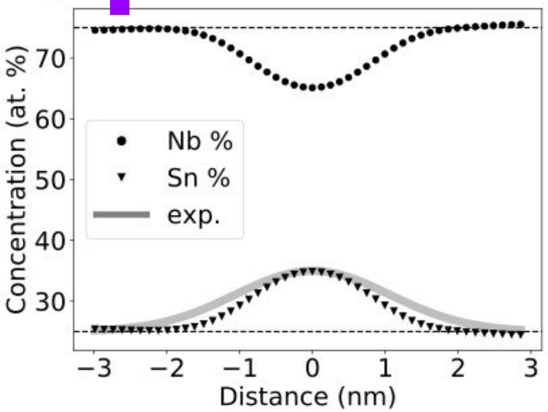

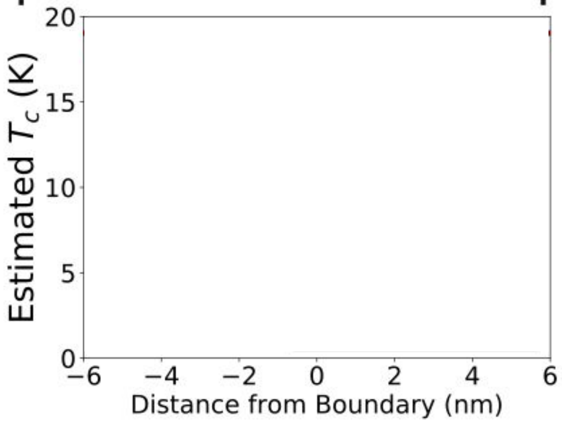

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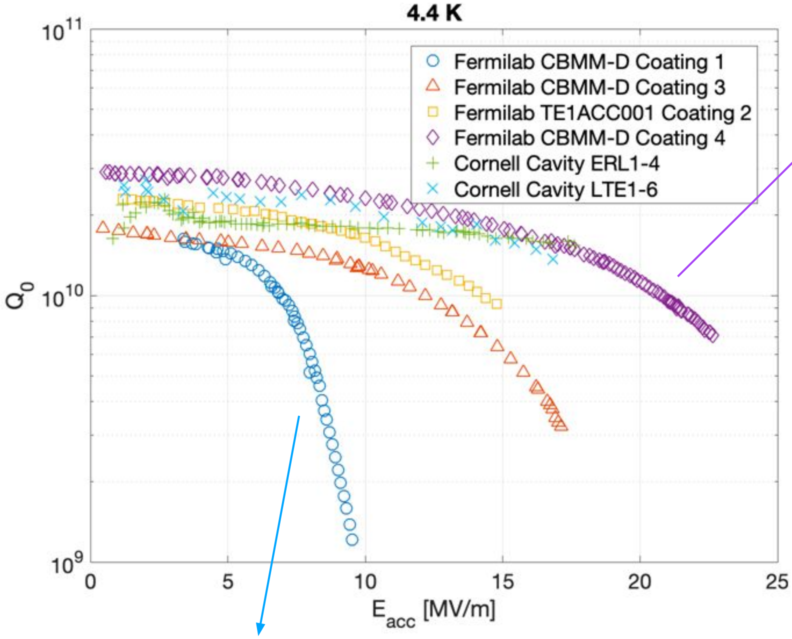

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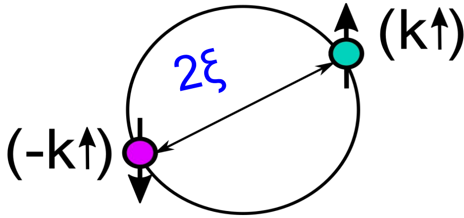

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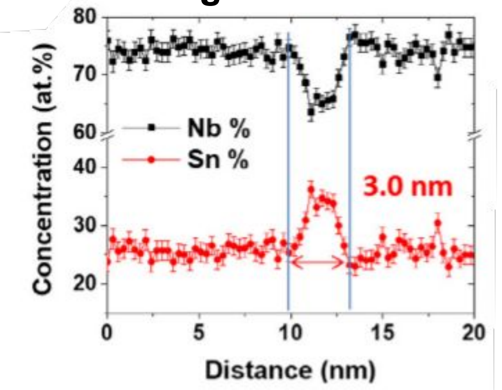

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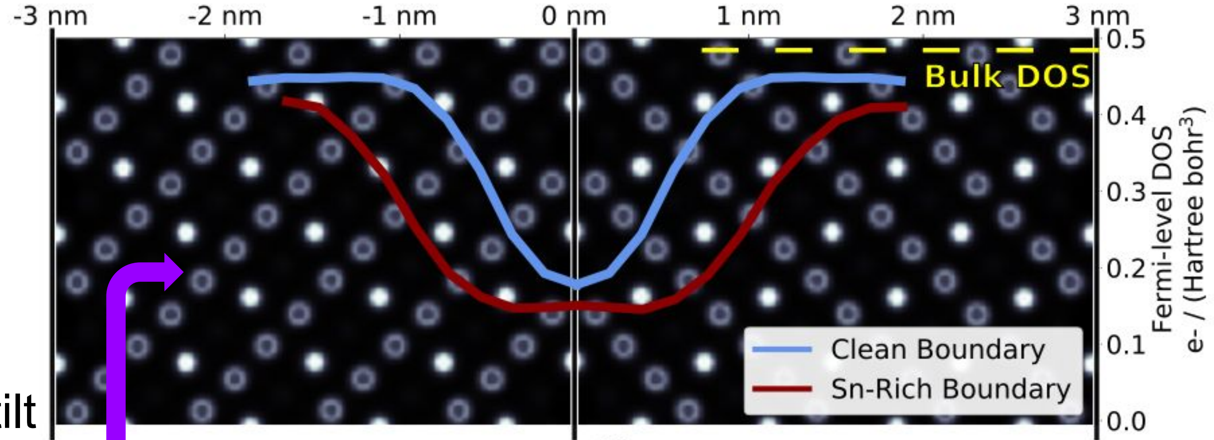

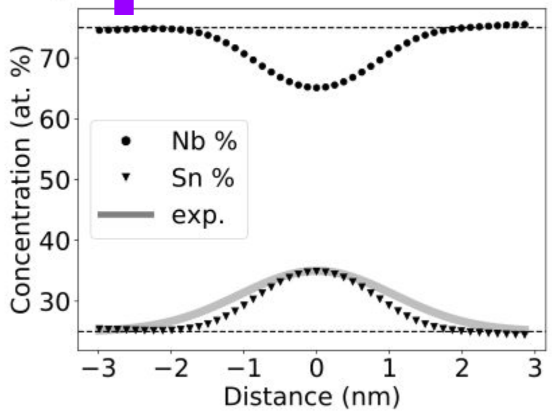

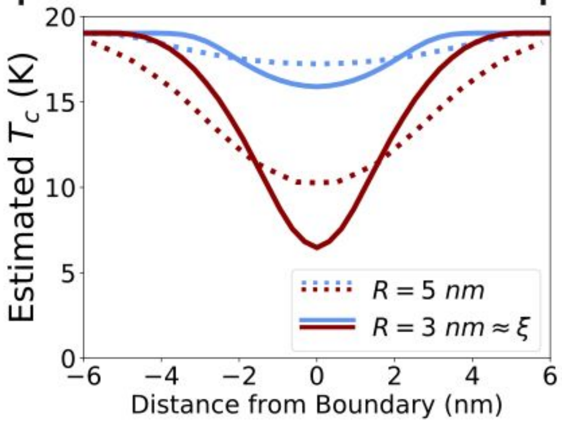

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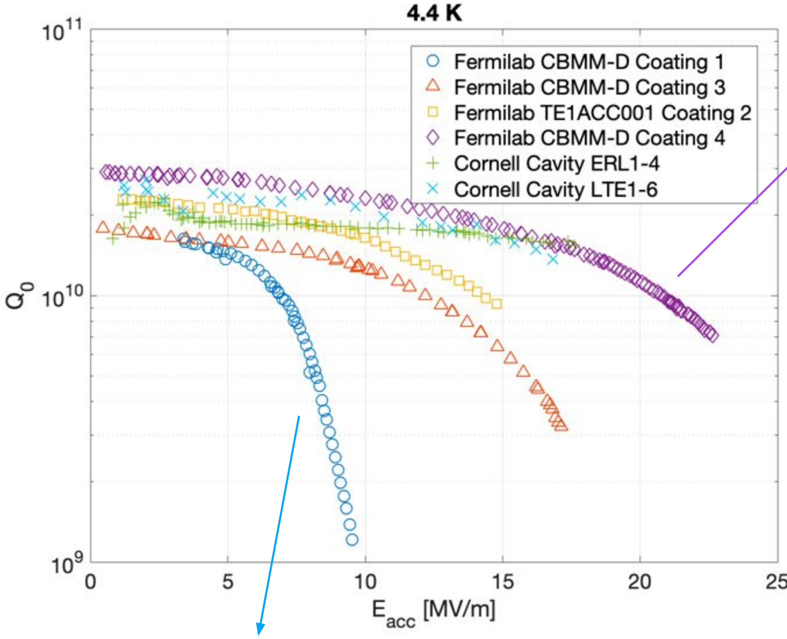

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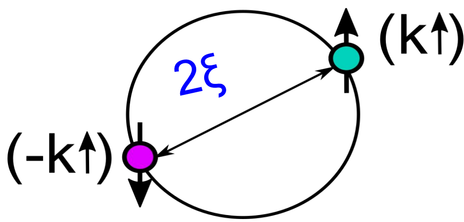

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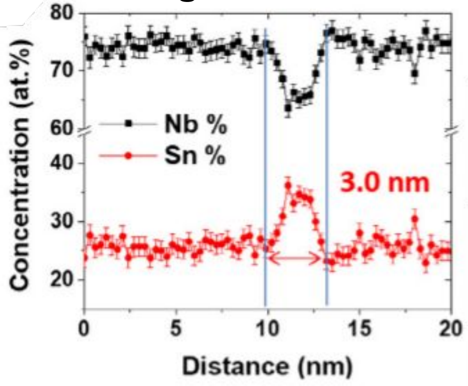

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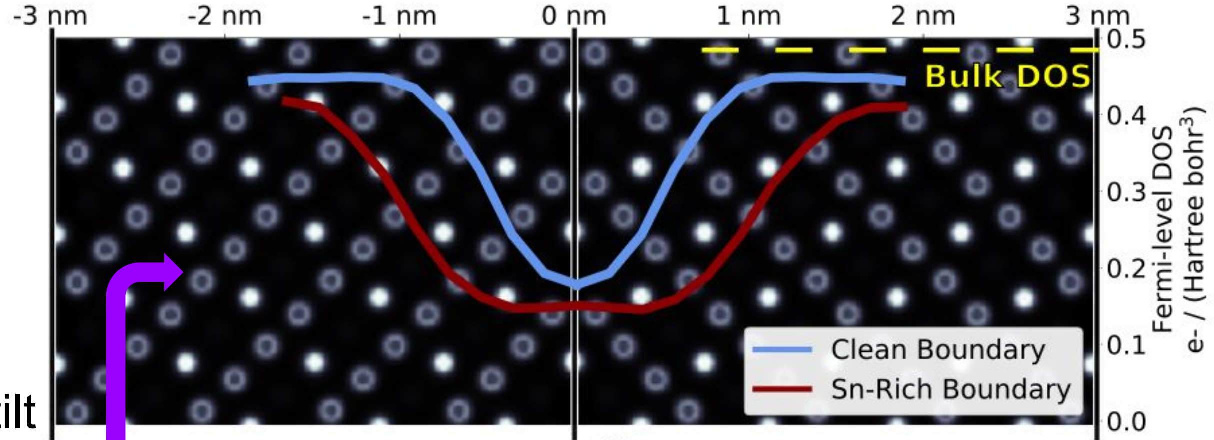

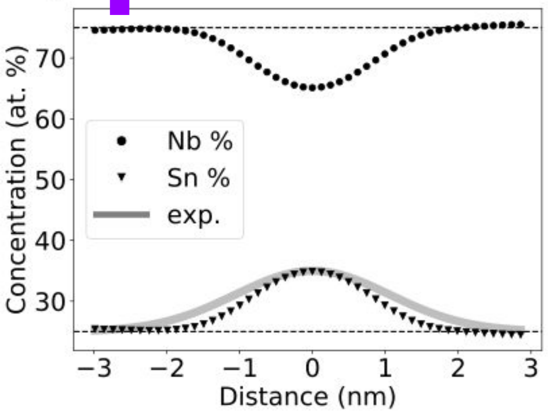

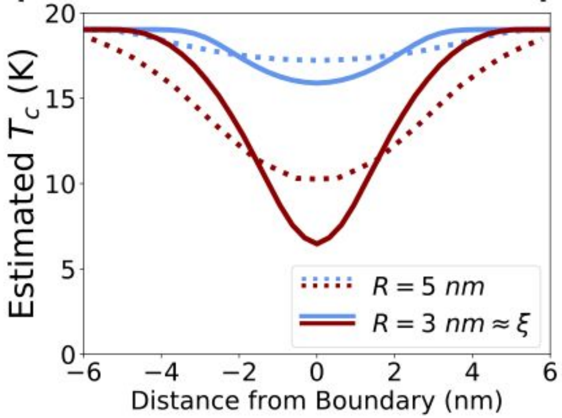

Clean GBs hardly affect Tc

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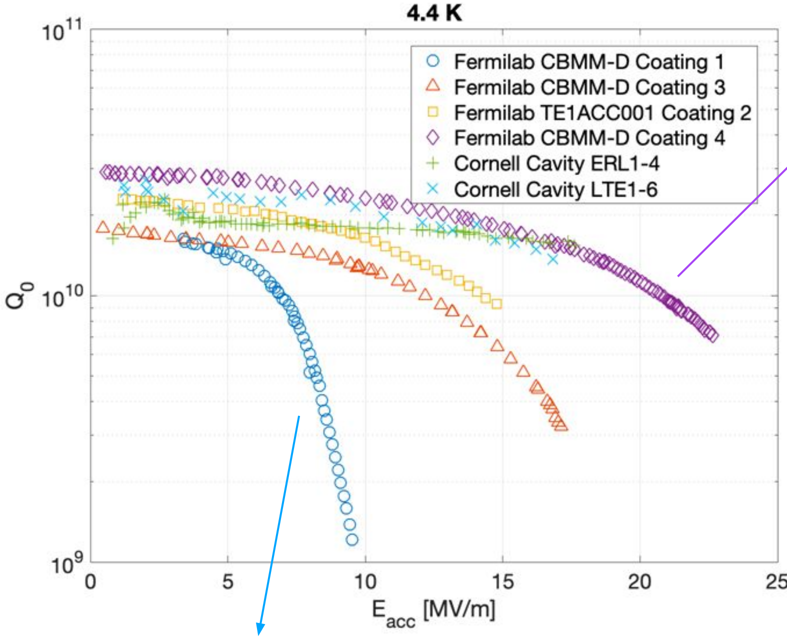

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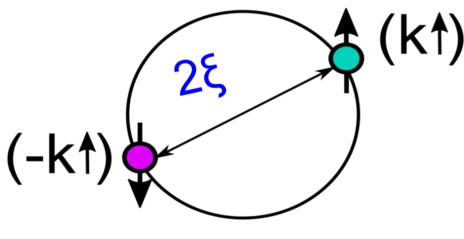

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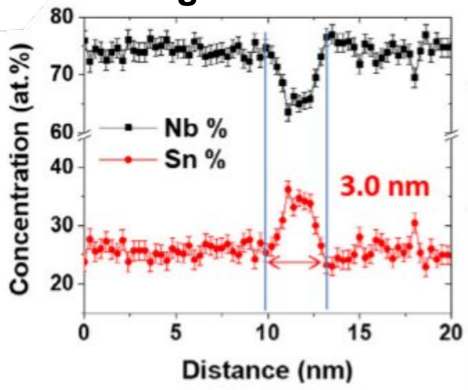

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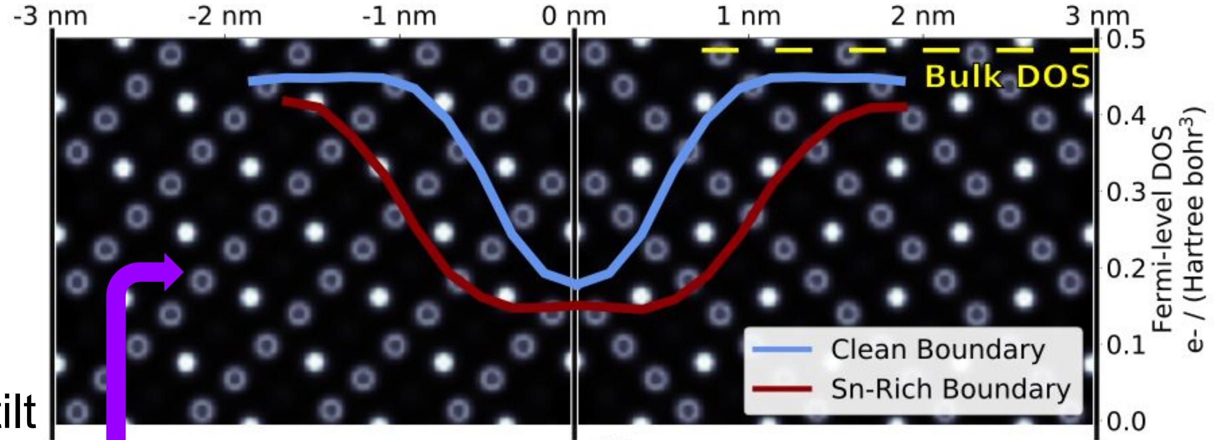

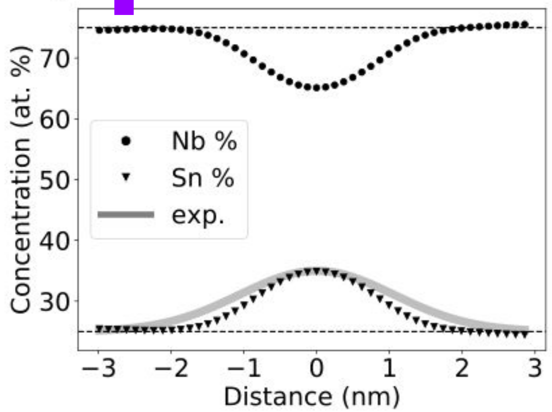

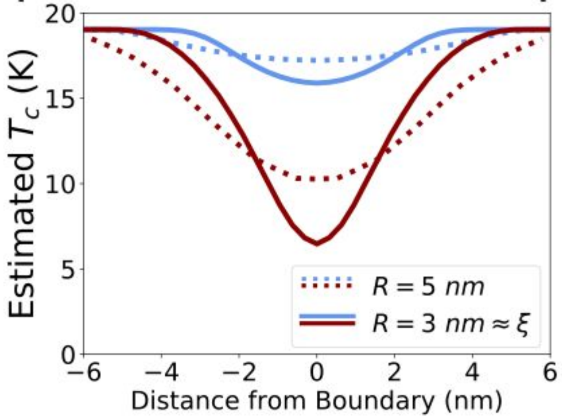

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Tin-rich GBs have large impact on Tc → highly degraded superconducting properties!

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Speculations:

ΔN(0) heavily influences properties of Nb_3Sn → inexpensive DFT calculations can help predict defect segregation behavior

Acknowledgments

Nathan Sitaraman (Cornell)
Prof. Tomás Arias (Cornell)
Ryan Porter, Prof. Matthias Liepe (Cornell)
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Prof. David Muller (Cornell)
& all of the collaborators in the CBB-SRF theme

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Jaeyel Lee, Prof. David Seidman (Northwestern)

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Kelley et al. 2020 *Supercond. Sci. Technol.*
https://doi.org/10.1088/1361-6668/abc8ce

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