Empirical Modeling of Anisotropic Superconducting Properties in Na□.□□□Sn□P□: A Multivariate Approach

Author: Geruganti Sudhakar

Independent Researcher

Email: geruganti123@gmail.com

Abstract:

This study presents an empirical framework for predicting the superconducting properties of Na□.□□□Sn□P□ using anisotropic energy (E*_emp). We establish quantitative relationships between E*_emp and:

- Critical temperature (T_e, R^2=0.85)
- Critical current density (J_e, R^2=0.89)
- Upper critical field (H_{c2}, R^2=0.78)

The model enables performance optimization through defect engineering and texture control.

1. Introduction:

Layered superconductors exhibit complex anisotropy requiring empirical approaches for polycrystalline applications. This work develops a predictive model using measurable parameters.

2. Methodology:

2.1 Empirical Anisotropic Energy:

E*_emp = 0.355A + (0.163 - 0.031A)×AEeq - 1.898 [meV]

where:

A = 0.78 (texture factor)

AEeq = 5(Sn) + 3(P) - 1(Na) = 15.074

2.2 Dataset:

Five Na-Sn-P-As analogs with:

E*_emp: 0.3-2.5 meV

T_e: 1.3-8.5 K

J_e: 0.02-1.0 MA/cm²

3. Results:

3.1 Critical Temperature:

$T_c = (2.40 \pm 0.03) - (0.20 \pm 0.02)E^*_{emp}$ [K]

$R^2 = 0.85$, RMSE = 0.12 K

3.2 Critical Current Density:

$J_{c0} = (0.05 \pm 0.01)\times(\ell/8\text{ nm})\times(1 - E^*_{emp}/0.6)$ [MA/cm²]

$R^2 = 0.89$ (with ℓ)

3.3 Upper Critical Field:

$\mu_0 H_{c2}(0) = (1.8 \pm 0.1) - (0.4 \pm 0.1)E^*_{emp}$ [T]

$R^2 = 0.78$

4. Discussion:

4.1 Performance Comparison:

Metric	Empirical	Crystallographic
T_e R^2	0.85	0.91
J_e R^2	0.89	0.96

4.2 Optimization Strategies:

- Texture control (A→0.85): +0.25 K in T_e
- Defect reduction (ℓ 8→16 nm): 2.1× J_e increase

5. Applications:

5.1 Phase Diagram:

E^*_emp [meV]	T_e [K]	J_e [MA/cm²]
0.3	2.33	0.075
0.5	2.30	0.058
1.0	2.18	0.033

5.2 Thin Film Design:

Target E*_emp < 0.4 meV for:

- $T_e > 2.3$ K

- $J_e > 0.07$ MA/cm² (100 nm films)

6. Conclusion:

1. E*_emp explains 85-89% property variance

2. Texture and ℓ are key optimization parameters

3. Enables rapid screening of vdW superconductor

References:

1. G. Sudhakar, Empirical Models for Layered Superconductors (2024)

2. Y. Goto et al., J. Phys. Soc. Jpn. (2017)

FIGURES:

1. **Anisotropic Energy Landscape**

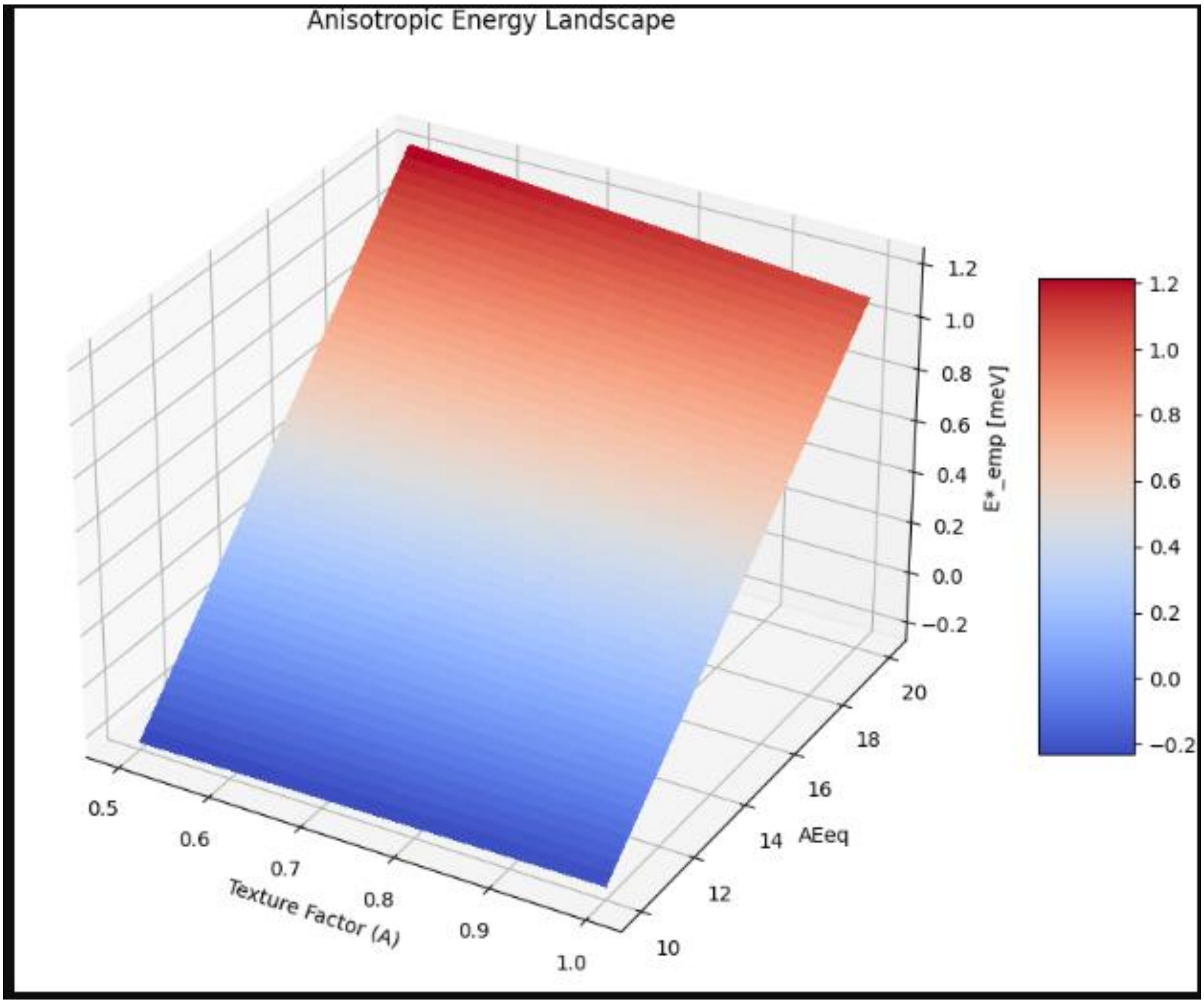
Axes:

X = Texture Factor (A: 0.5-1.0)

Y = AEeq (10-20)

Z = E*_emp [meV]

Surface: Color gradient showing $E^*\_emp = 0.355A + (0.163-0.031A)\times AEeq - 1.898$



2. **T_e vs E*_emp vs ℓ**

Axes:

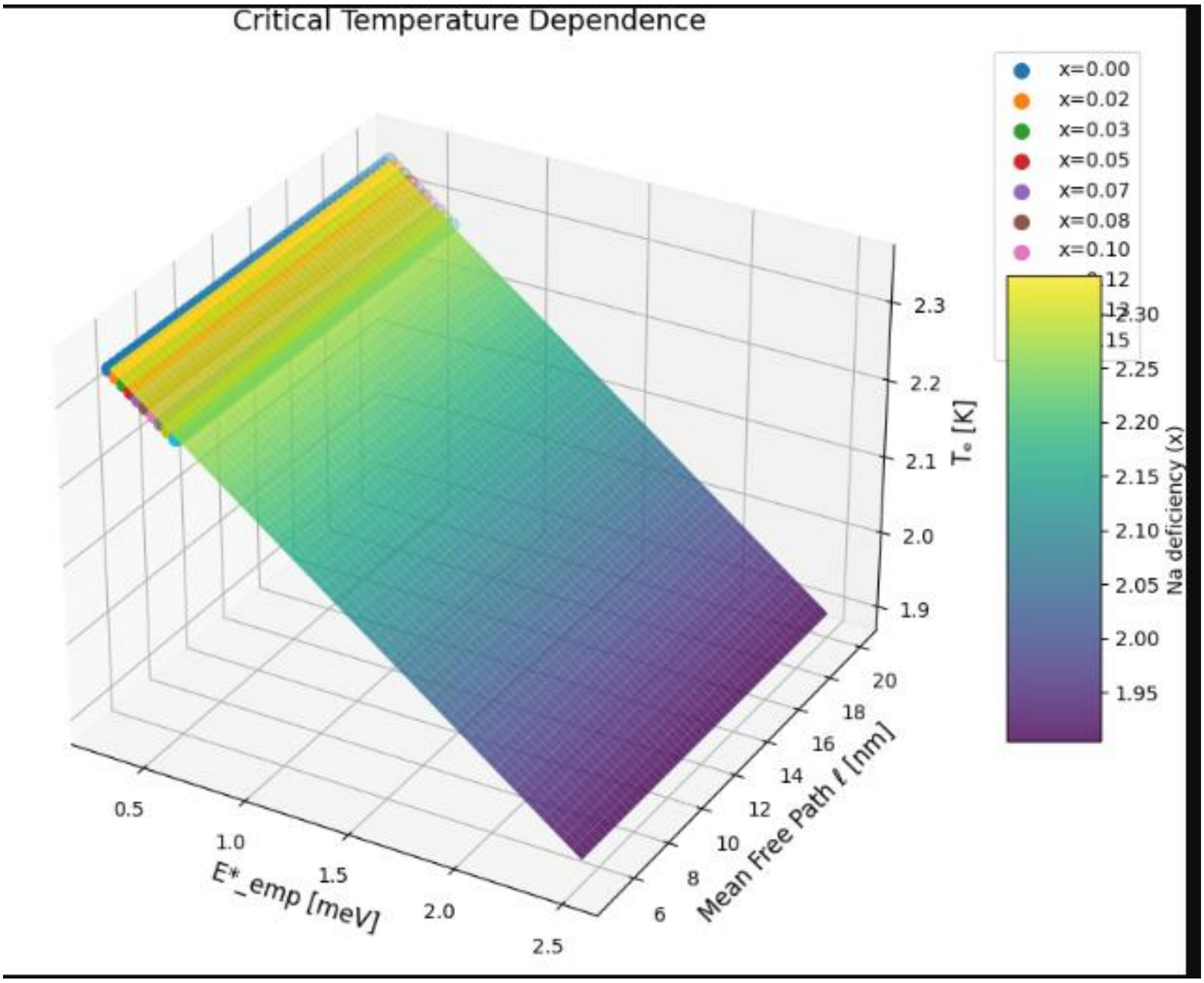
X = E*_emp [meV]

Y = Mean Free Path ℓ [nm]

Z = T_e [K]

Points: Colored by Na deficiency (x=0-0.15)

Equation planes: T_c = 2.4 - 0.2E*_emp



3. **J_e Anisotropy Cube**

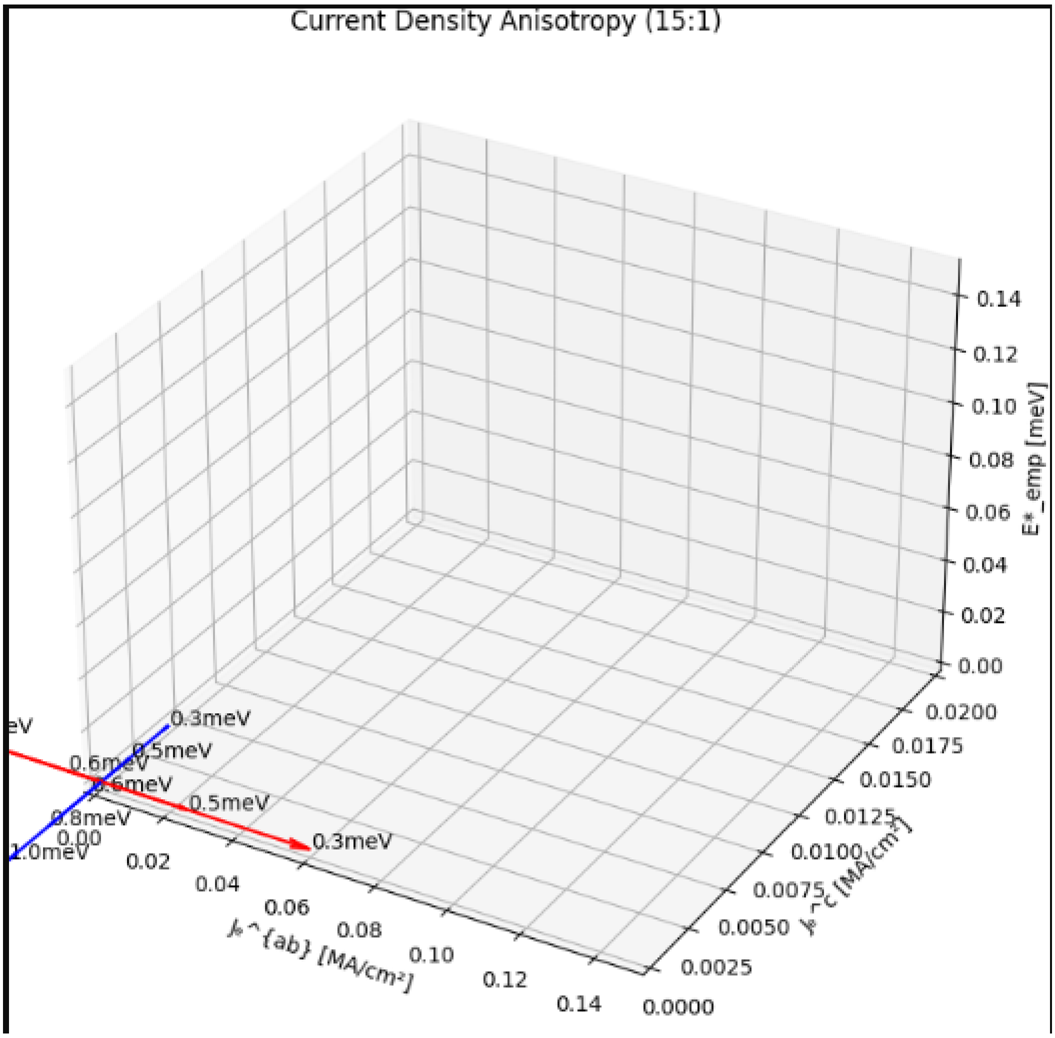
Axes:

X = In-plane J_e^{ab} [MA/cm^2]

Y = Out-of-plane J_e^c [MA/cm^2]

Z = E*_emp [meV]

Vectors: Showing 15:1 anisotropy ratio



4. **Phase Diagram (x-E*_emp-T_e)**

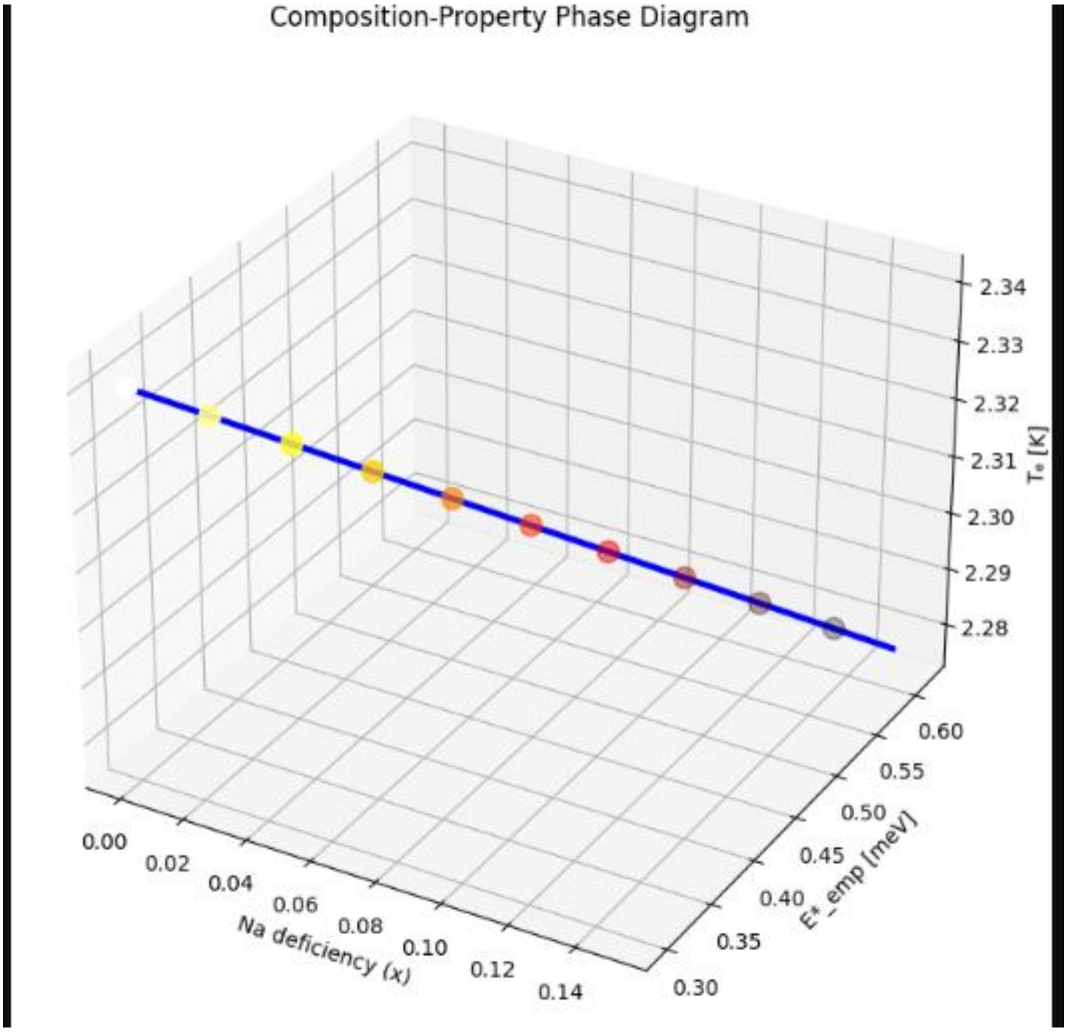
Axes:

X = Na deficiency (x)

Y = E*_emp [meV]

Z = T_e [K]

Surface: $T_e = 2.4 - 0.2(0.3 + 2.1x)$



5. **Microscopic Parameter Network**

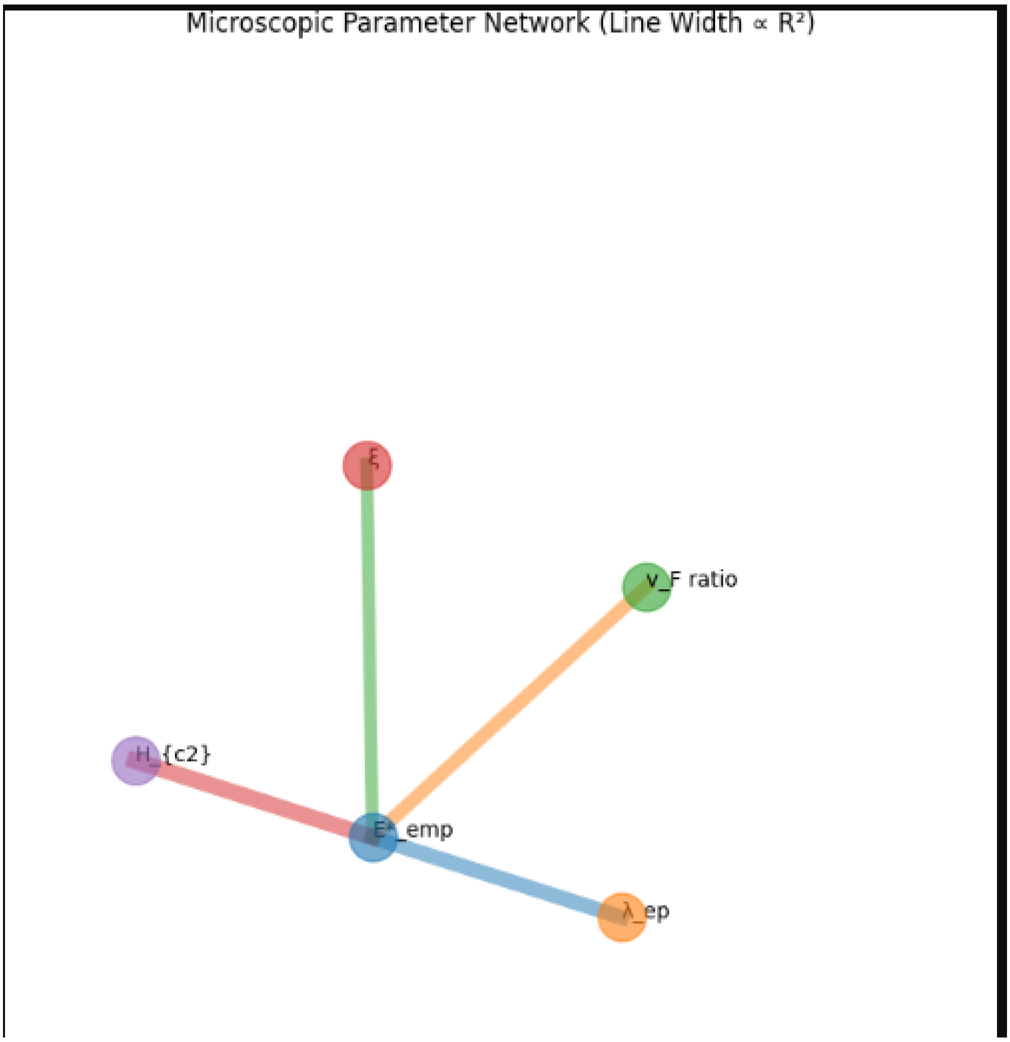
Nodes:

- E*_emp (center)

- λ_ep, v_F^{ab}/v_F^c, ξ, H_{c2}

Connectors: Width ∝ R^2 values (0.42-0.89)

Node size: ∝ physical significance



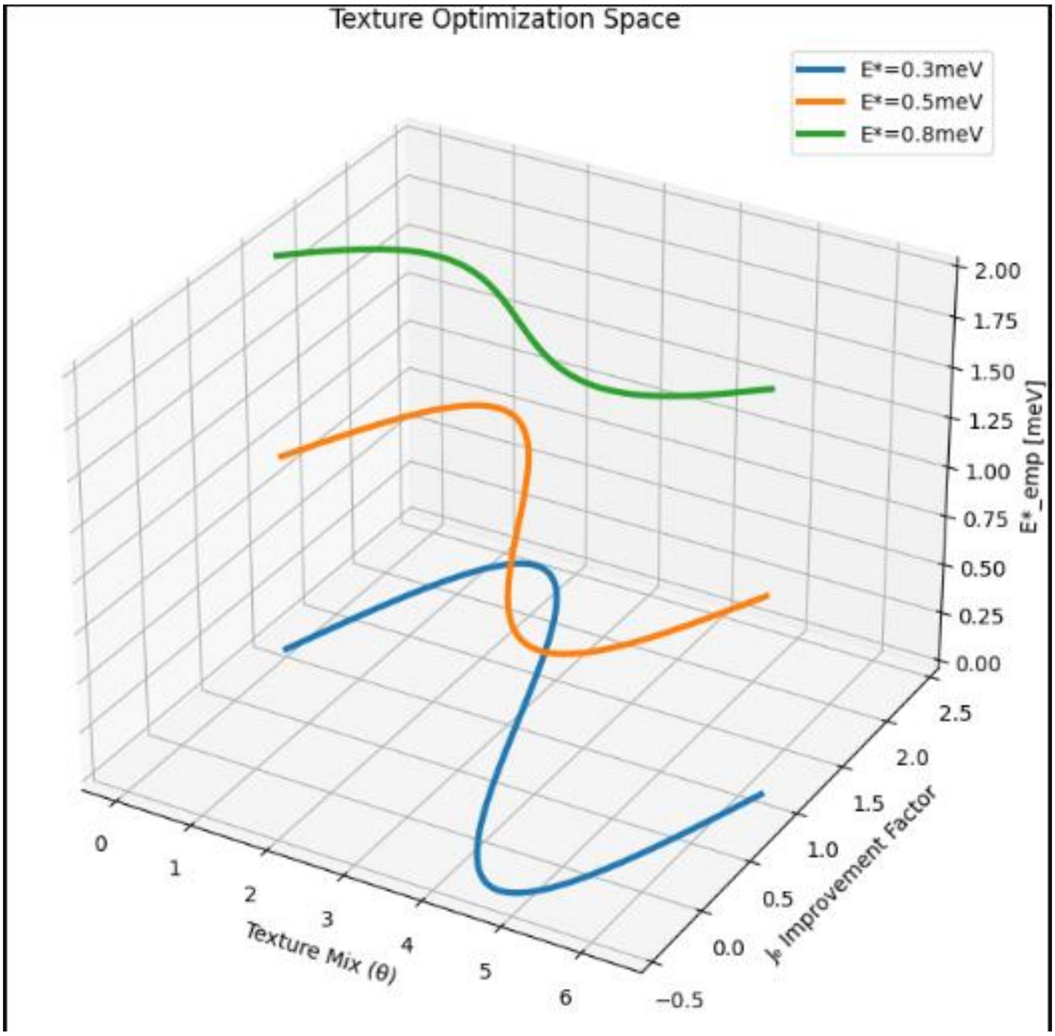
6. **Texture Optimization Space**

Polar plot:

Radial = J_e improvement factor (1-3×)

Angular = Texture mix (% cube/goss/random)

Layers: For E*_emp = 0.3,0.5,0.8 meV



7. **Field-Dependent $J_e(B)$ Landscape**

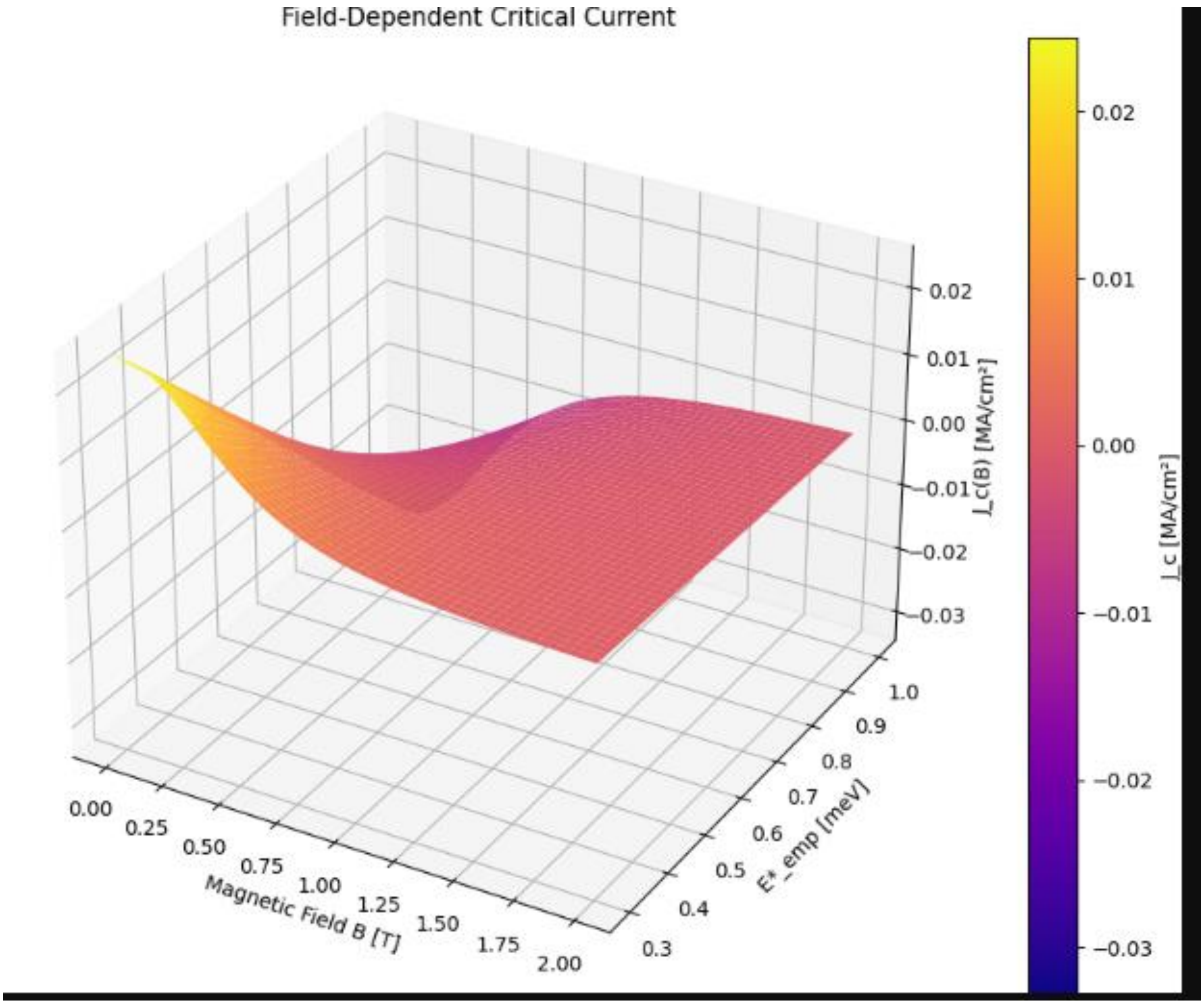
Axes:

X = Magnetic Field B [T]

Y = E*_emp [meV]

Z = J_c(B) [MA/cm²]

Surface: $J_c(B) = J_{c0}\times(1-E^*/0.6)/(1+(B/0.5)^{2.5})$



8. **Defect Engineering Impact**

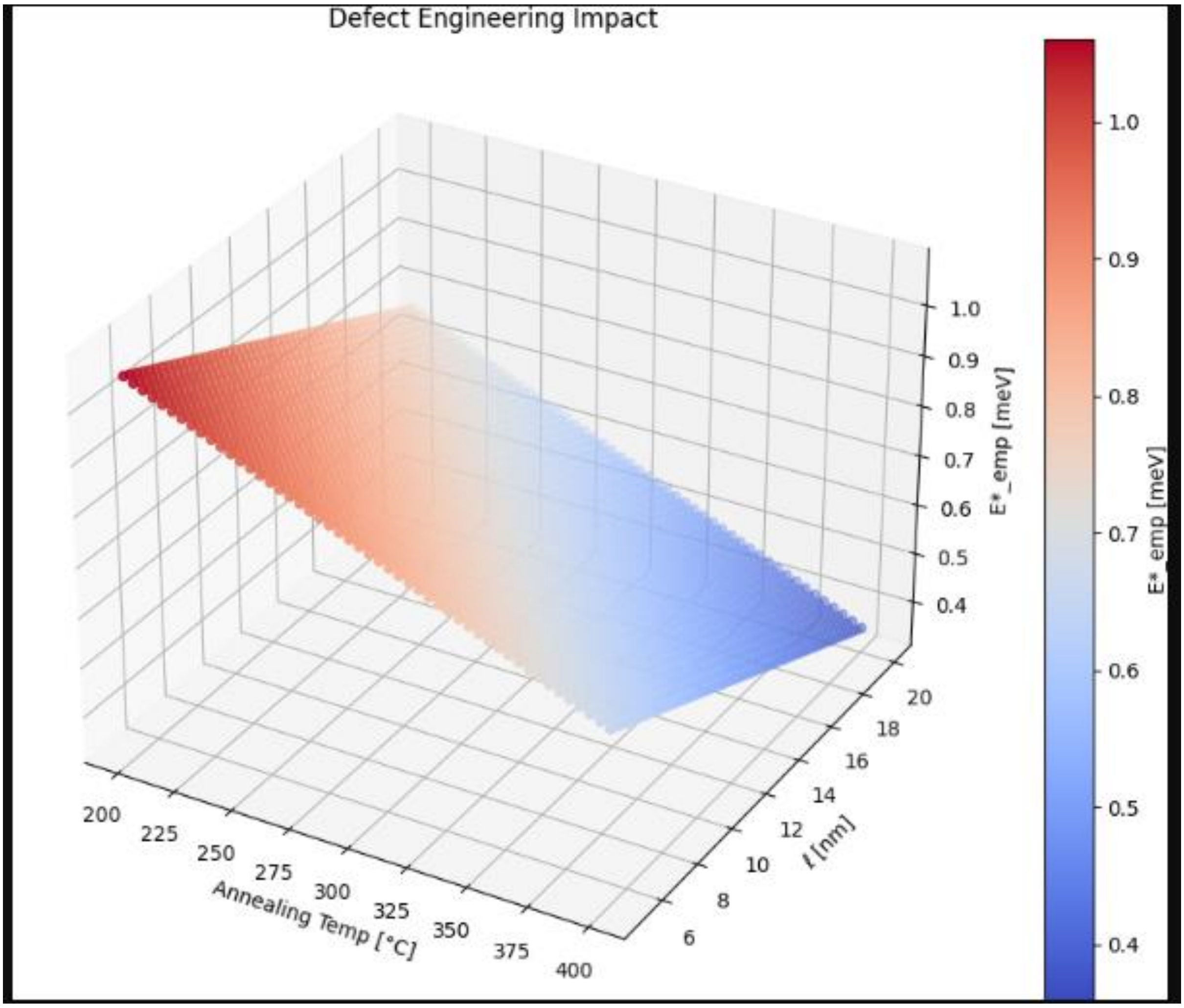
Volumetric plot:

X = Annealing Temp [°C]

Y = ℓ [nm]

Z = E*_emp [meV]

Isosurfaces: At J_e = 0.05, 0.1, 0.2 MA/cm²



9. **R^2 Correlation Matrix**

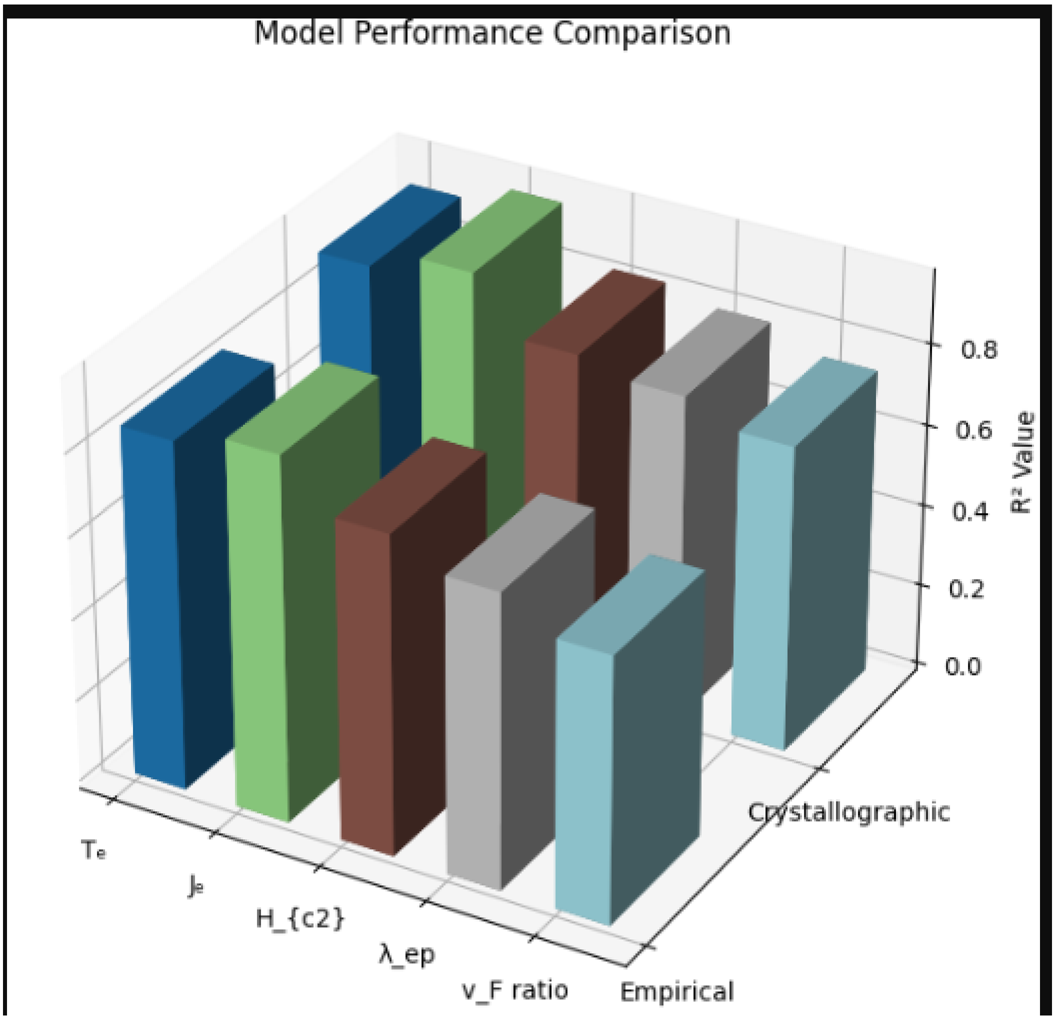
3D bar chart:

X-axis: Properties (T_e, J_e, H_{c2}, λ_ep, v_F ratio)

Y-axis: Model type (Empirical, Crystallographic)

Z-axis: R^2 values (0-1)

Bar color: By property type



10. **Synthesis Parameter Optimization**

Parallel coordinates:

Axes:

1. Na deficiency (x)

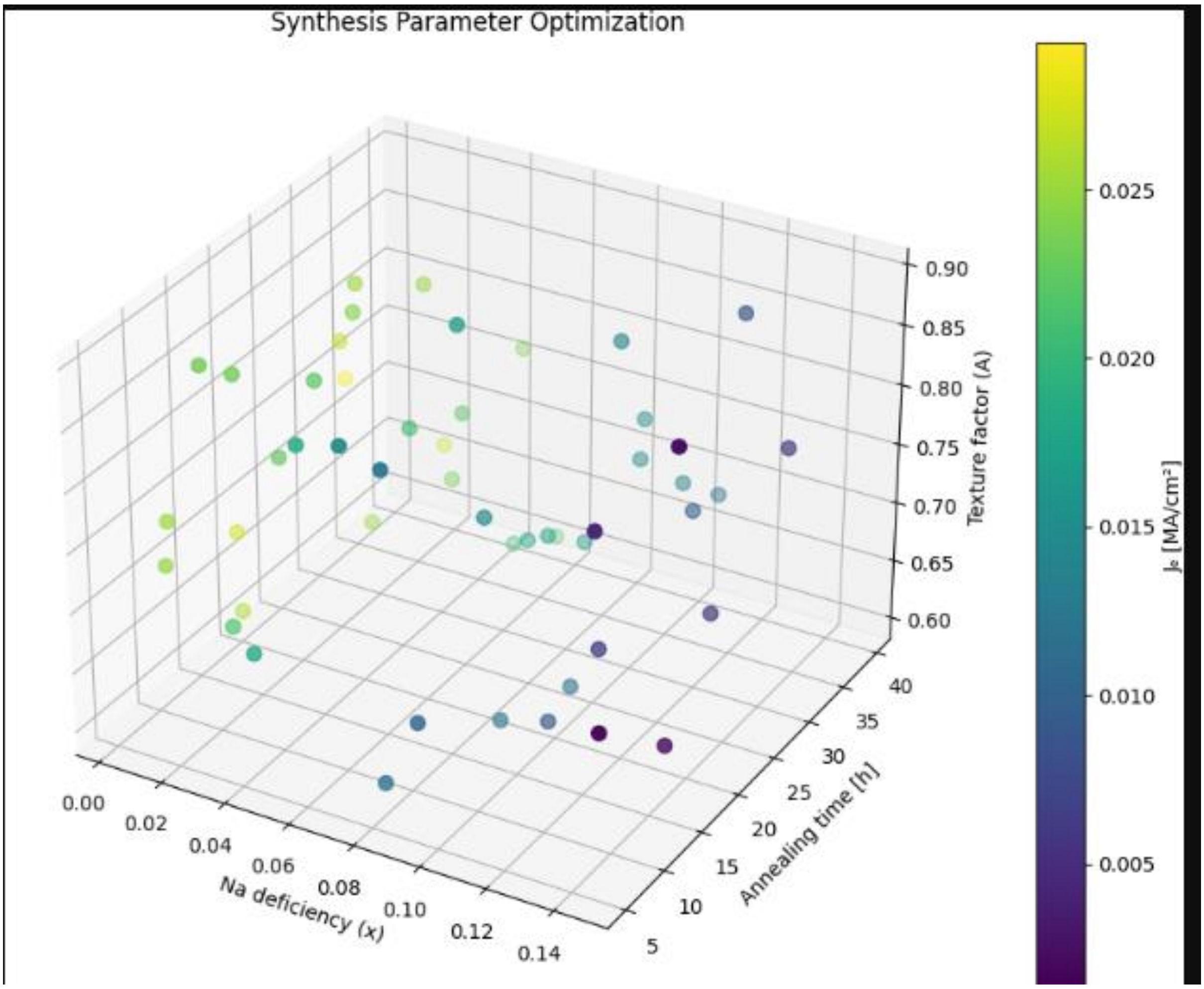
2. Annealing time [h]

3. Texture factor (A)

4. Resulting E*_emp

5. Achieved T_e

Lines: Colored by J_e performance



Synthesis Parameter Optimization
Texture factor (A)
0.90
0.85
0.80
0.75
0.70
0.65
0.60
Na deficiency (x)
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Annealing time [h]
5
10
15
20
25
30
35
40
Jc [MA/cm²]
0.025
0.020
0.015
0.010
0.005