



北京大學
PEKING UNIVERSITY



WEIAA02

Temperature Responses of Superconducting Niobium Properties in Experiment and Simulation

Presenter: Zhitao Yang
Advisor: Jiankui Hao
On behalf of PKU SRF team

2023.06.28

Conclusion

5

First-Principles
Calculation

4

In-situ ARXPS

3

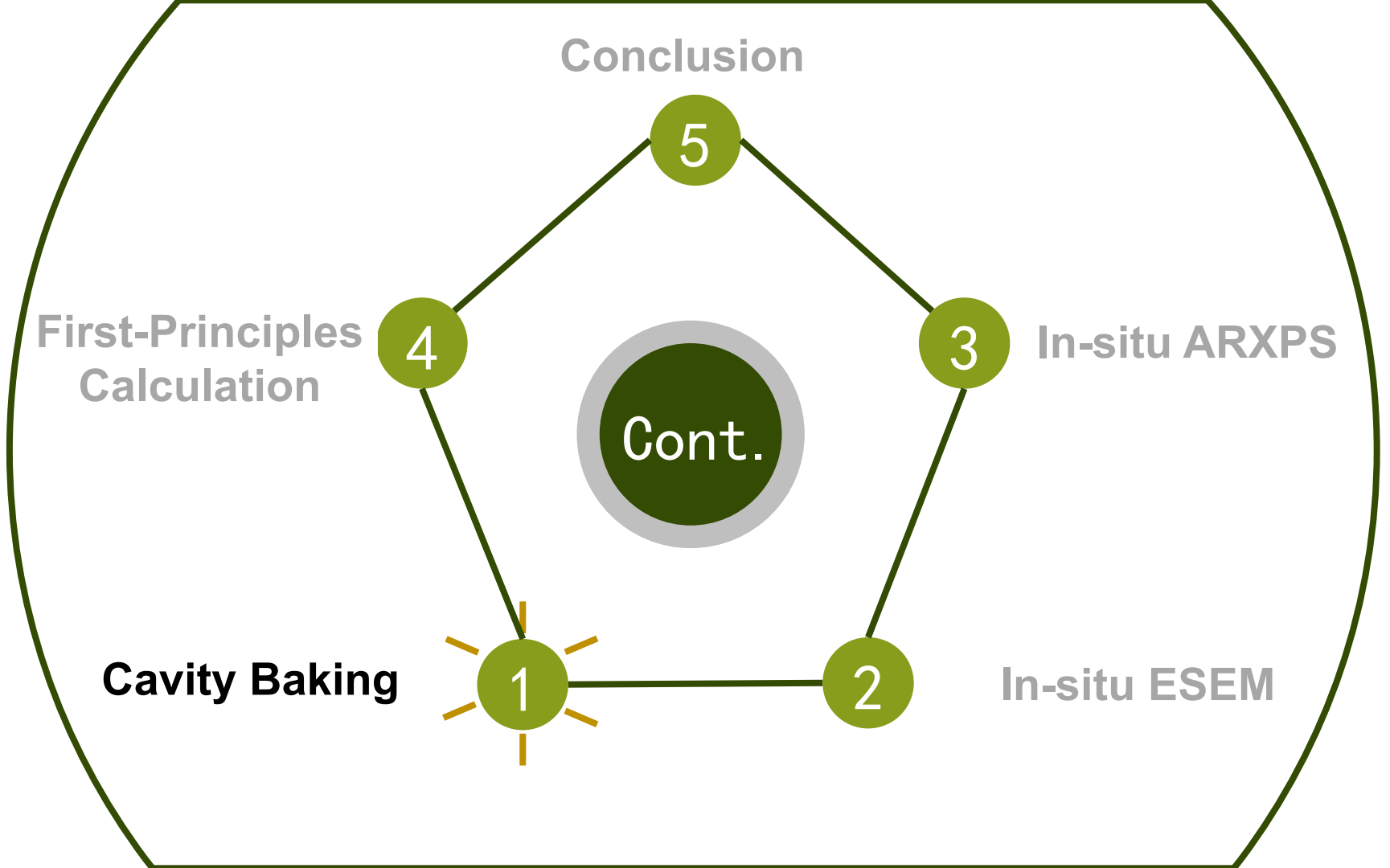
Cont.

Cavity Baking

1

In-situ ESEM

2



1.4

Baking Temperature



3

1.4

Baking Temperature



a 75-100°C

- 4 h - Pre-Baking
- Improve max E_{acc} effectively



3

1.4

Baking Temperature



a 75-100°C

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- Improve max E_{acc} effectively



b 120-180°C

- 48 h - Low Temperature Baking
- Suppress HFQS effectively
- 48 h - Nitrogen Infusion
- Improve Q_0

1.4

Baking Temperature



a 75-100°C

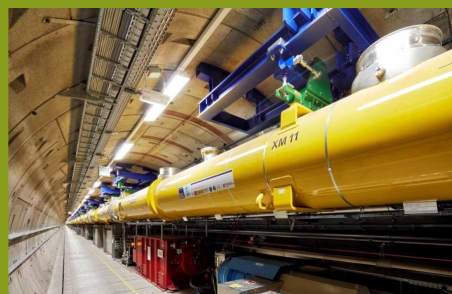
- 4 h - Pre-Baking
- Improve max E_{acc} effectively

c 300-400°C

- 1-3 h - Medium Temperature Baking
- High Q_0 and Acceptable E_{acc}

b 120-180°C

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Baking Temperature



a 75-100°C

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b 120-180°C

- 48 h - Low Temperature Baking
- Suppress HFQS effectively
- 48 h - Nitrogen Infusion
- Improve Q_0

d 800-900°C

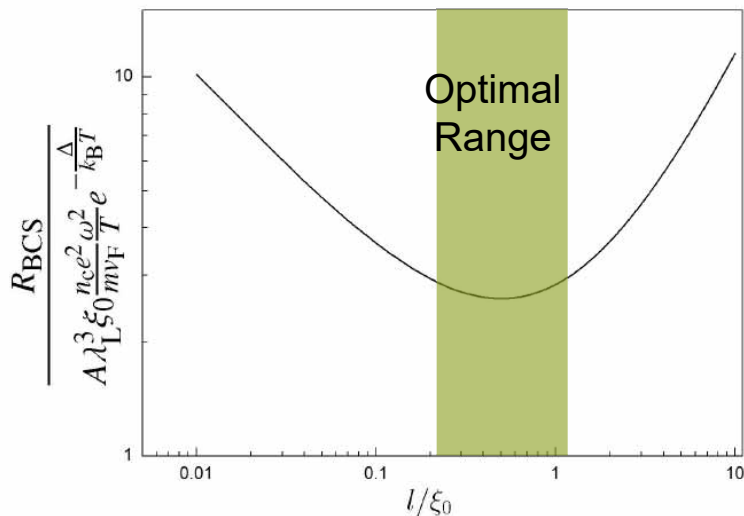
- 3 h - High Temperature Annealing
- Hydrogen degassing and Recrystallization
- 2/0, 2/6, 10/20, 20/30, 3/60, Nitrogen Doping
- Improve Q_0



1980

Cornell
F.
Palmer

8.6 GHz Nb cavity, 250-300°C 5-10 min, $R_{\text{BCS}} \downarrow$ 10-20%;
 350°C 10 min, $R_{\text{res}} \downarrow$;
 Nb-O compounds \downarrow , Interstitial O \uparrow , MFP Opt





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2008

Jlab
G.V.Eremeev

1.5 GHz Nb Cavity, 400°C 1 h, HFQS, high R_{res} ,
Nb-O compounds $\downarrow \uparrow$, Non-stoichiometric Nb-O,
Interstitial O not enough;



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F.
Palmer

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Nb-O compounds \downarrow , Interstitial O \uparrow , MFP Opt

2008

Jlab
G.V.Eremeev

1.5 GHz Nb Cavity, 400°C 1 h, HFQS, high R_{res} ,
Nb-O compounds $\downarrow \uparrow$, Non-stoichiometric Nb-O,
Interstitial O not enough;

2020

FNAL
S. Posen

1.3 GHz Nb Cavity, 250-400°C 2.5 h, $R_{BCS} \downarrow$, $R_{res} \downarrow$;
KEK, IHEP, repetitious results;
Nb-O compounds \downarrow , Interstitial O & N \uparrow , MFP Opt;

Conclusion

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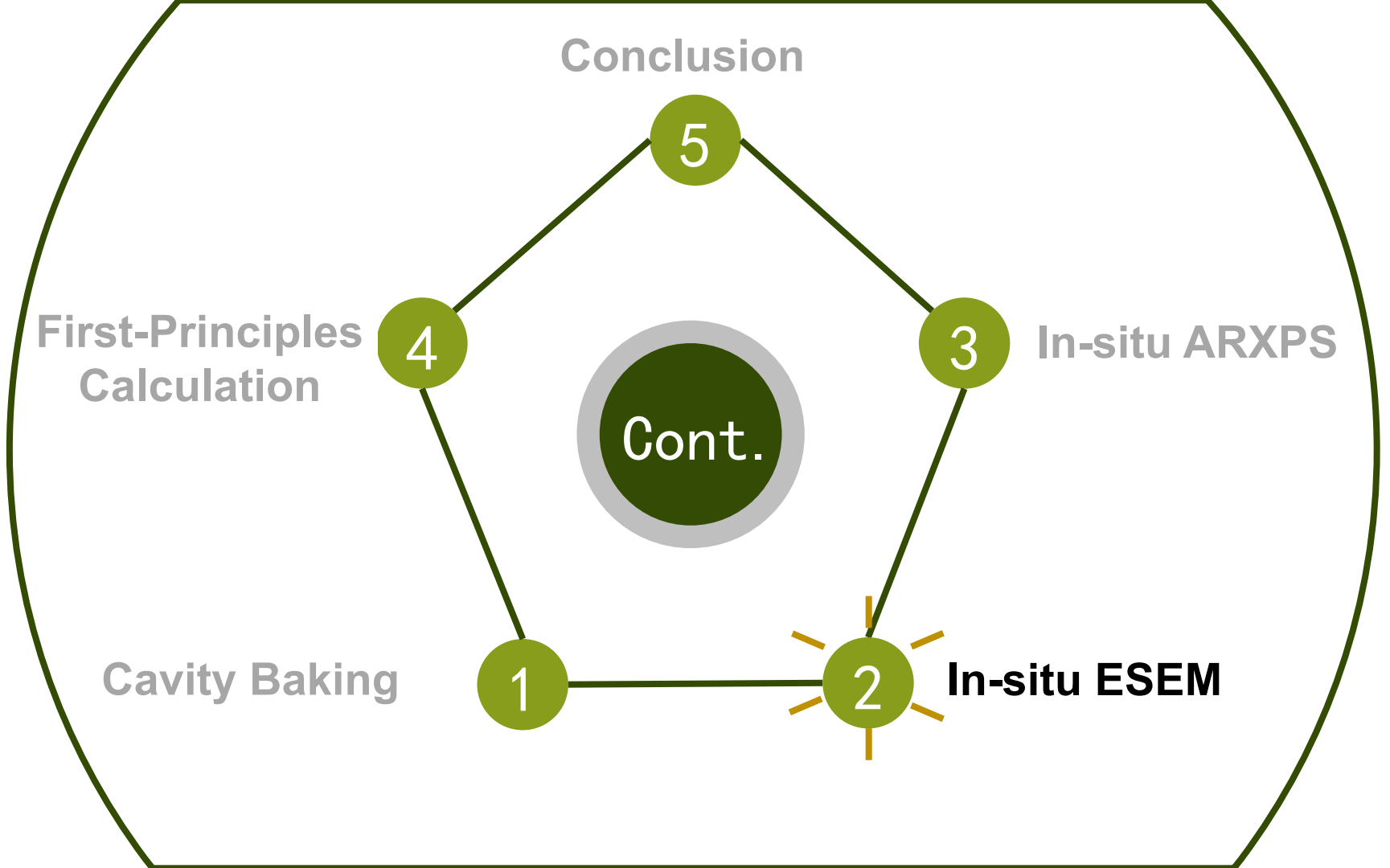
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Cavity Baking

1

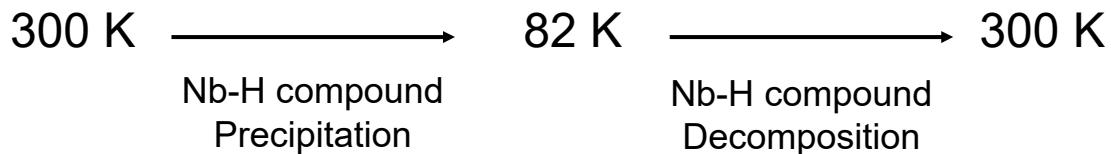
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In-situ ESEM





- Heavily chemically polished baseline samples
- In-situ environmental scanning electron spectroscopy (ESEM)
- Liquid nitrogen cooling platform



- Observation while cooling and heating
- First round of cooling: precipitation and scars
- Second round of cooling: repeatable scars and precipitation

2.2

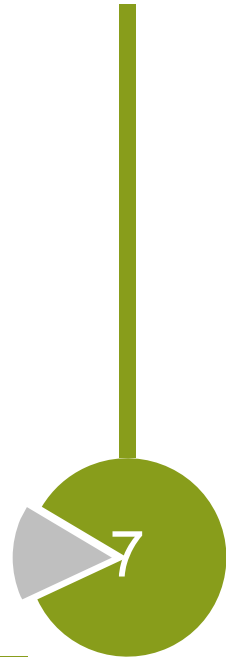
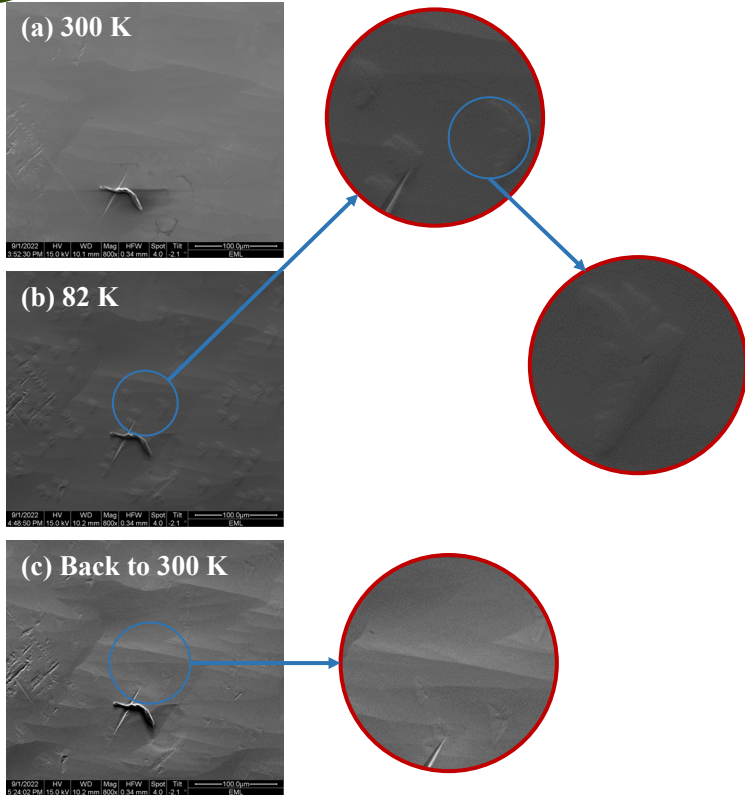
Nb-H precipitation Observation



7

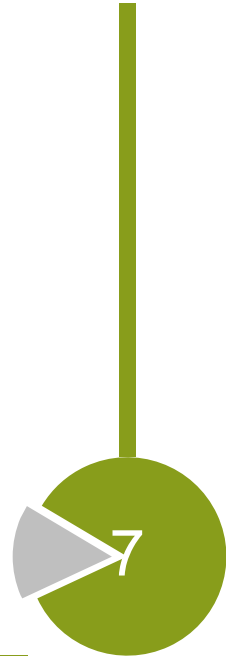
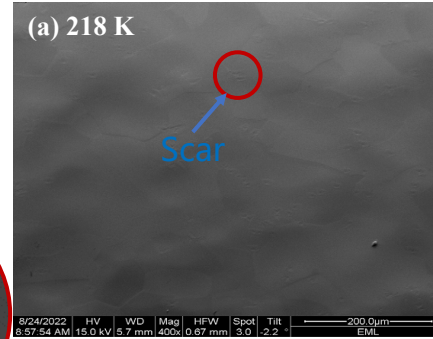
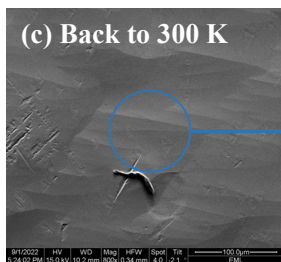
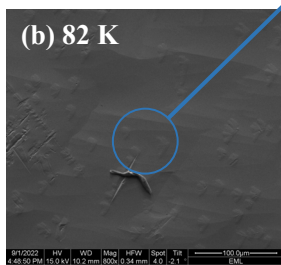
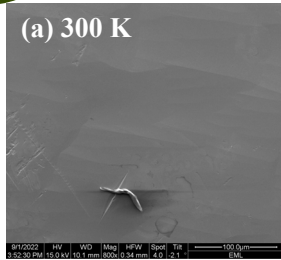
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Nb-H precipitation Observation



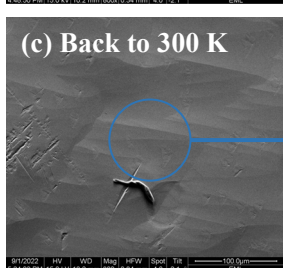
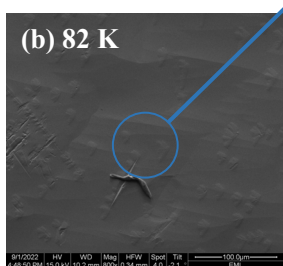
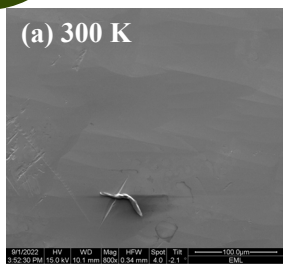
2.2

Nb-H precipitation Observation



2.2

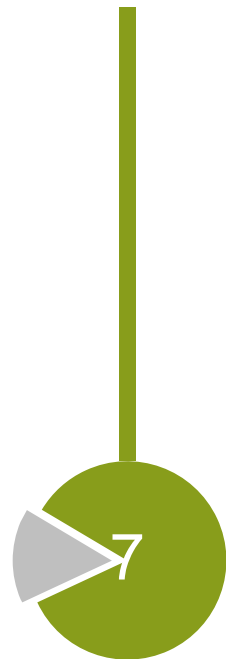
Nb-H precipitation Observation



(a) 218 K

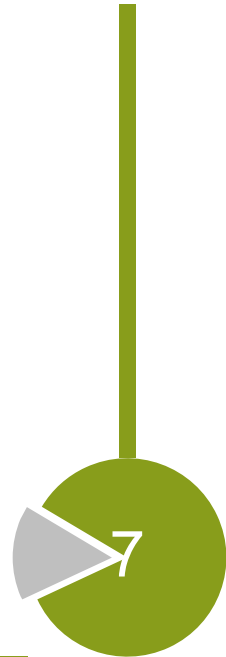
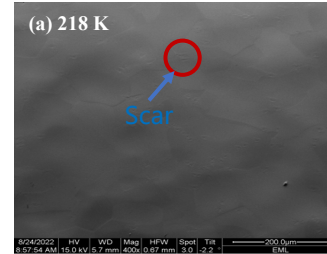
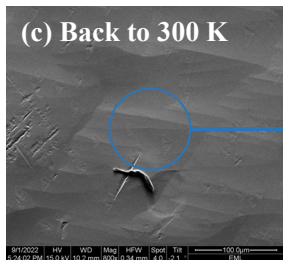
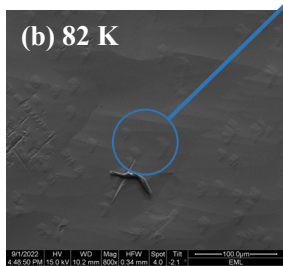
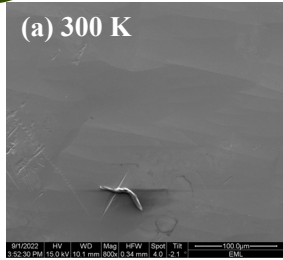


8/24/2022	HV	WD	Mag	HFWD	Spot	Tilt	200.0µm
8:57:54 AM	15.0 kV	5.7 mm	400x	0.67 mm	3.0	-2.2 °	EML



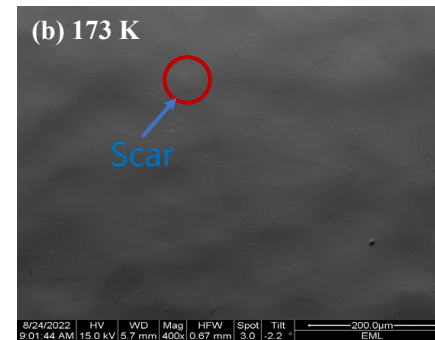
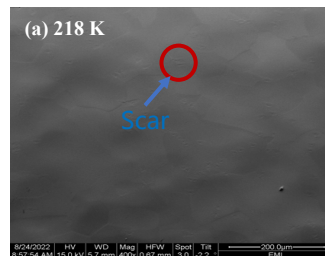
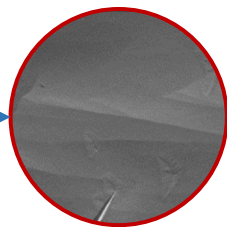
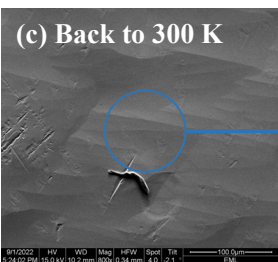
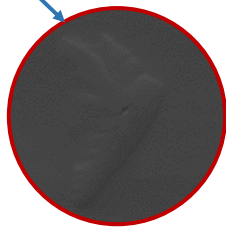
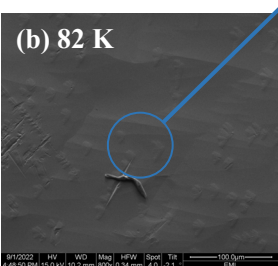
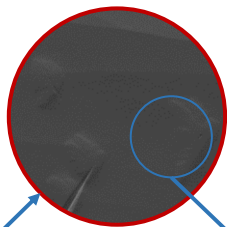
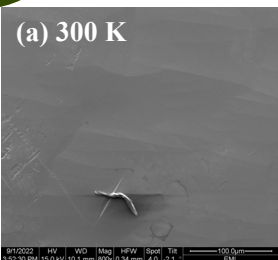
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Nb-H precipitation Observation



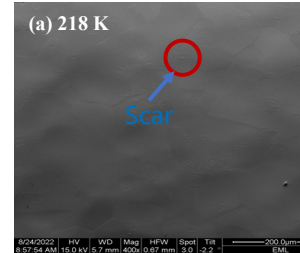
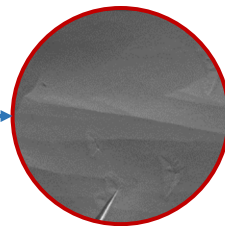
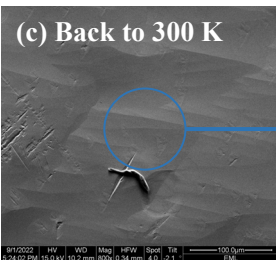
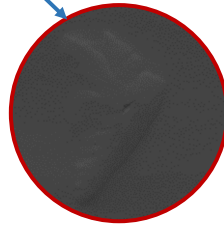
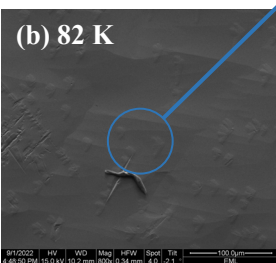
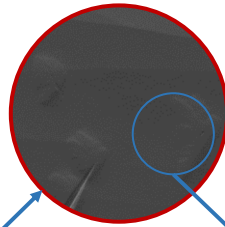
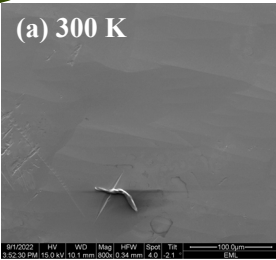
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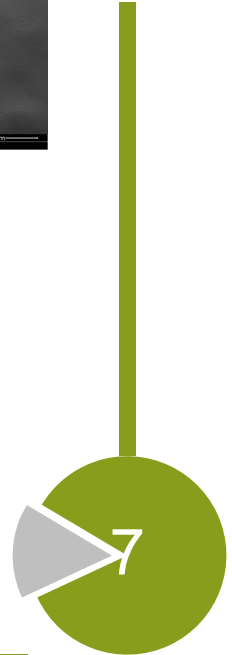
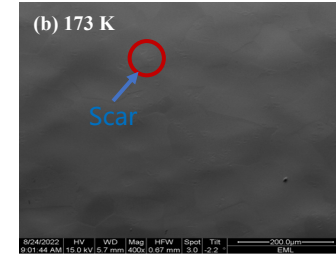
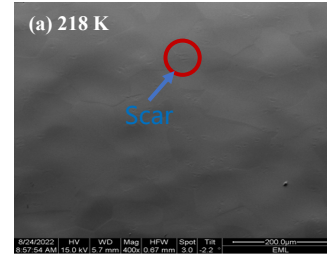
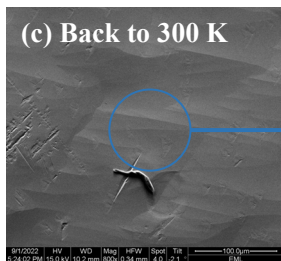
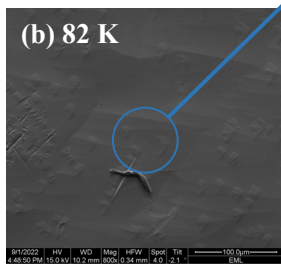
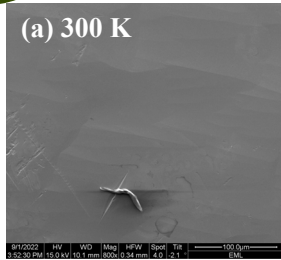
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Nb-H precipitation Observation



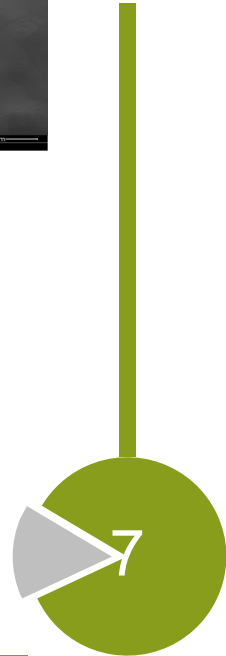
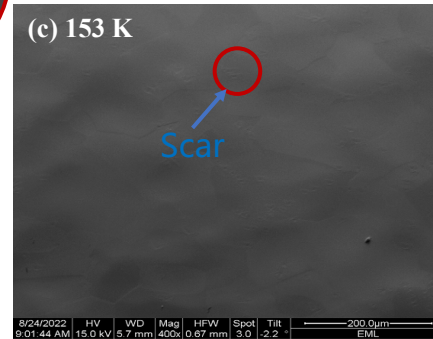
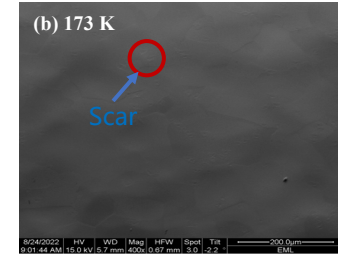
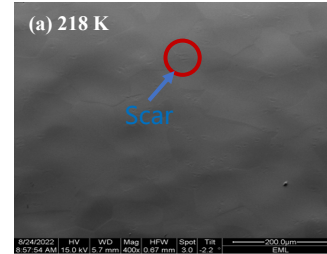
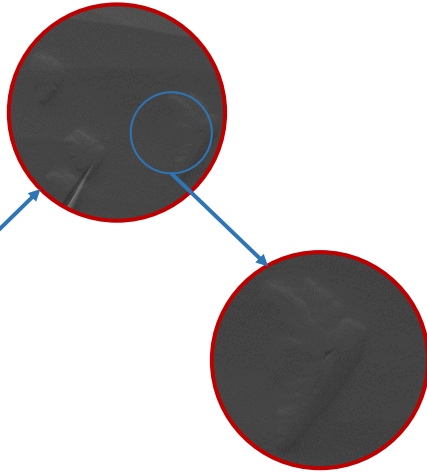
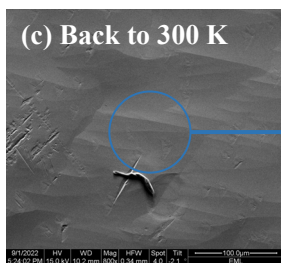
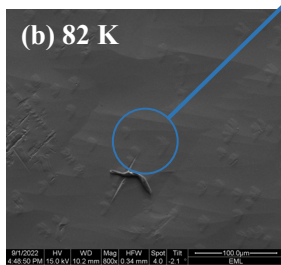
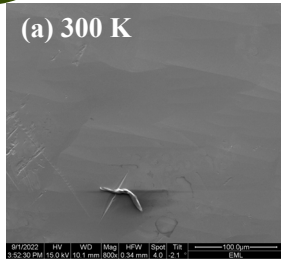
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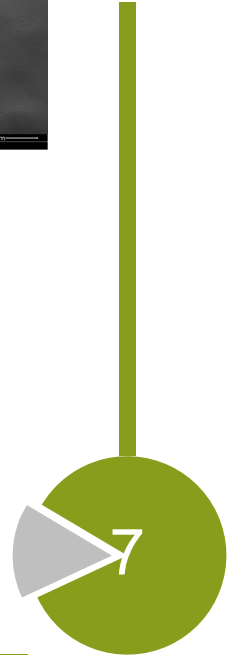
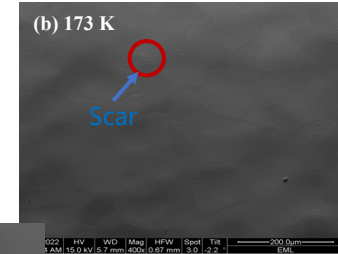
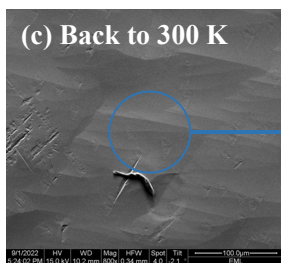
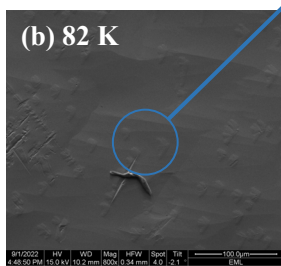
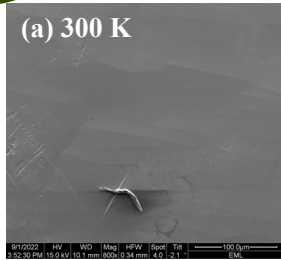
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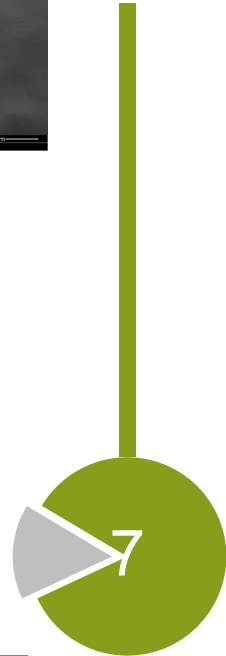
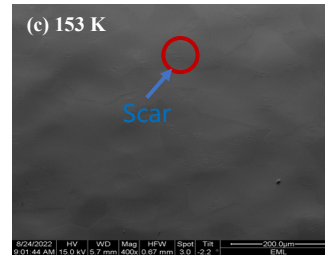
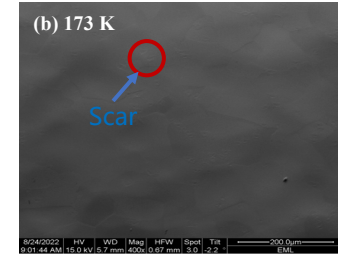
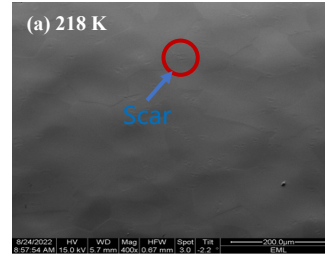
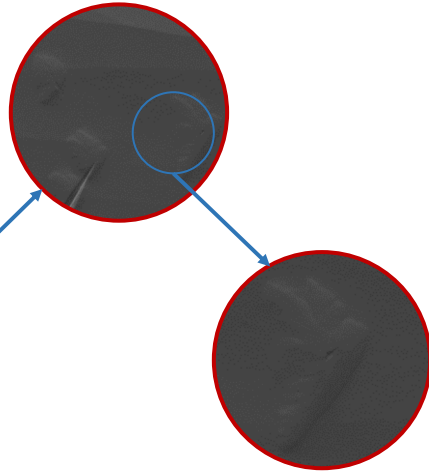
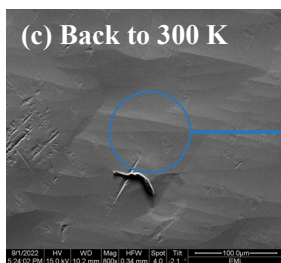
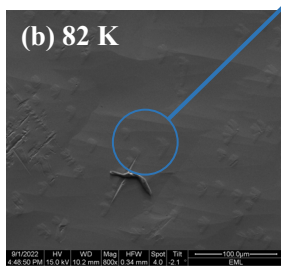
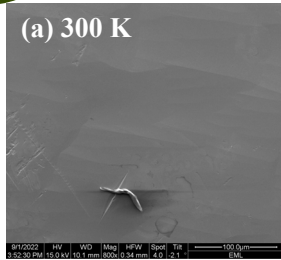
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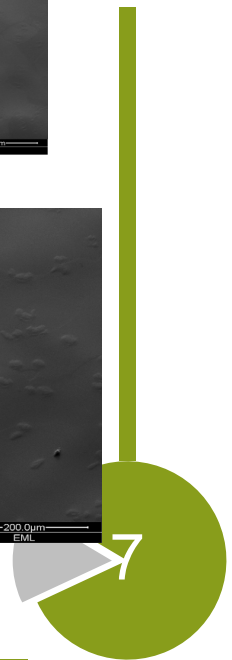
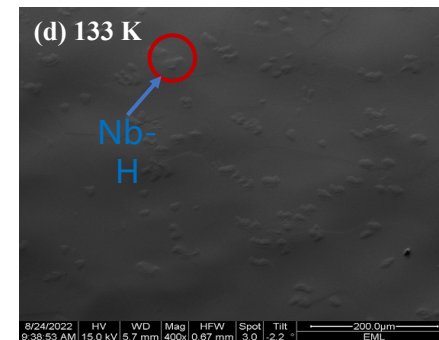
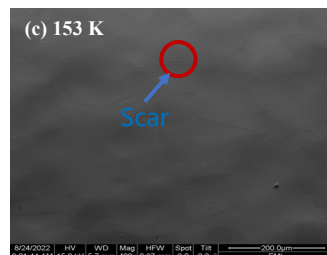
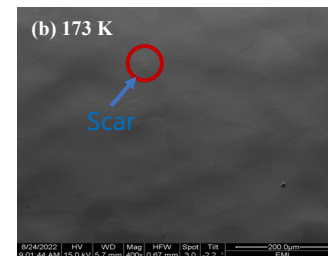
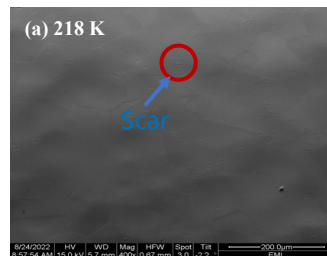
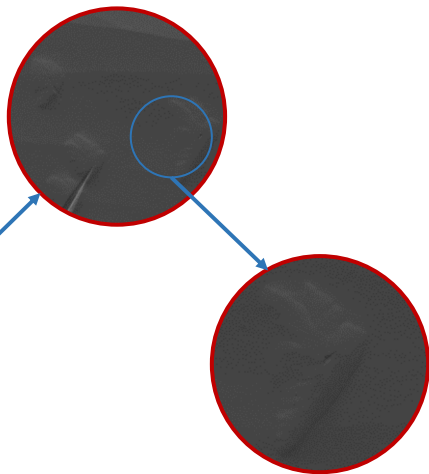
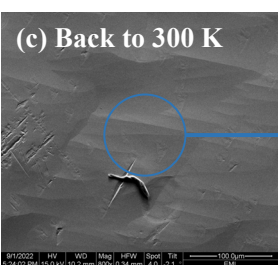
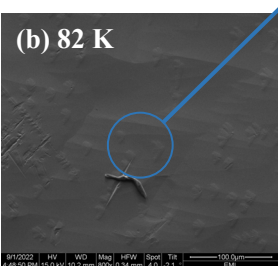
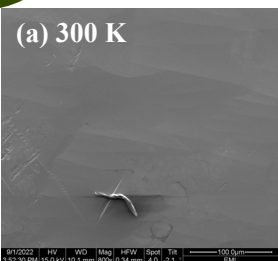
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Nb-H precipitation Observation



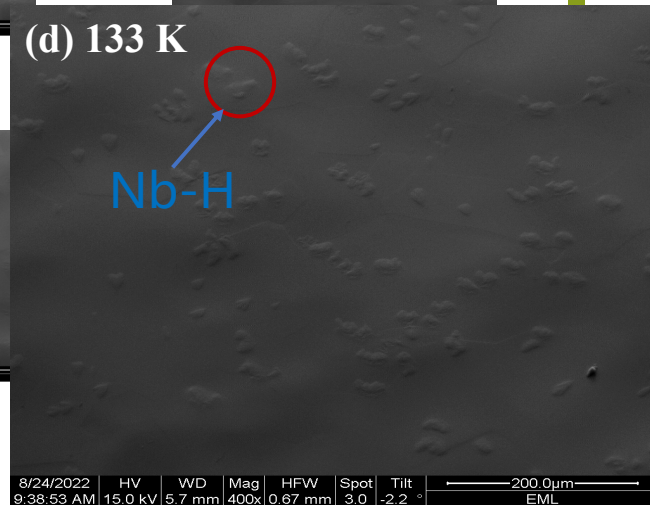
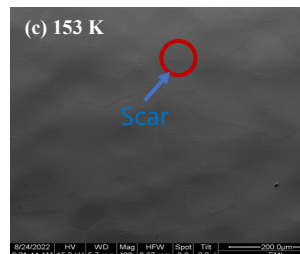
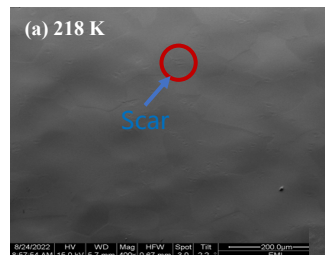
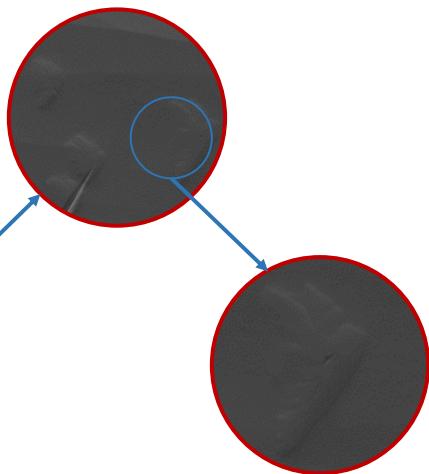
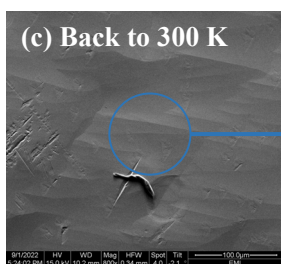
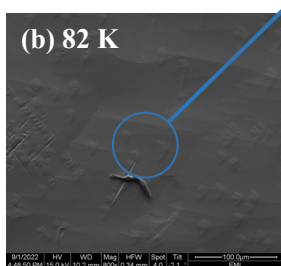
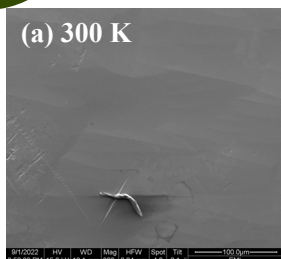
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Nb-H precipitation Observation



2.2

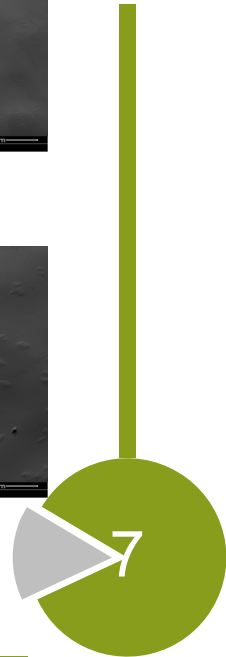
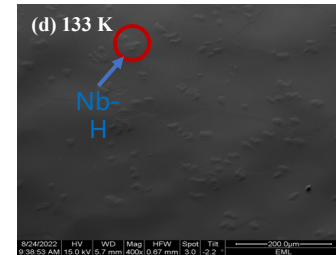
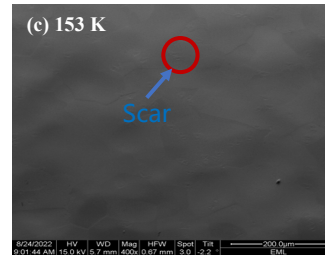
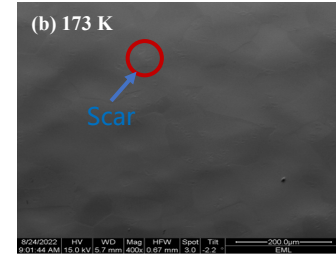
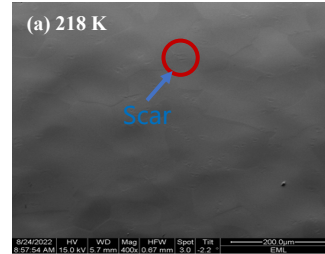
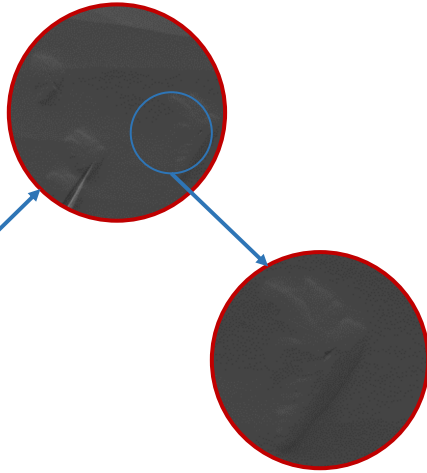
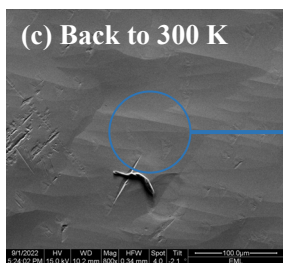
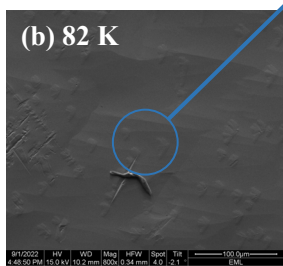
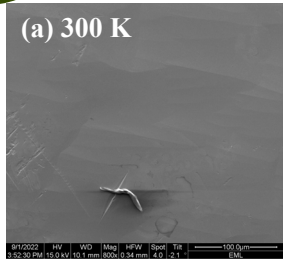
Nb-H precipitation Observation



8/24/2022 HV WD Mag HFW Spot Tilt
9:38:53 AM 15.0 kV 5.7 mm 400x 0.67 mm 3.0 -2.2 °
200.0µm
EML

2.2

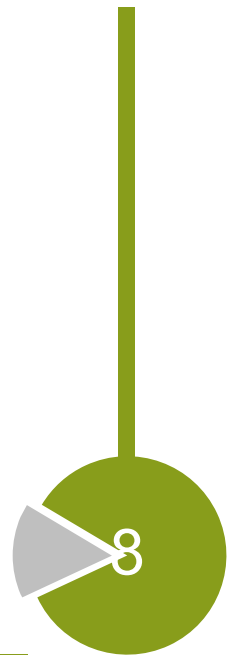
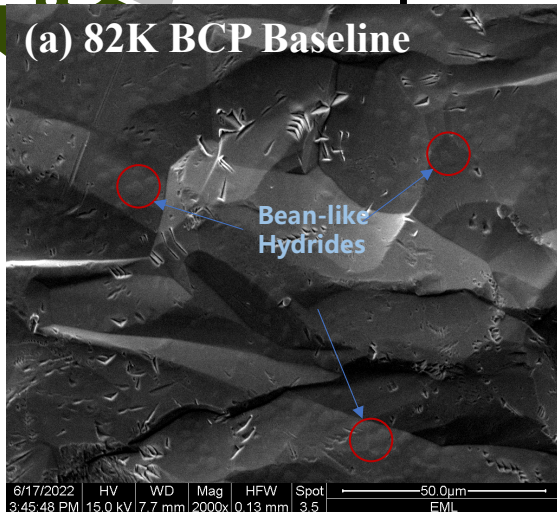
Nb-H precipitation Observation



2.3 Comparisons among baked samples

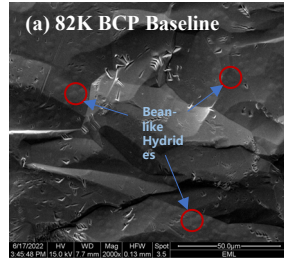


(a) 82K BCP Baseline



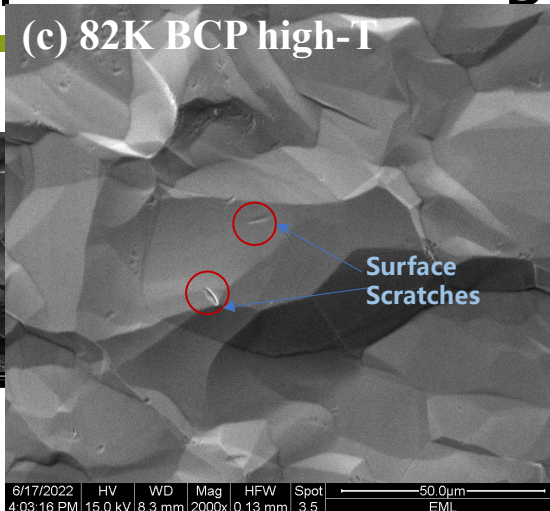
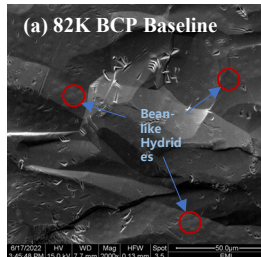
2.3

Comparisons among baked samples



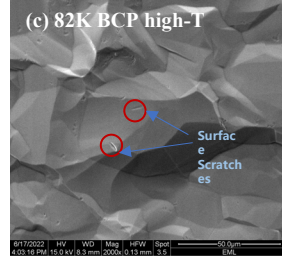
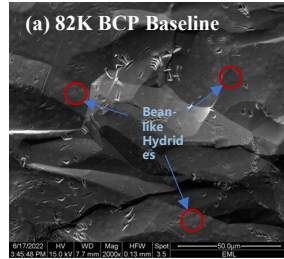
2.3

Comparisons among baked samples

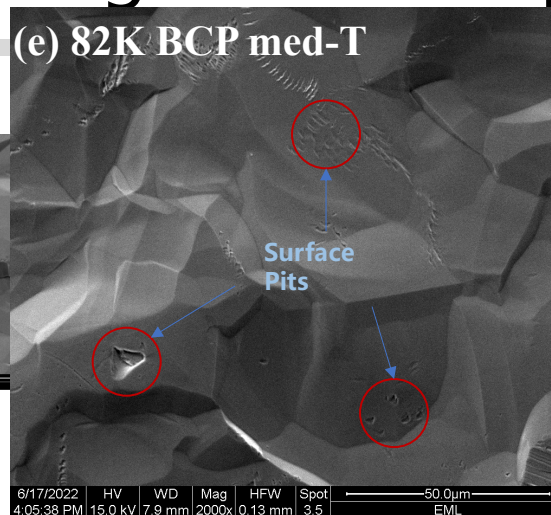
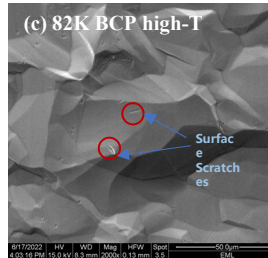
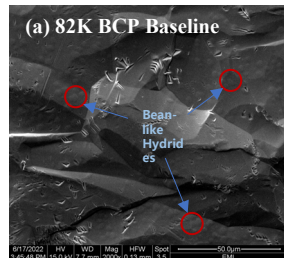


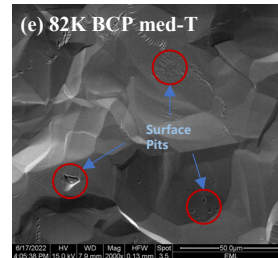
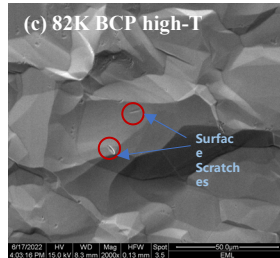
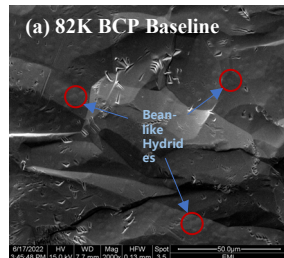
2.3

Comparisons among baked samples

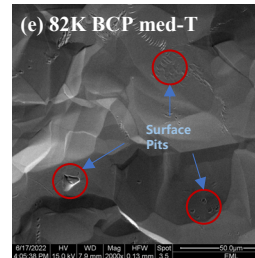
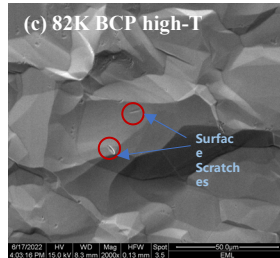
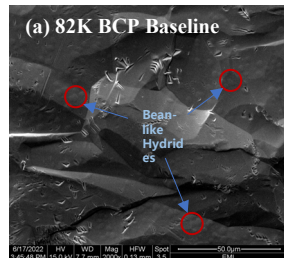


Comparisons among baked samples

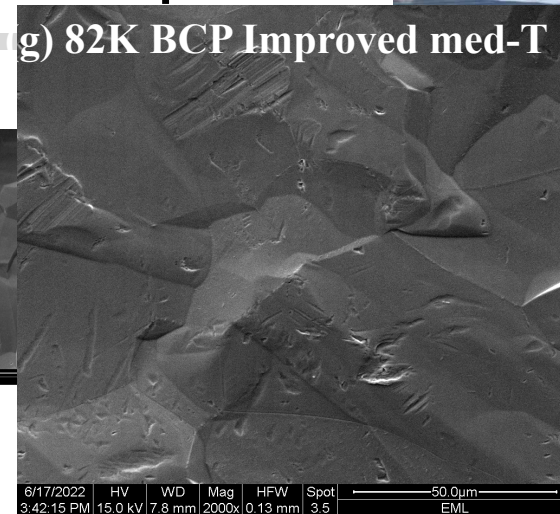


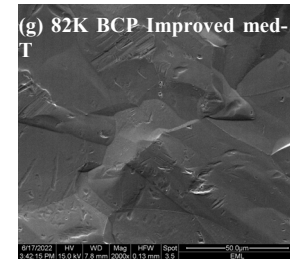
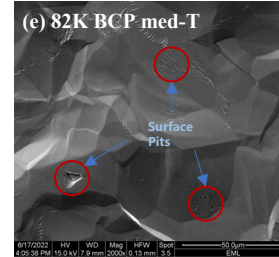
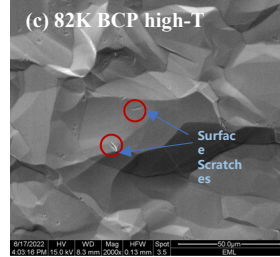
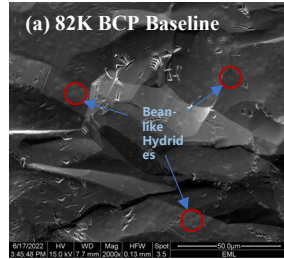


Comparisons among baked samples



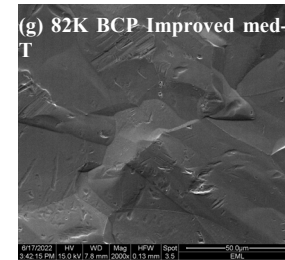
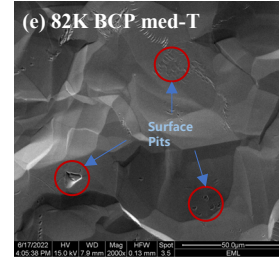
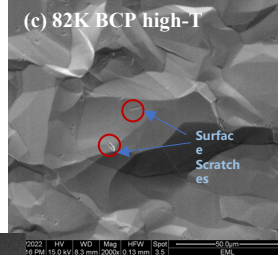
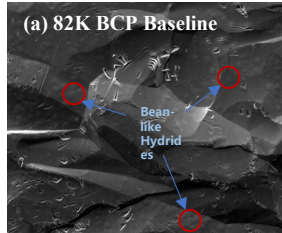
(g) 82K BCP Improved med-T



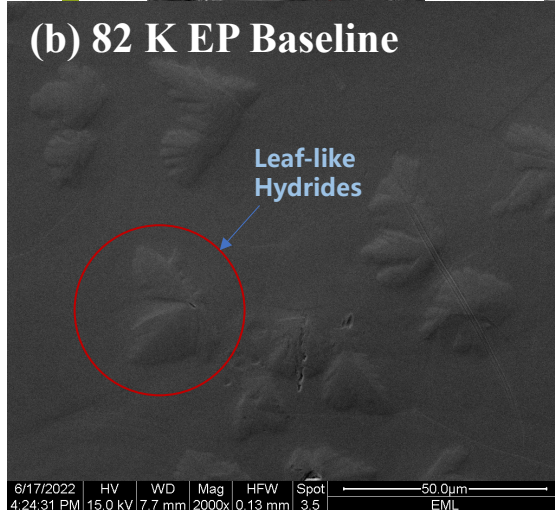


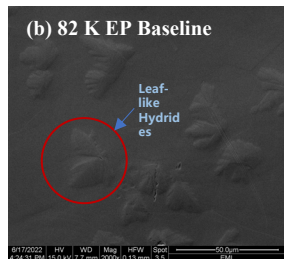
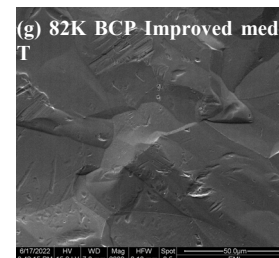
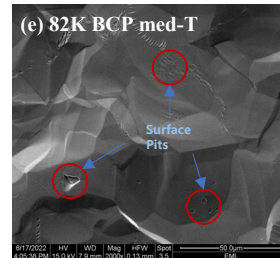
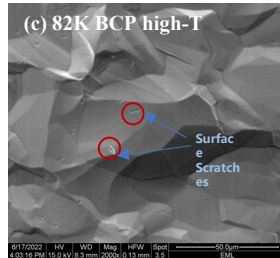
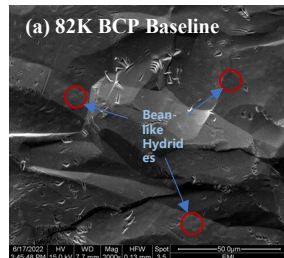
2.3

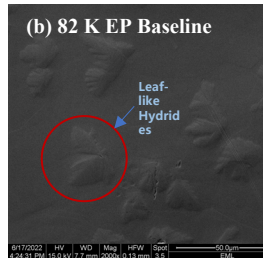
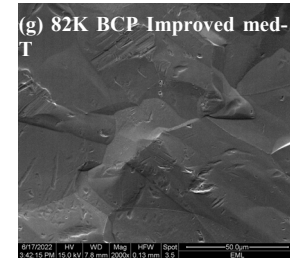
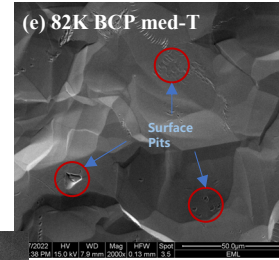
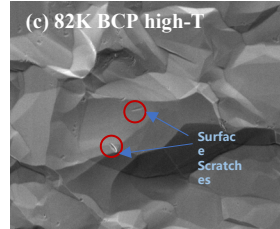
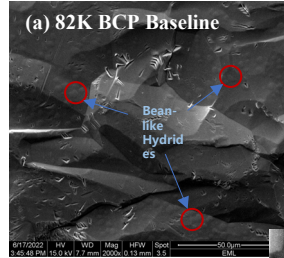
Comparisons among baked samples



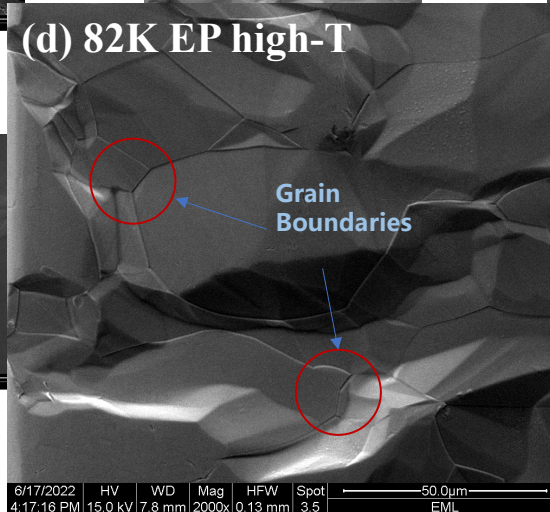
(b) 82 K EP Baseline





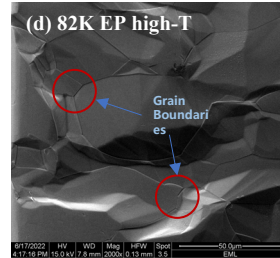
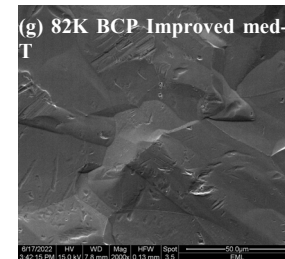
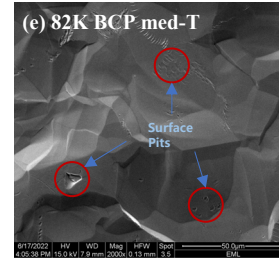
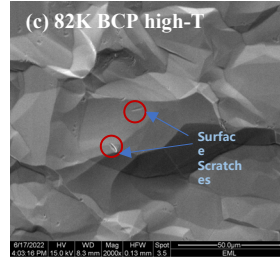
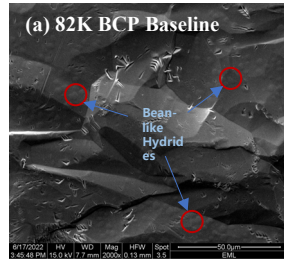


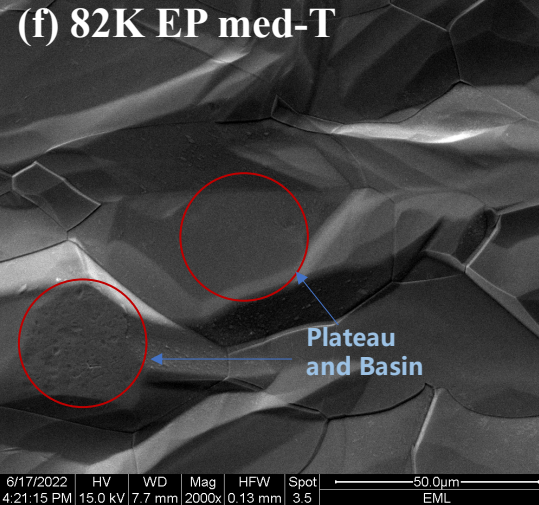
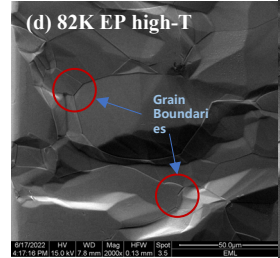
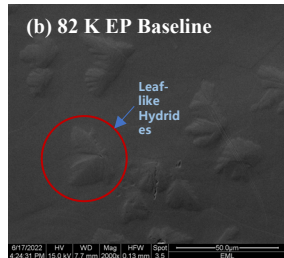
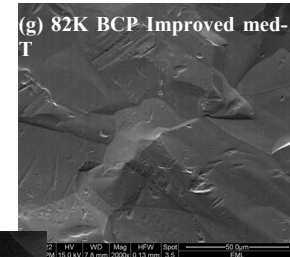
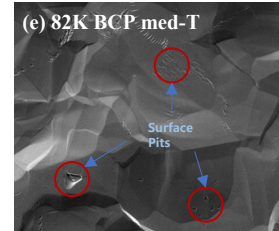
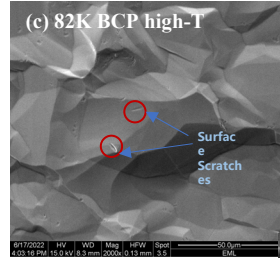
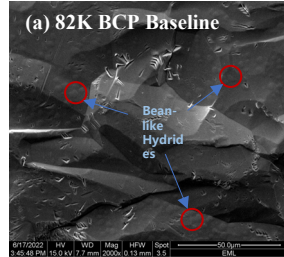
(d) 82K EP high-T

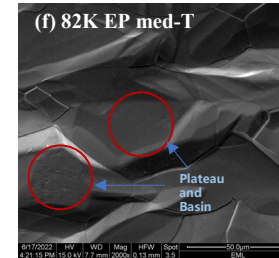
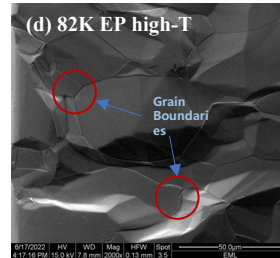
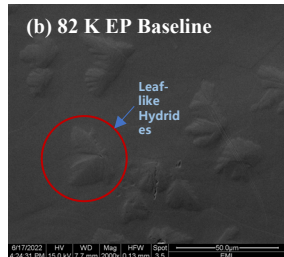
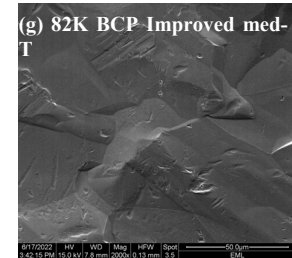
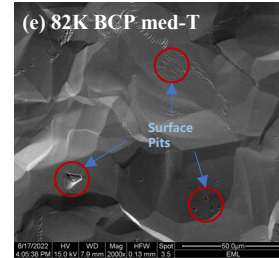
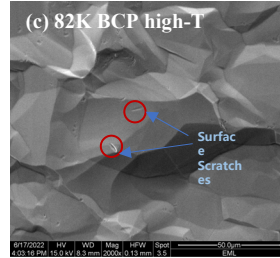
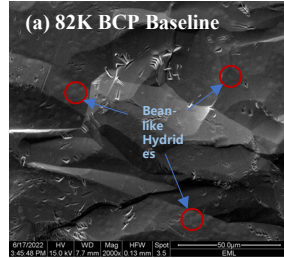


2.3

Comparisons among baked samples

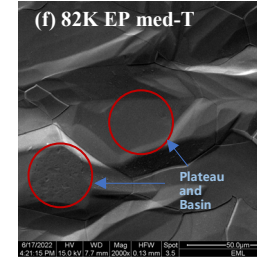
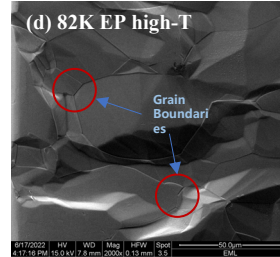
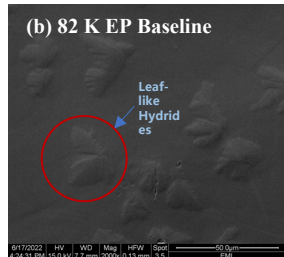
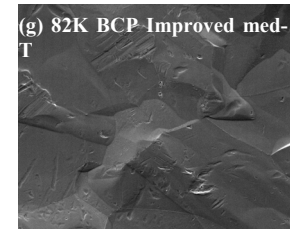
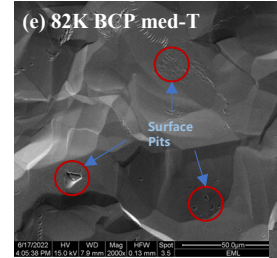
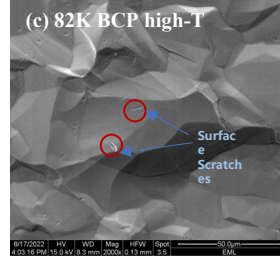
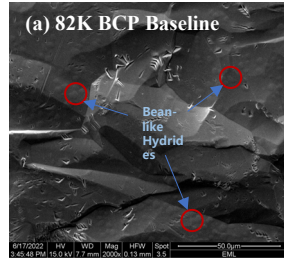




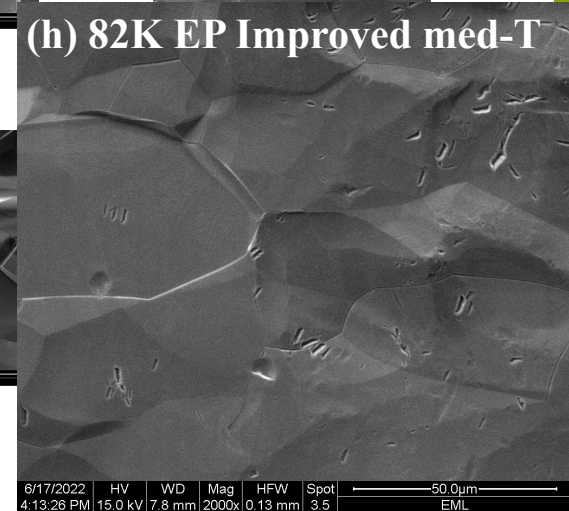


2.3

Comparisons among baked samples

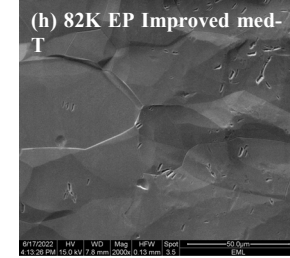
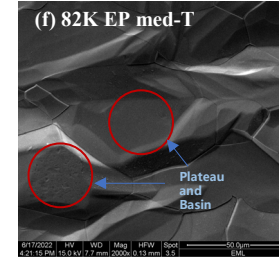
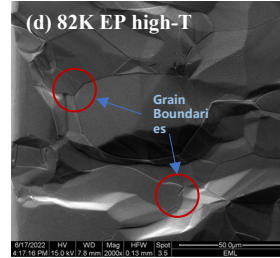
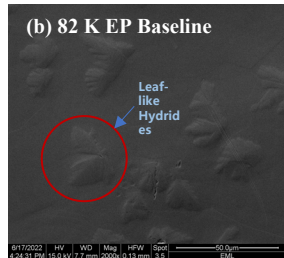
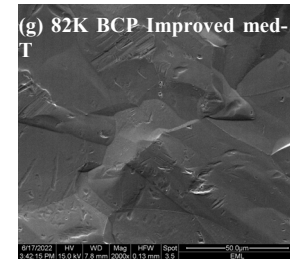
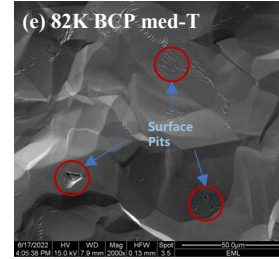
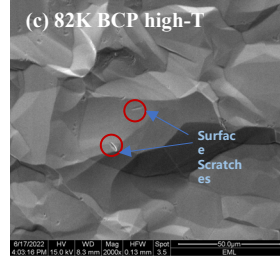
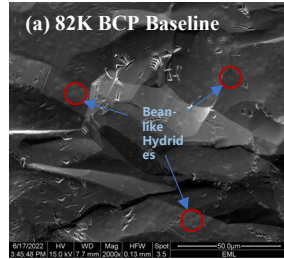


(h) 82K EP Improved med-T

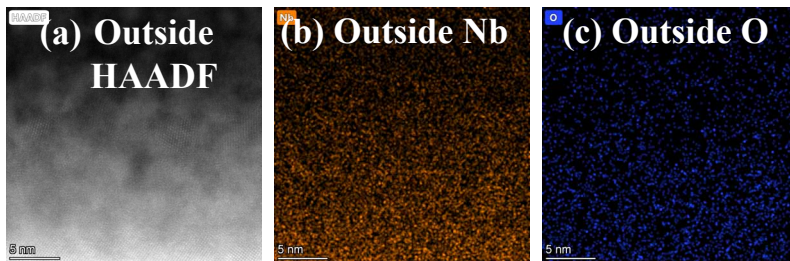


2.3

Comparisons among baked samples



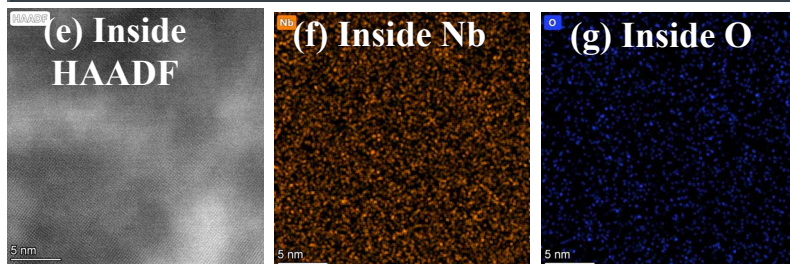
High-T, Medium-T, and Improved med-T can reduce Nb-H effectively



2022-11-02 09:46:18 Analysis of spectrum: Spectra from Area #1

(d) Outside EDS

Z	Element	Family	Atomic Fraction (%)	Atomic Error (%)	Mass Fraction (%)	Mass Error (%)	Fit error (%)
6	C	K	67.78	8.12	83.23	2.71	3.25
8	O	K	17.65	4.08	11.53	2.46	0.57
41	Nb	K	14.57	2.50	55.25	8.16	0.57



2022-11-02 09:45:18 Analysis of spectrum: Spectra from Area #1

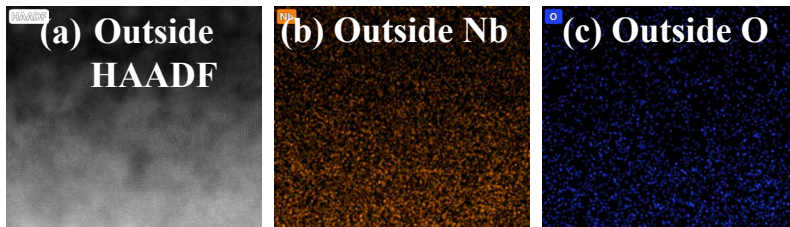
(h) Inside EDS

Z	Element	Family	Atomic Fraction (%)	Atomic Error (%)	Mass Fraction (%)	Mass Error (%)	Fit error (%)
6	C	K	0.00	0.24	0.00	0.03	0.00
8	O	K	8.27	2.42	1.53	0.36	1.29
41	Nb	K	91.73	22.76	98.47	17.59	0.11

2.4

Cross section

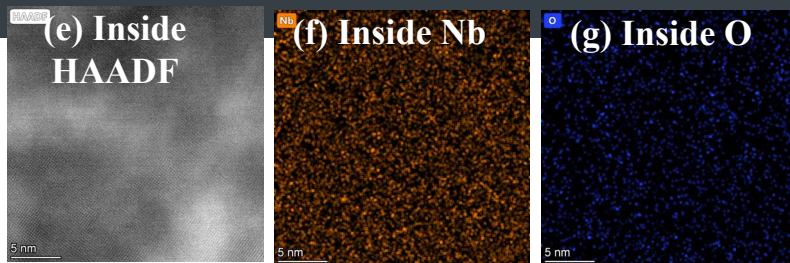
Baseline Nb sample



2022-11-02 09:46:18 Analysis of spectrum: Spectra from Area #1

(d) Outside EDS

Z	Element	Family	Atomic Fraction (%)	Atomic Error (%)	Mass Fraction (%)	Mass Error (%)	Fit error (%)
6	C	K	67.78	8.12	33.23	2.71	3.25
8	O	K	17.65	4.08	11.53	2.46	0.57
41	Nb	K	14.57	2.50	55.25	8.16	0.57



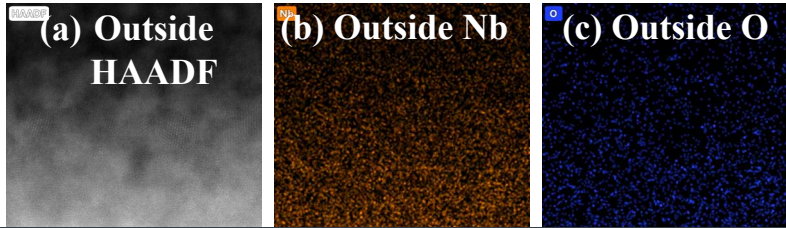
2022-11-02 09:45:18 Analysis of spectrum: Spectra from Area #1

(h) Inside EDS

Z	Element	Family	Atomic Fraction (%)	Atomic Error (%)	Mass Fraction (%)	Mass Error (%)	Fit error (%)
6	C	K	0.00	0.24	0.00	0.03	0.00
8	O	K	8.27	2.42	1.53	0.36	1.29
41	Nb	K	91.73	22.76	98.47	17.59	0.11

2.4

Cross section

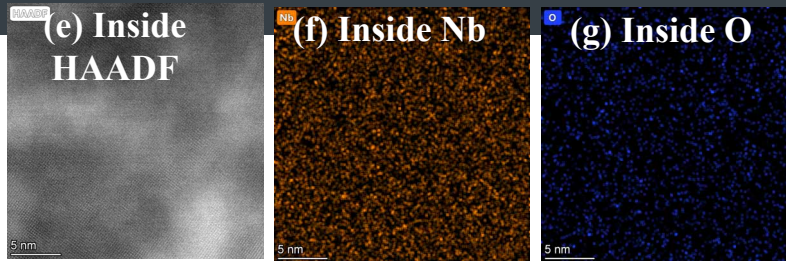
 Baseline Nb sample


- Out side $O:Nb > 1$, $C:O > 1$

2022-11-02 09:46:18 Analysis of spectrum: Spectra from Area #1

(d) Outside EDS

Z	Element	Family	Atomic Fraction (%)	Atomic Error (%)	Mass Fraction (%)	Mass Error (%)	Fit error (%)
6	C	K	67.78	8.12	33.23	2.71	3.25
8	O	K	17.65	4.08	11.53	2.46	0.57
41	Nb	K	14.57	2.50	55.25	8.16	0.57



2022-11-02 09:45:18 Analysis of spectrum: Spectra from Area #1

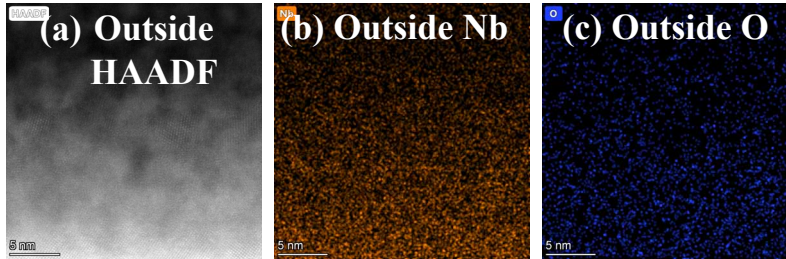
(h) Inside EDS

Z	Element	Family	Atomic Fraction (%)	Atomic Error (%)	Mass Fraction (%)	Mass Error (%)	Fit error (%)
6	C	K	0.00	0.24	0.00	0.03	0.00
8	O	K	8.27	2.42	1.53	0.36	1.29
41	Nb	K	91.73	22.76	98.47	17.59	0.11

2.4

Cross section

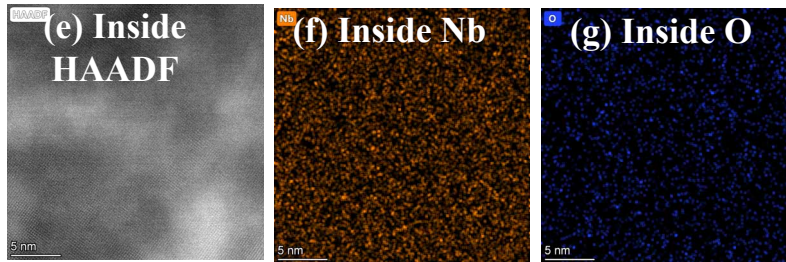
Baseline Nb sample



2022-11-02 09:46:18 Analysis of spectrum: Spectra from Area #1

(d) Outside EDS

Z	Element	Family	Atomic Fraction (%)	Atomic Error (%)	Mass Fraction (%)	Mass Error (%)	Fit error (%)
6	C	K	67.78	8.12	83.33	12.71	8.25
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2022-11-02 09:45:18 Analysis of spectrum: Spectra from Area #1

(h) Inside EDS

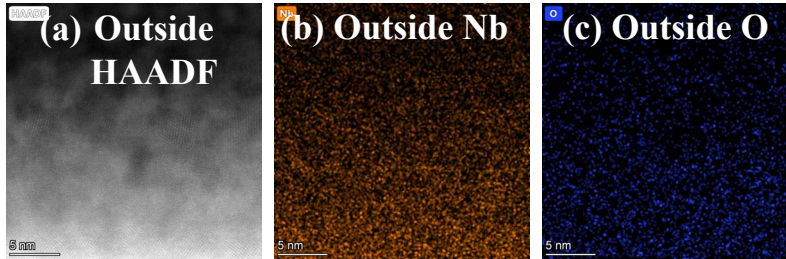
Z	Element	Family	Atomic Fraction (%)	Atomic Error (%)	Mass Fraction (%)	Mass Error (%)	Fit error (%)
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41	Nb	K	91.73	22.76	98.47	17.59	0.11

- Out side O:Nb > 1, C:O > 1

2.4

Cross section

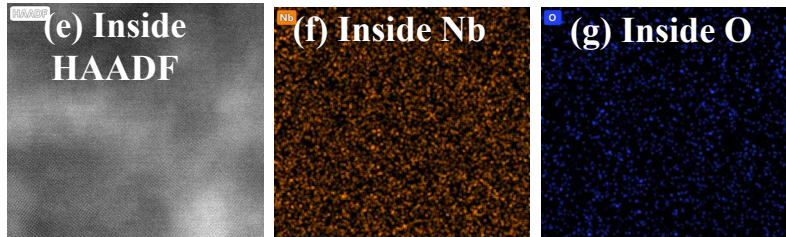
Baseline Nb sample



2022-11-02 09:46:18 Analysis of spectrum: Spectra from Area #1

(d) Outside EDS

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2022-11-02 09:45:18 Analysis of spectrum: Spectra from Area #1

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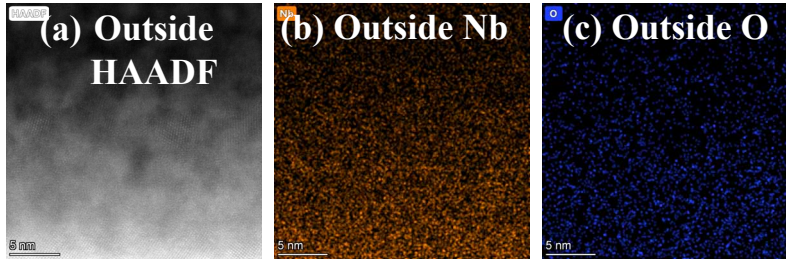
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41	Nb	K	91.73	22.76	98.47	17.59	0.11

- Out side O:Nb > 1, C:O > 1

2.4

Cross section

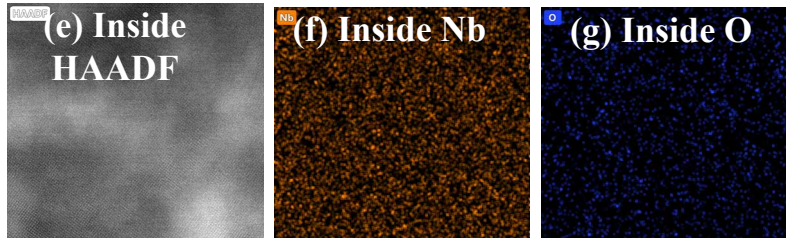
Baseline Nb sample



2022-11-02 09:46:18 Analysis of spectrum: Spectra from Area #1

(d) Outside EDS

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2022-11-02 09:45:18 Analysis of spectrum: Spectra from Area #1

(h) Inside EDS

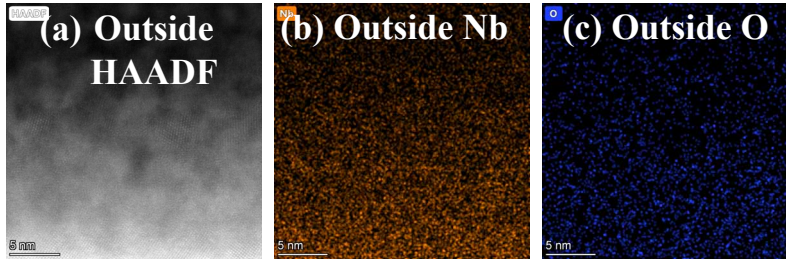
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8	O	K	8.27	2.42	1.53	0.36	1.29
41	Nb	K	91.73	22.76	98.47	17.59	0.11

- Out side O:Nb > 1, C:O > 1
- Inside O:Nb << 1, C:O ≈ 0

2.4

Cross section

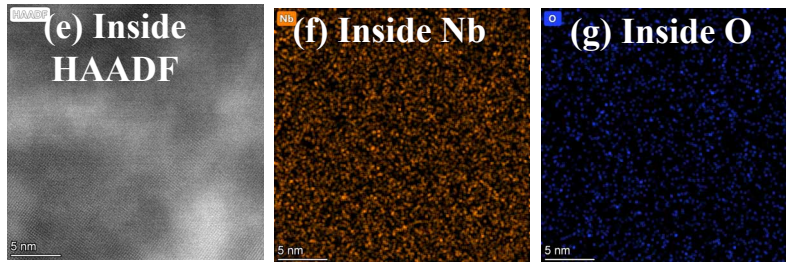
Baseline Nb sample



2022-11-02 09:46:18 Analysis of spectrum: Spectra from Area #1

(d) Outside EDS

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2022-11-02 09:45:18 Analysis of spectrum: Spectra from Area #1

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8	O	K	9.27	1.42	11.53	0.38	11.29
41	Nb	K	91.73	22.76	88.47	17.59	0.11

- Out side O:Nb > 1, C:O > 1
- Inside O:Nb << 1, C:O ≈ 0
- Protection layer, Nb-O compounds, suppress the release of Hydrogen
- Inevitable adventitious carbon
- Interstitial O/C sources during baking

Conclusion

5

First-Principles
Calculation

4

In-situ ARXPS

3

Cont.

Cavity Baking

1

In-situ ESEM

2

Introduction of in-situ ARXPS



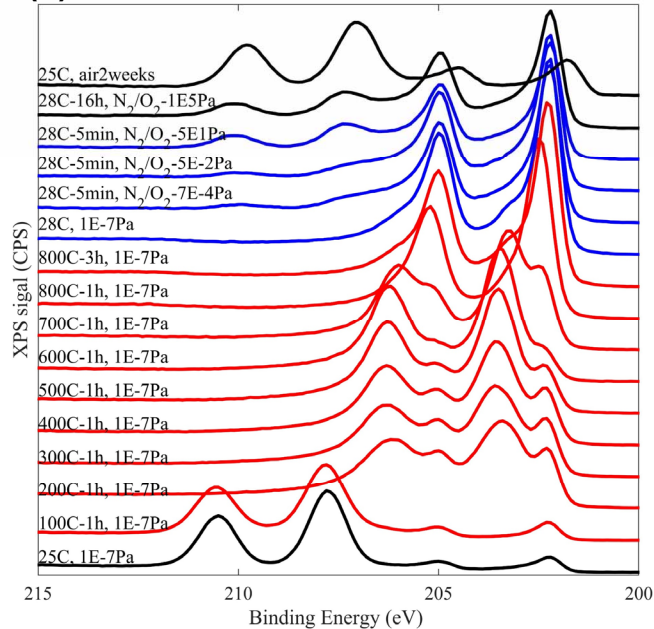
- Heavily chemically polished baseline samples
- In-situ angular resolved X-ray photoelectron spectroscopy (ARXPS): the larger the detection angle, the shallower the detection depth
- Baking chamber is separated from measurement chamber for high vacuum detection, quasi in-situ with accurate movement
- Raising from room temperature to 800°C with the gradient of 100°C, baking and measuring
- Focus on the peaks of Nb (mainly Nb-O compounds) and C (adventitious carbon and Nb-C compounds)

3.4

Temperature response of Nb-O



(a) 100-800°C

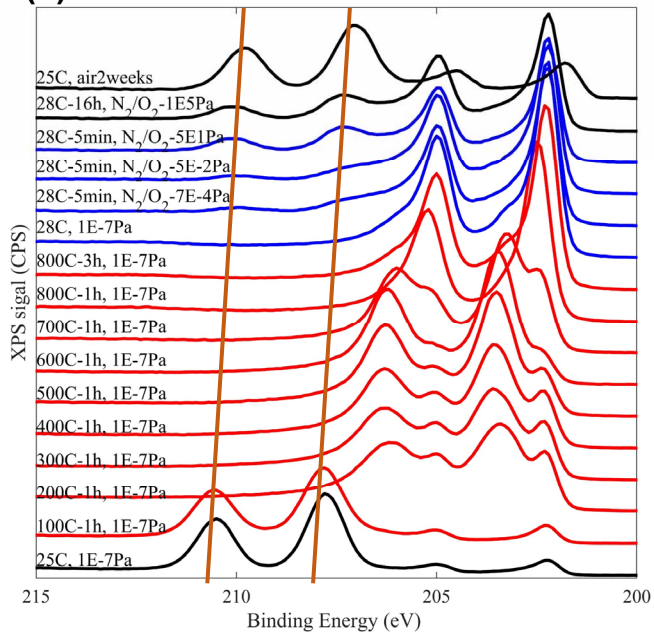


3.4

Temperature response of Nb-O



(a) 100-800°C

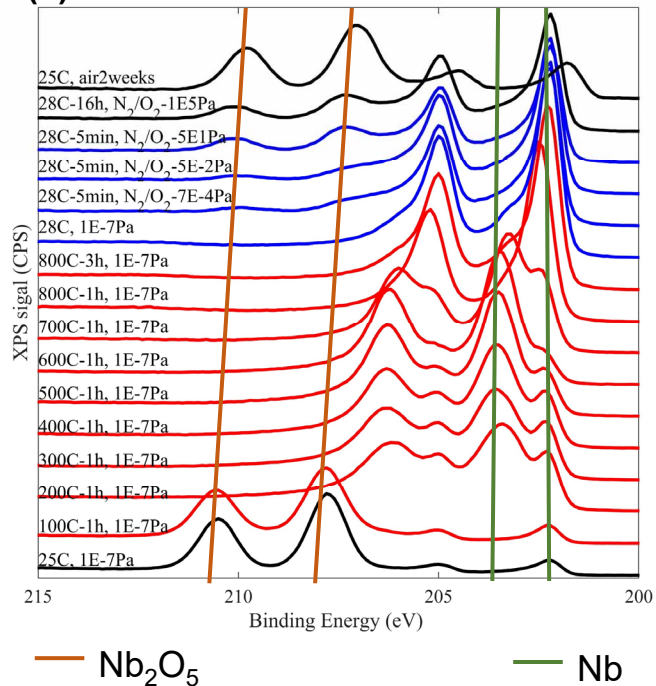
— Nb₂O₅

3.4

Temperature response of Nb-O



(a) 100-800°C

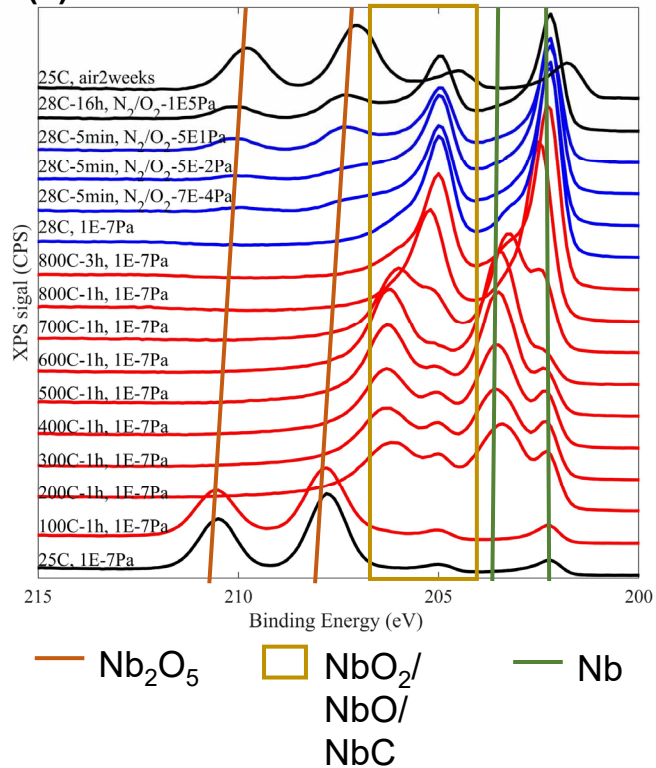


3.4

Temperature response of Nb-O



(a) 100-800°C



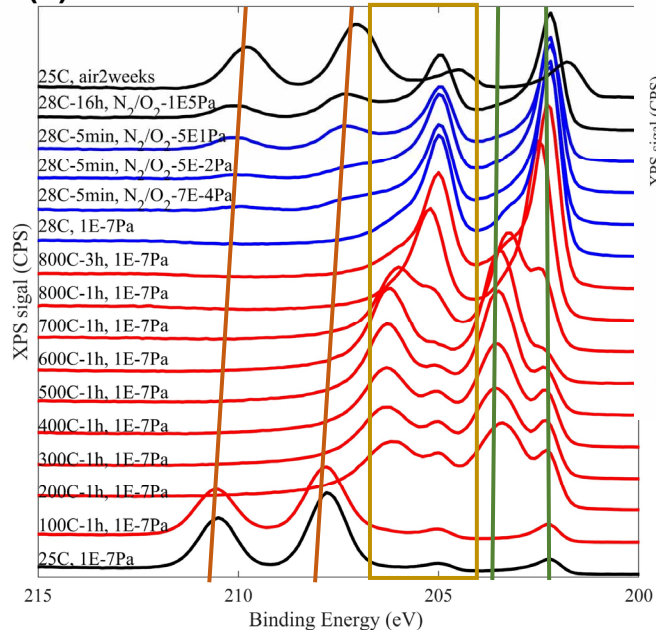
3.4

Temperature response of Nb-O

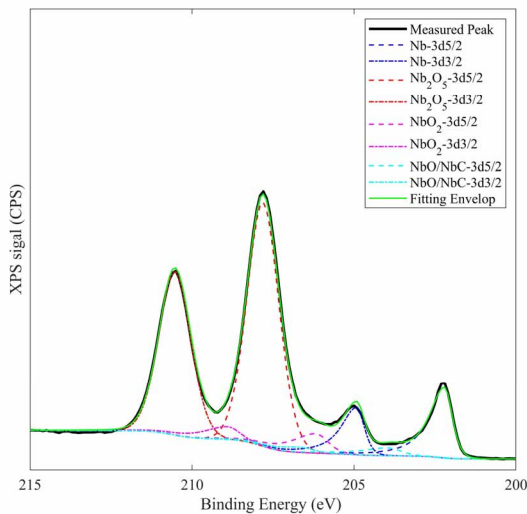
(b) 25°C



(a) 100-800°C



— Nb_2O_5
 □ $\text{NbO}_2/$
 $\text{NbO}/$
 NbC
 — Nb

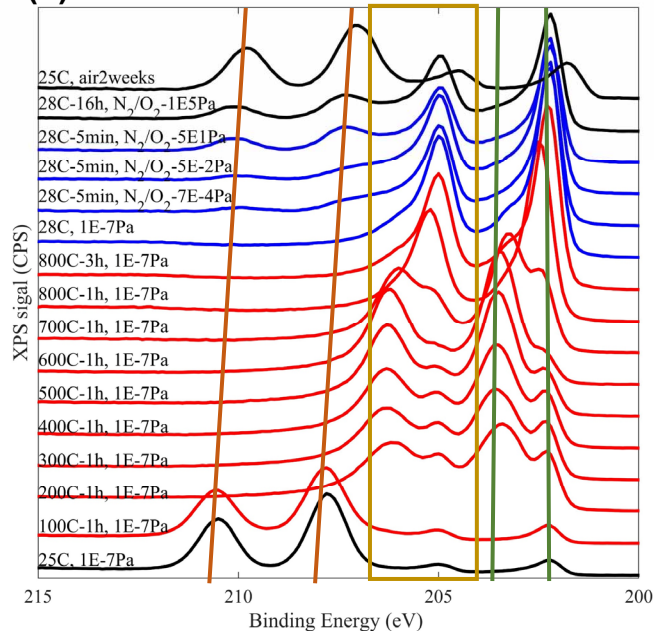


3.4

Temperature response of Nb-O

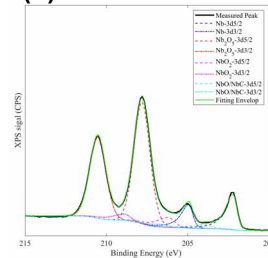


(a) 100-800°C



— Nb_2O_5
 $\text{NbO}_2/\text{NbO}/\text{NbC}$
 — Nb

(b) 25°C



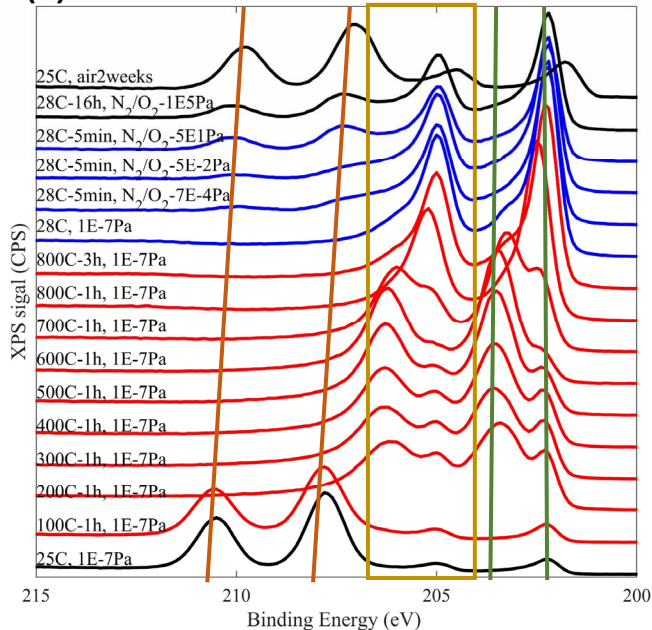
3.4

Temperature response of Nb-O

(c) 400°C 1 h

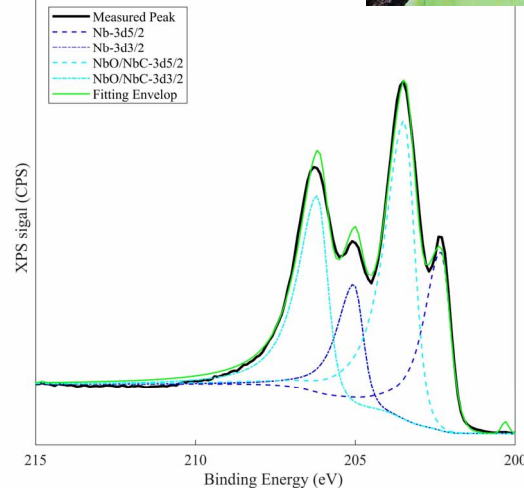
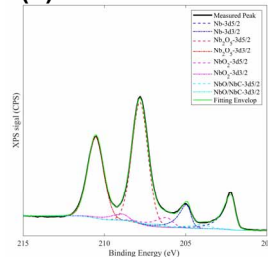


(a) 100-800°C



— Nb_2O_5
 — $\text{NbO}_2/\text{NbO}/\text{NbC}$
 — Nb

(b) 25°C

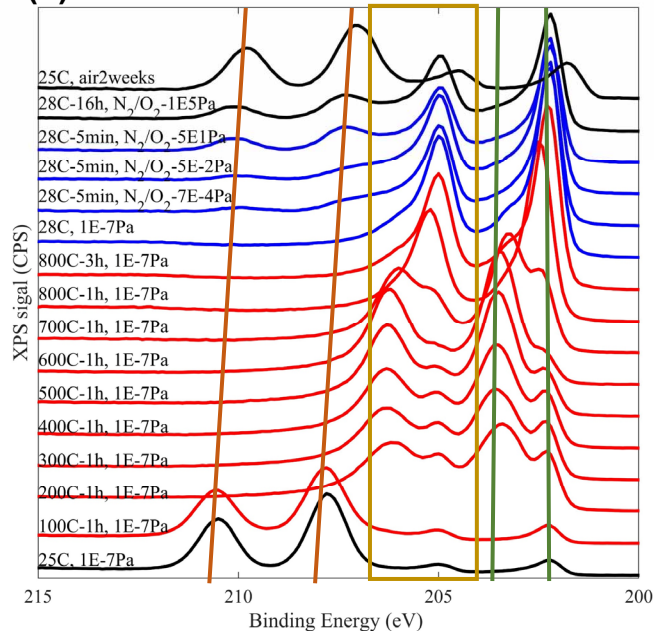


3.4

Temperature response of Nb-O

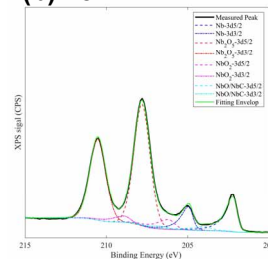


(a) 100-800°C

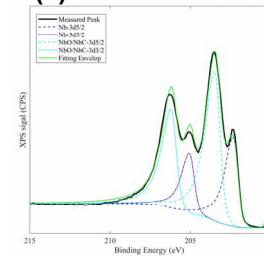


— Nb₂O₅ □ NbO₂/NbO/NbC — Nb

(b) 25°C



(c) 400°C 1 h

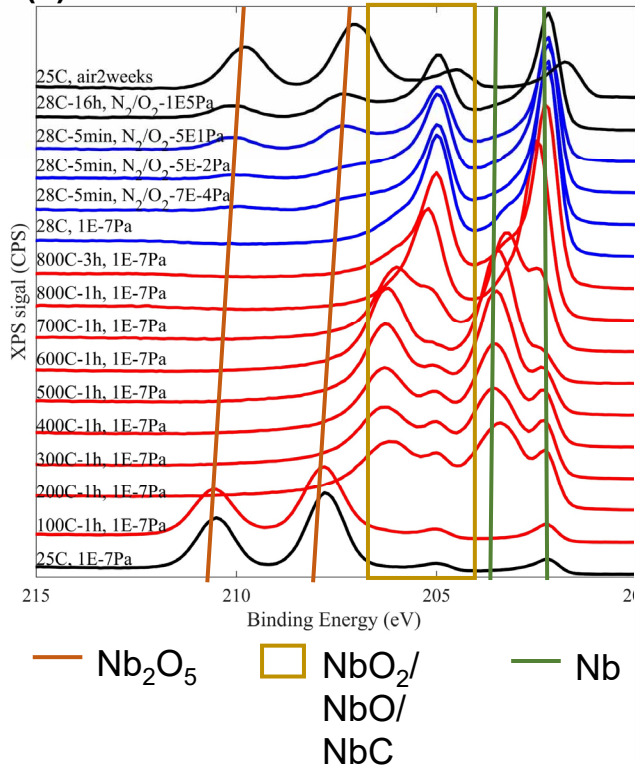


3.4

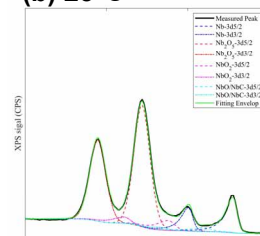
Temperature response of Nb-O



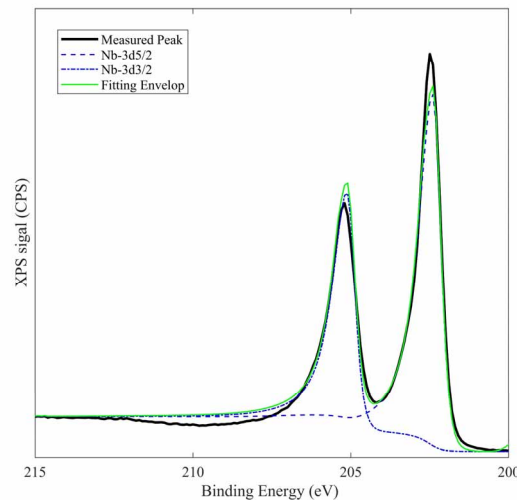
(a) 100-800°C



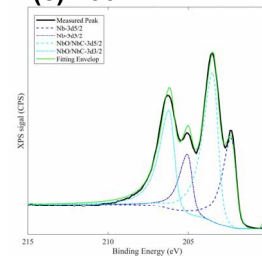
(b) 25°C



(d) 800°C 3 h



(c) 400°C 1 h

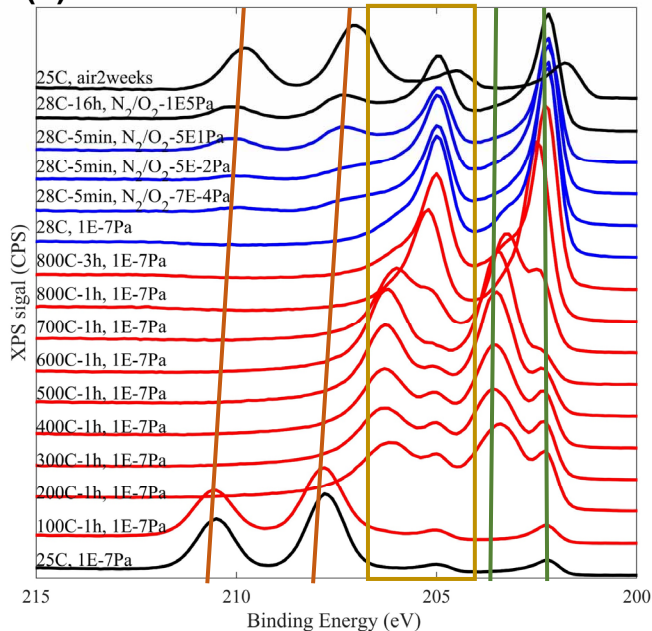


3.4

Temperature response of Nb-O

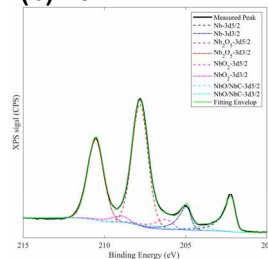


(a) 100-800°C

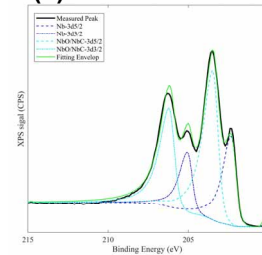


— Nb_2O_5
 — $\text{NbO}_2/\text{NbO}/\text{NbC}$
 — Nb

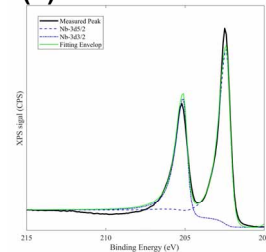
(b) 25°C



(c) 400°C 1 h



(d) 800°C 3 h

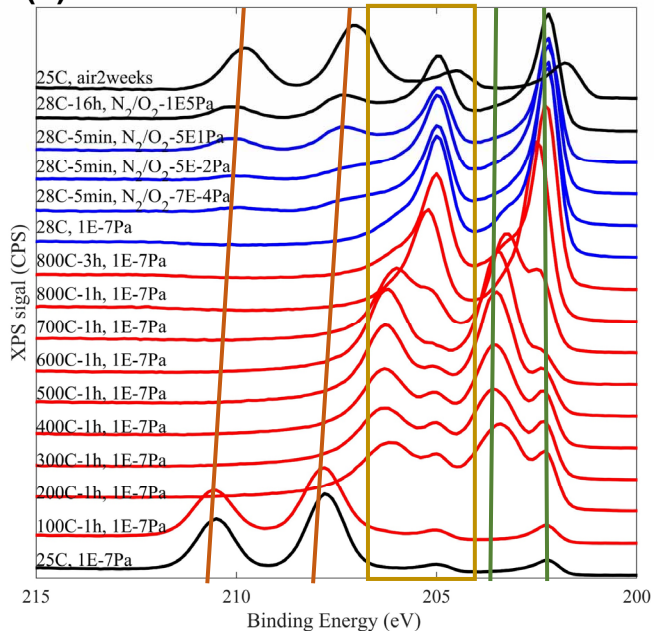


3.4

Temperature response of Nb-O

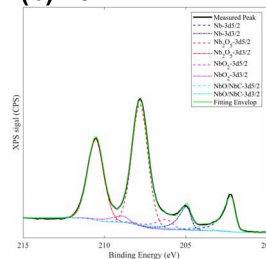


(a) 100-800°C

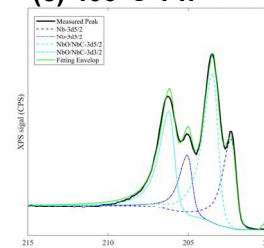


— Nb₂O₅ □ NbO₂/
 NbO/
 NbC — Nb

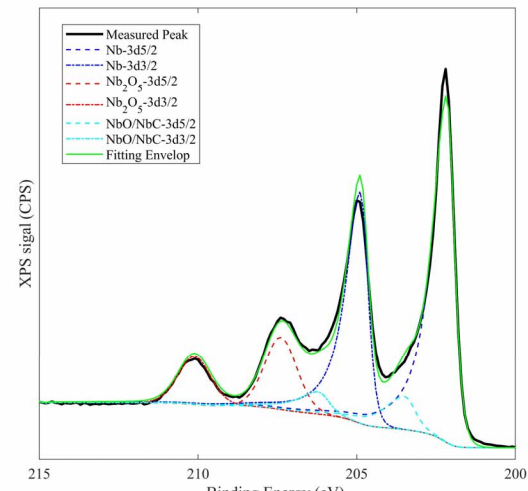
(b) 25°C



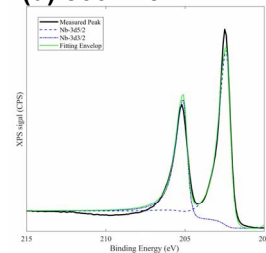
(c) 400°C 1 h



(e) 28°C N-O 16 h



(d) 800°C 3 h

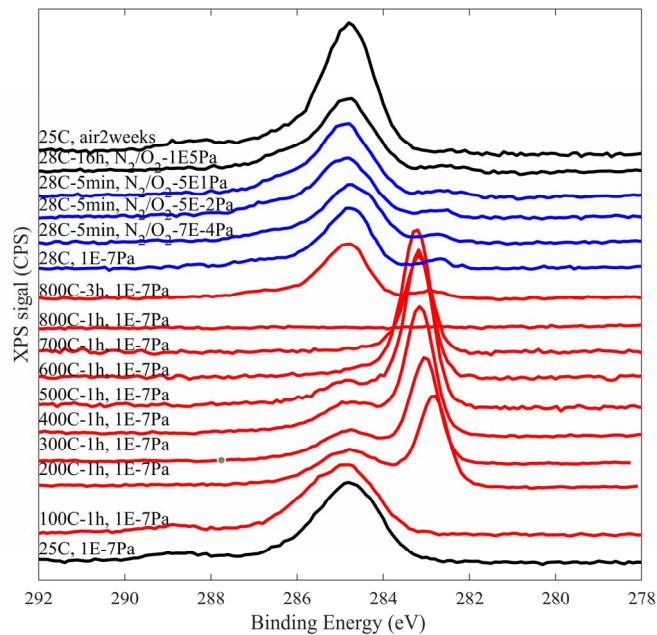


3.2

Temperature response of C



(a) 100-800°C

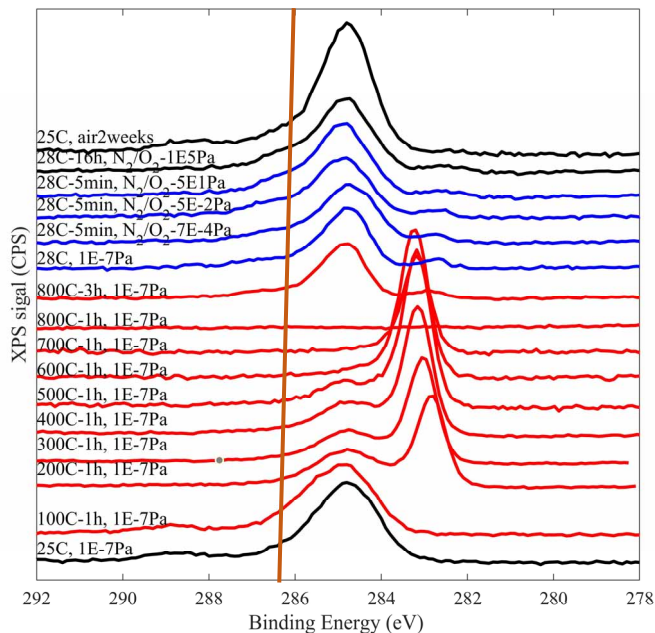


3.2

Temperature response of C



(a) 100-800°C



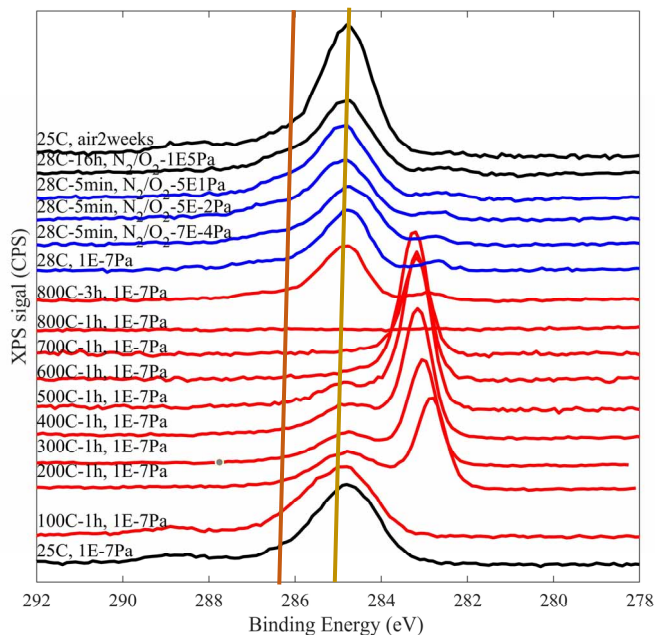
— C=O/
O=C-O/

3.2

Temperature response of C



(a) 100-800°C



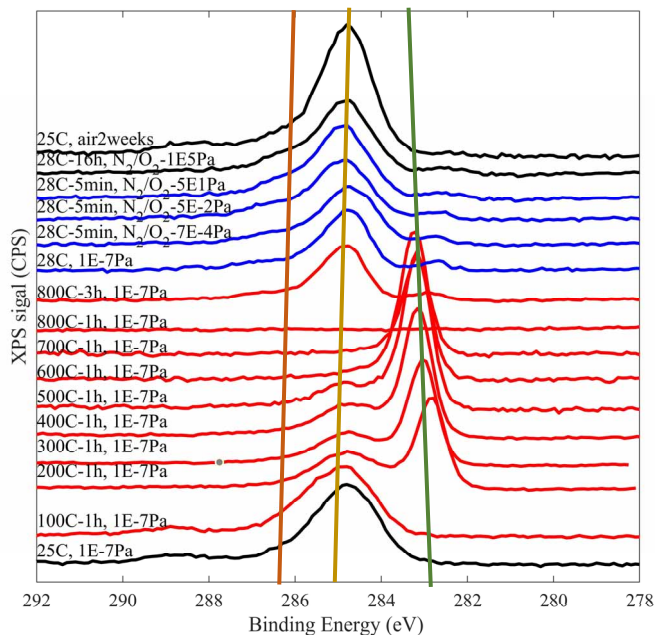
— C=O/
O=C-O/ — C-H

3.2

Temperature response of C



(a) 100-800°C



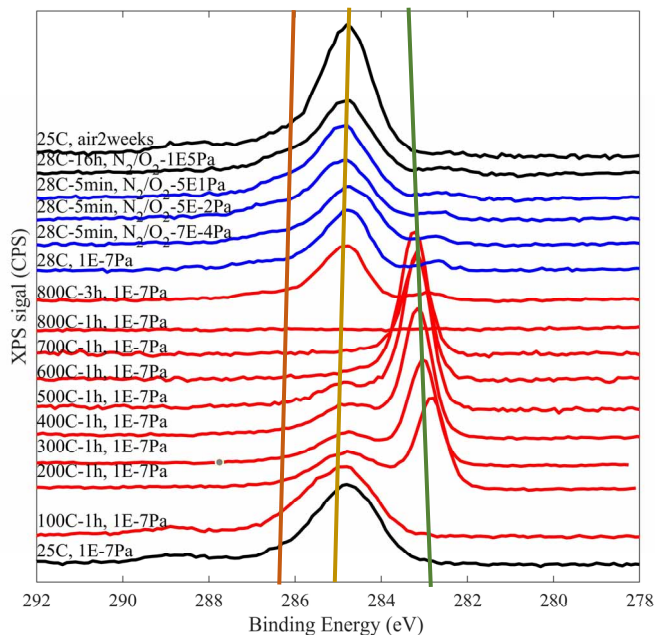
— C=O/
O=C-O/ — C-H — NbC

Temperature response of C

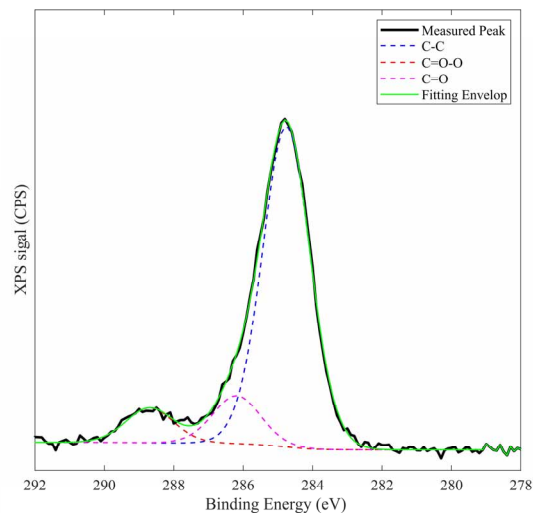
(b) 25°C



(a) 100-800°C



— C=O/
O=C-O/ — C-H — NbC

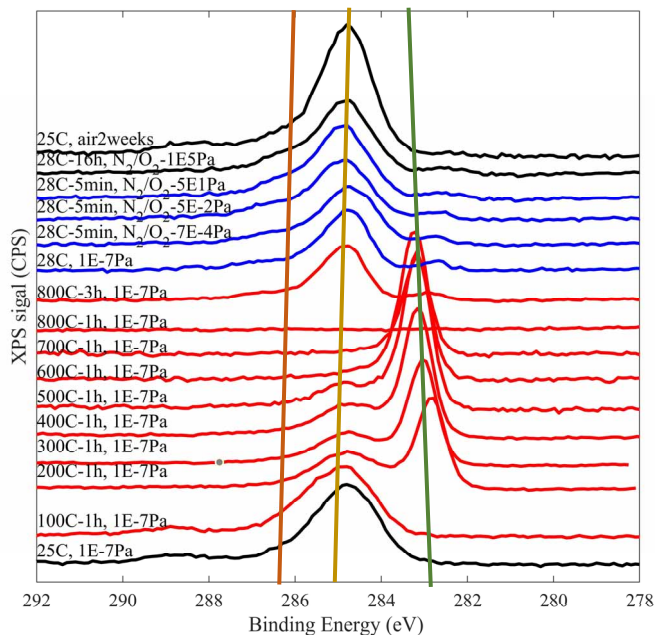


3.2

Temperature response of C

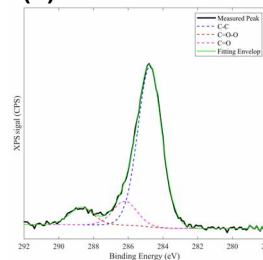


(a) 100-800°C



— C=O/
O=C-O/ — C-H — NbC

(b) 25°C



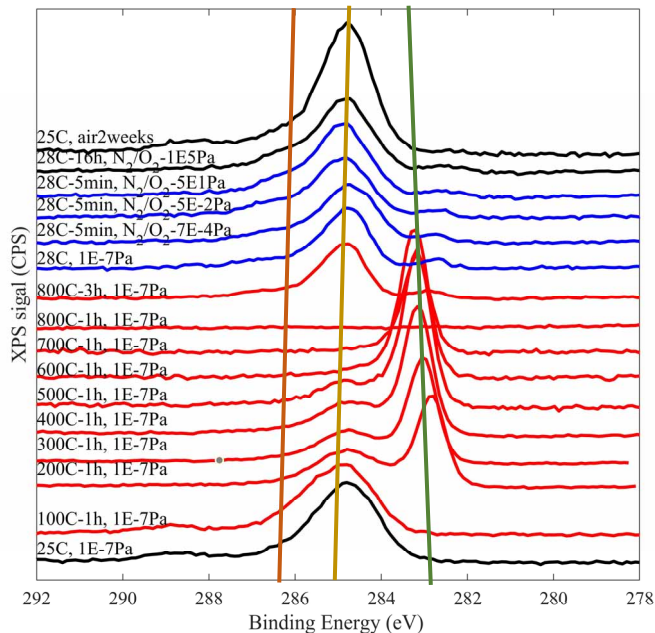
3.2

Temperature response of C

(c) 400°C 1 h

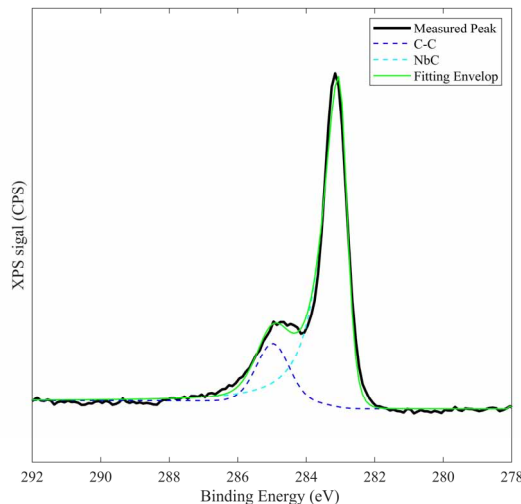
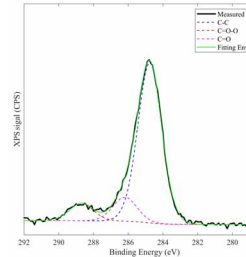


(a) 100-800°C



— C=O/
O=C-O/ — C-H — NbC

(b) 25°C

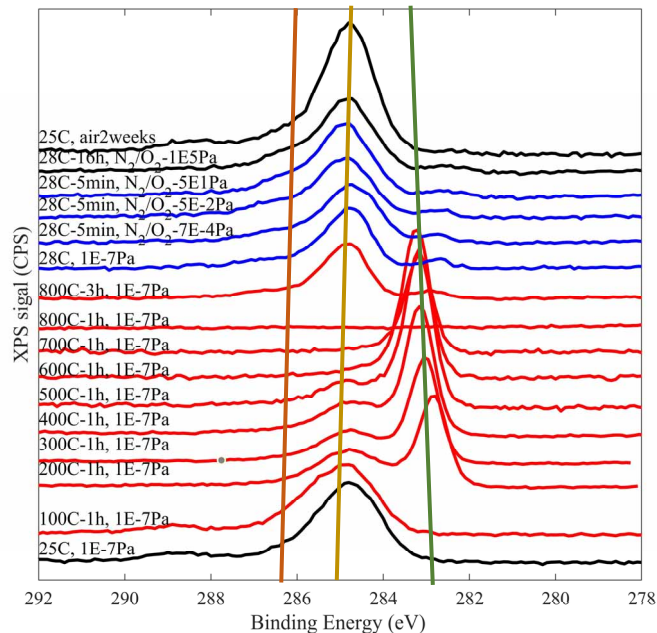


3.2

Temperature response of C

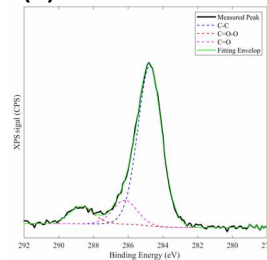


(a) 100-800°C

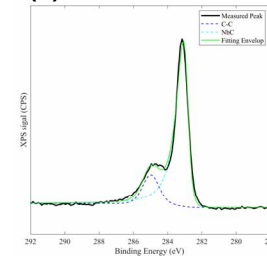


— C=O/
O=C-O/ — C-H — NbC

(b) 25°C



(c) 400°C 1 h

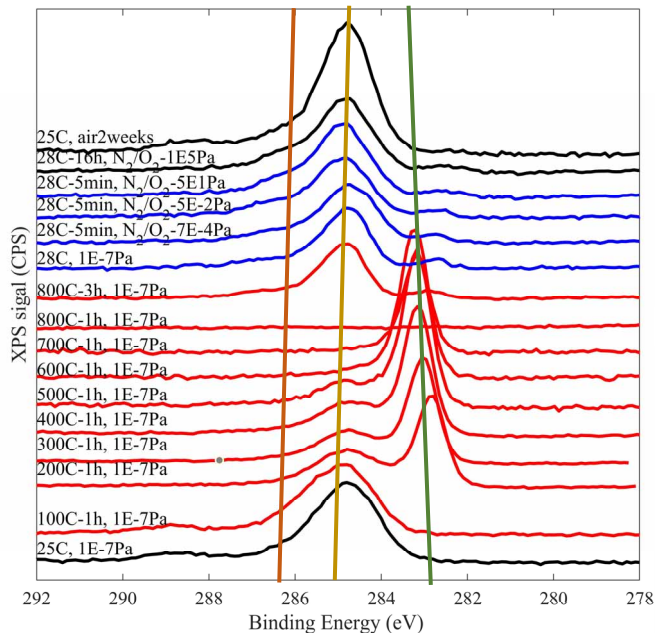


3.2

Temperature response of C

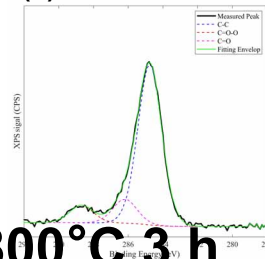


(a) 100-800°C

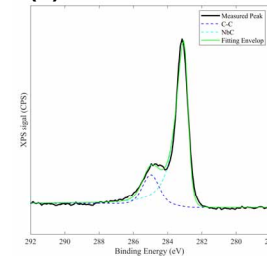


— C=O/
 O=C-O/
— C-H
— NbC

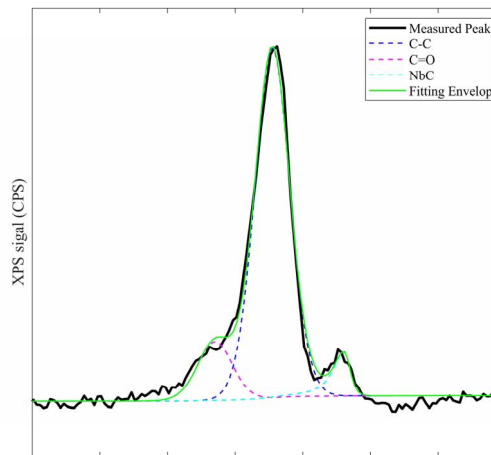
(b) 25°C



(c) 400°C 1 h

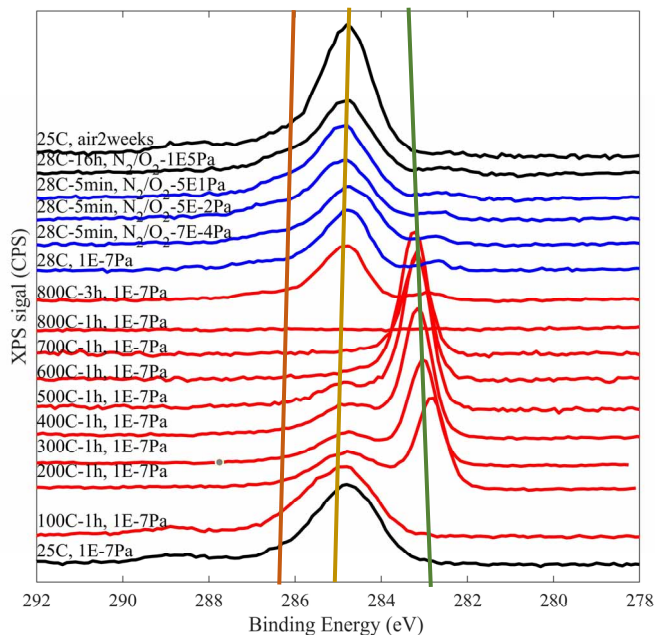


(d) 800°C 3 h



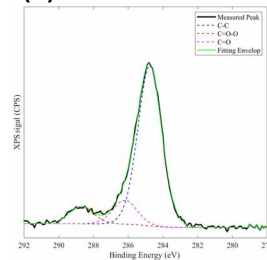


(a) 100-800°C

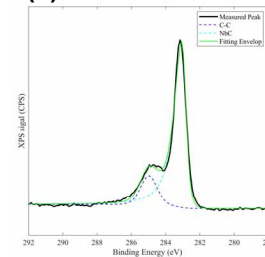


— C=O/
O=C-O/ — C-H — NbC

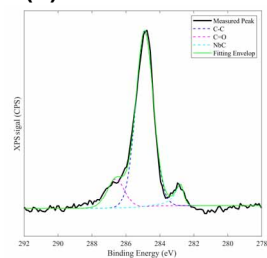
(b) 25°C



(c) 400°C 1 h



(d) 800°C 3 h

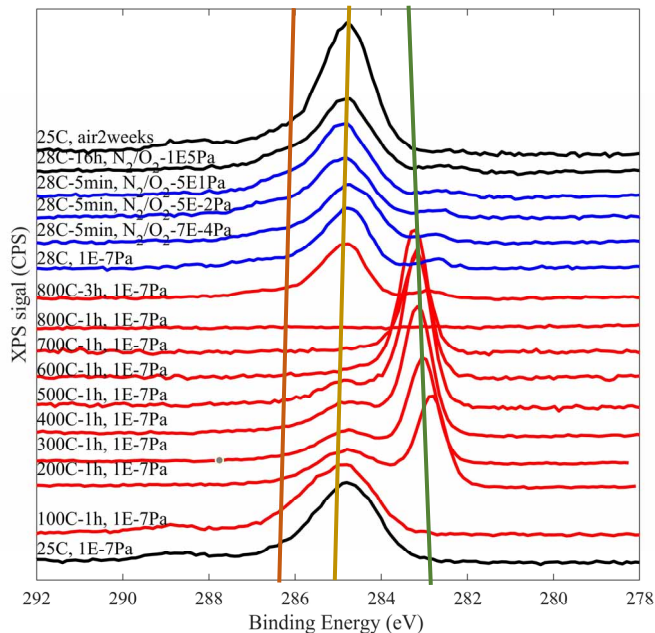


3.2

Temperature response of C

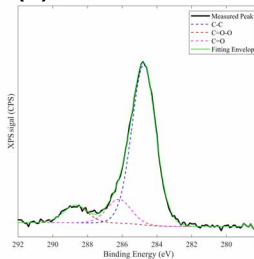


(a) 100-800°C

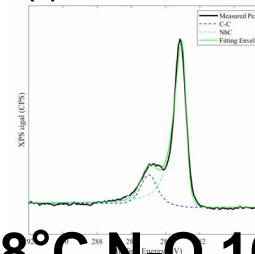


— C=O/
O=C-O/ — C-H — NbC

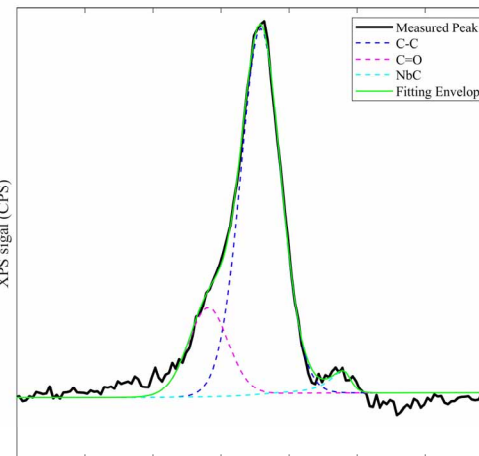
(b) 25°C



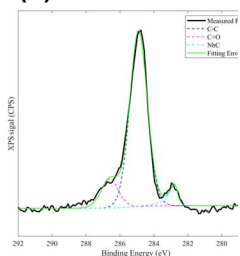
(c) 400°C 1 h



(e) 28°C N-O 16 h

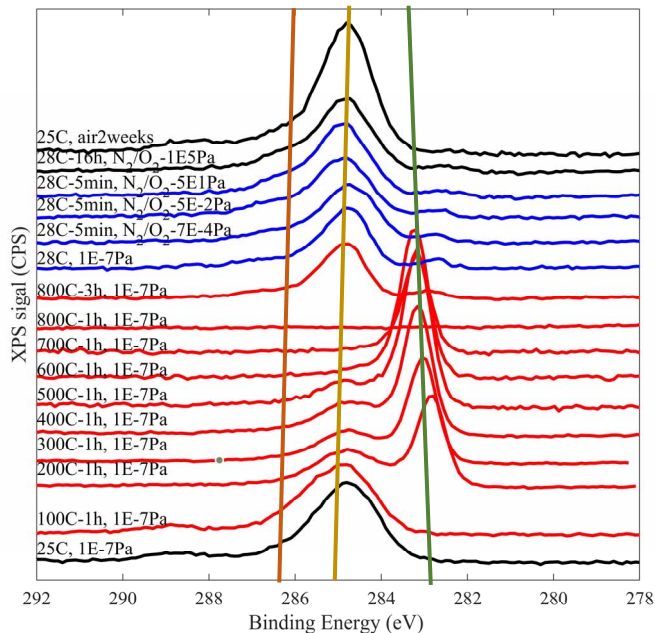


(d) 800°C 3 h



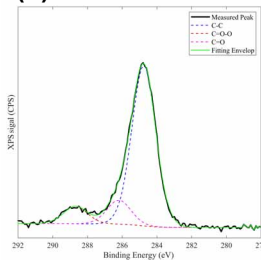


(a) 100-800°C

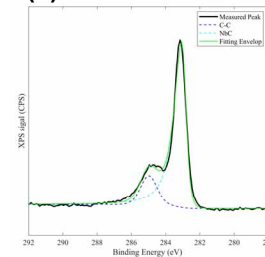


— C=O/
O=C-O/ — C-H — NbC

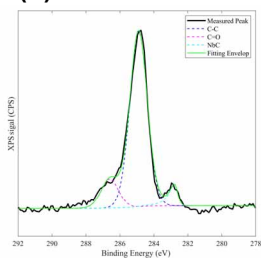
(b) 25°C



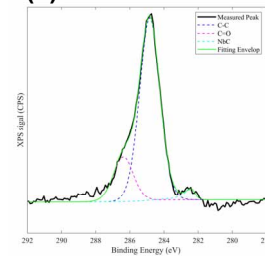
(c) 400°C 1 h



(d) 800°C 3 h

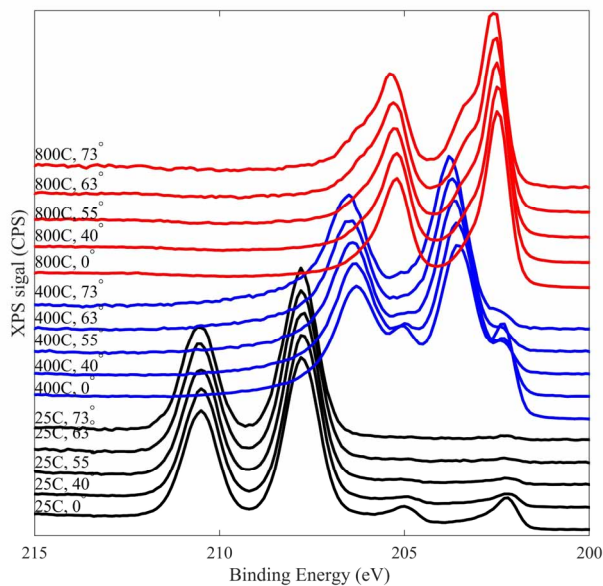


(e) 28°C N-O 16 h





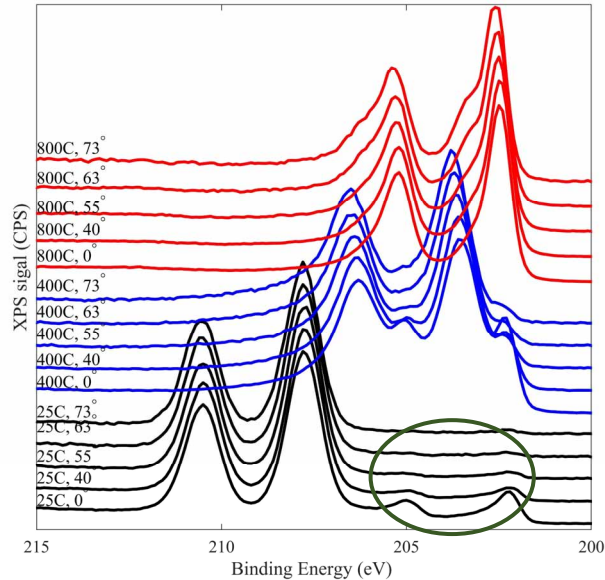
(a) 25, 400, 800°C - Nb Peaks



Depth resolution by changing angle



(a) 25, 400, 800°C - Nb Peaks

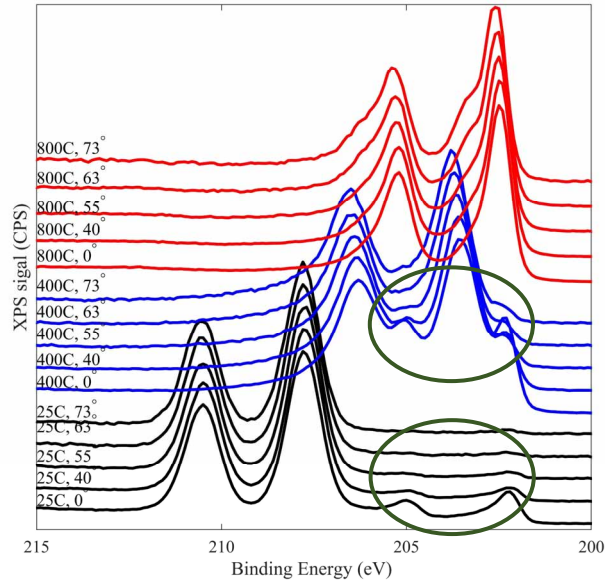


3.3

Depth resolution by changing angle



(a) 25, 400, 800°C - Nb Peaks

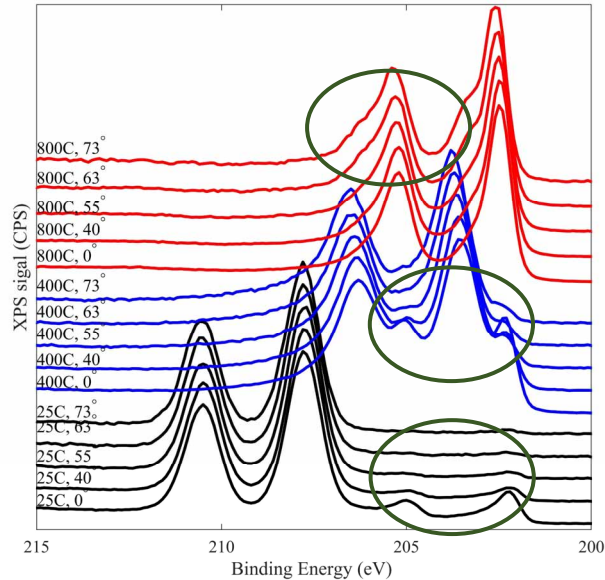


3.3

Depth resolution by changing angle



(a) 25, 400, 800°C - Nb Peaks

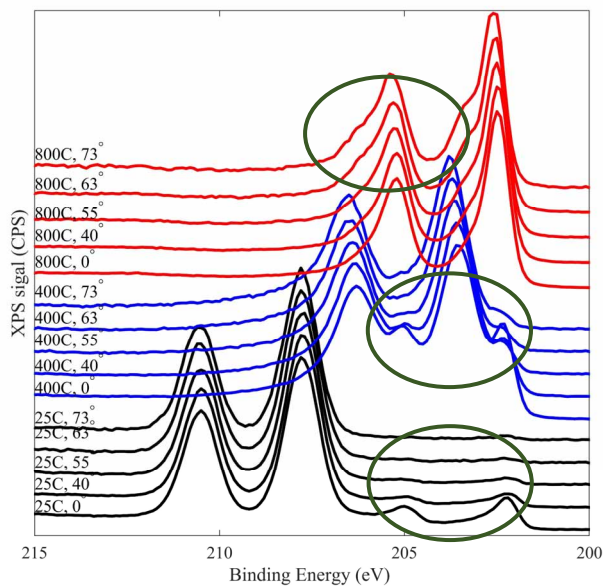


3.3

Depth resolution by changing angle



(a) 25, 400, 800°C - Nb Peaks



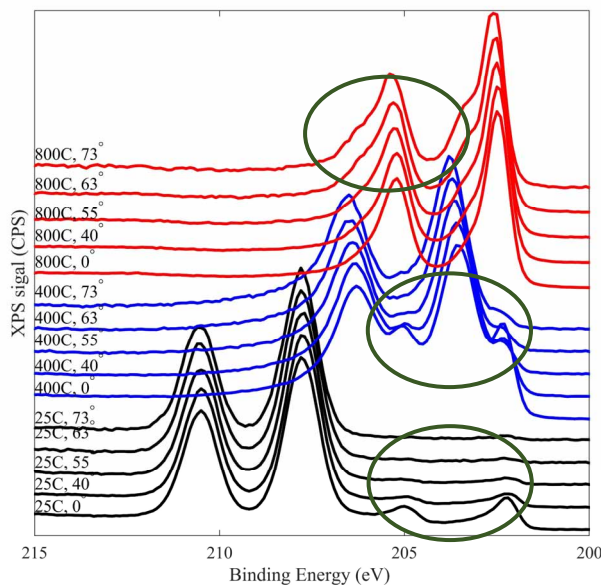
- Surface-Higher valence Nb
- Inner-Lower valence Nb

3.3

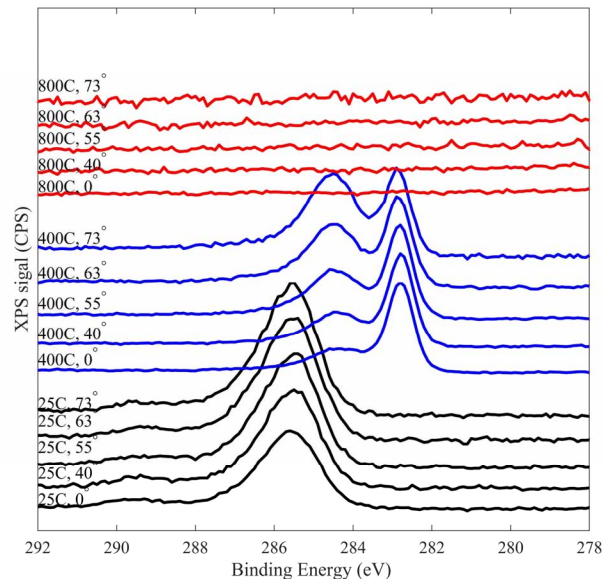
Depth resolution by changing angle



(a) 25, 400, 800°C - Nb Peaks



(b) 25, 400, 800°C - C Peaks



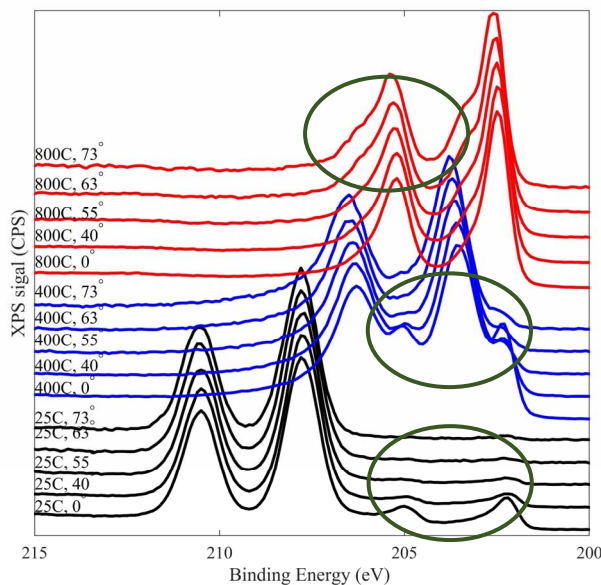
- Surface-Higher valence Nb
- Inner-Lower valence Nb

3.3

Depth resolution by changing angle

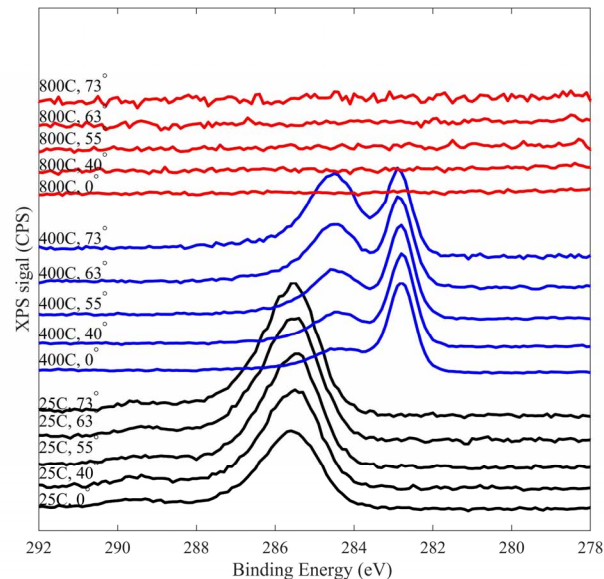


(a) 25, 400, 800°C - Nb Peaks



- Surface-Higher valence Nb
- Inner-Lower valence Nb

(b) 25, 400, 800°C - C Peaks



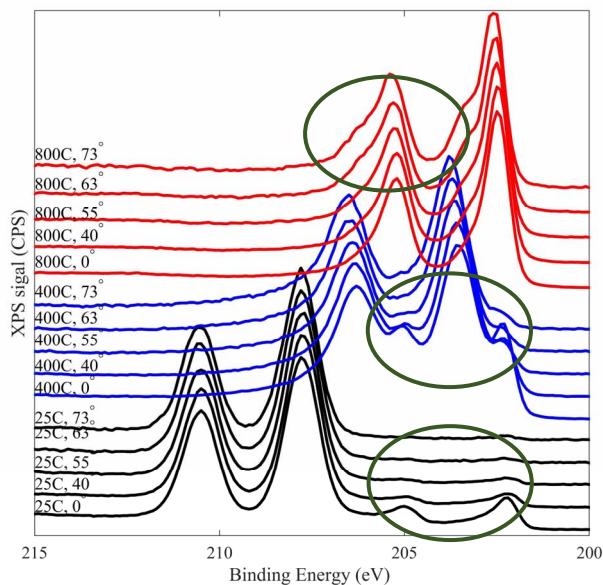
- Surface-Adventitious C
- Inner-Nb-C Compound

3.3

Depth resolution by changing angle

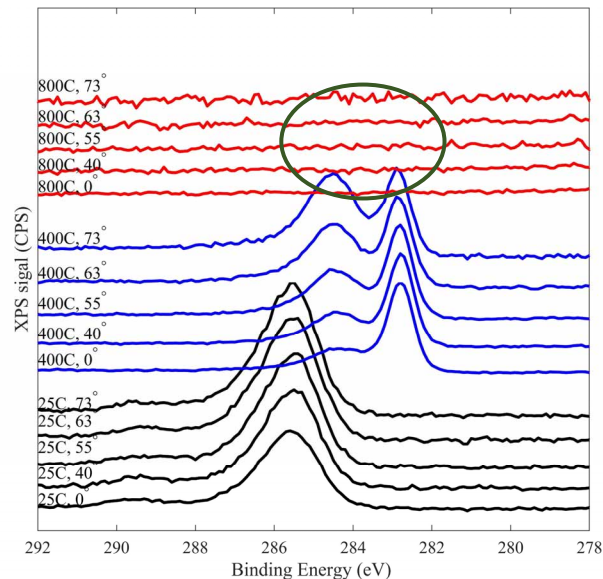


(a) 25, 400, 800°C - Nb Peaks

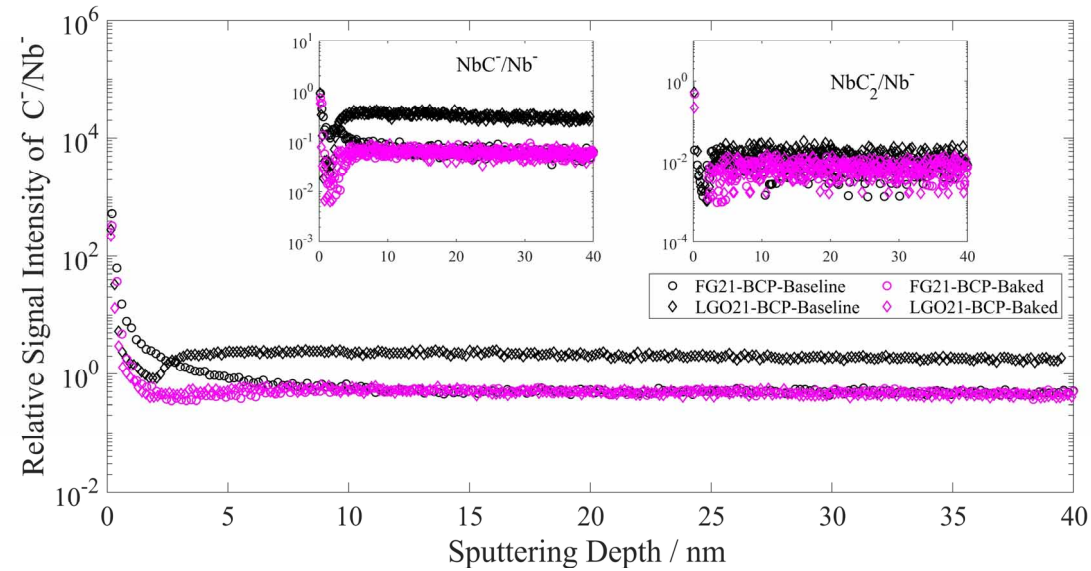


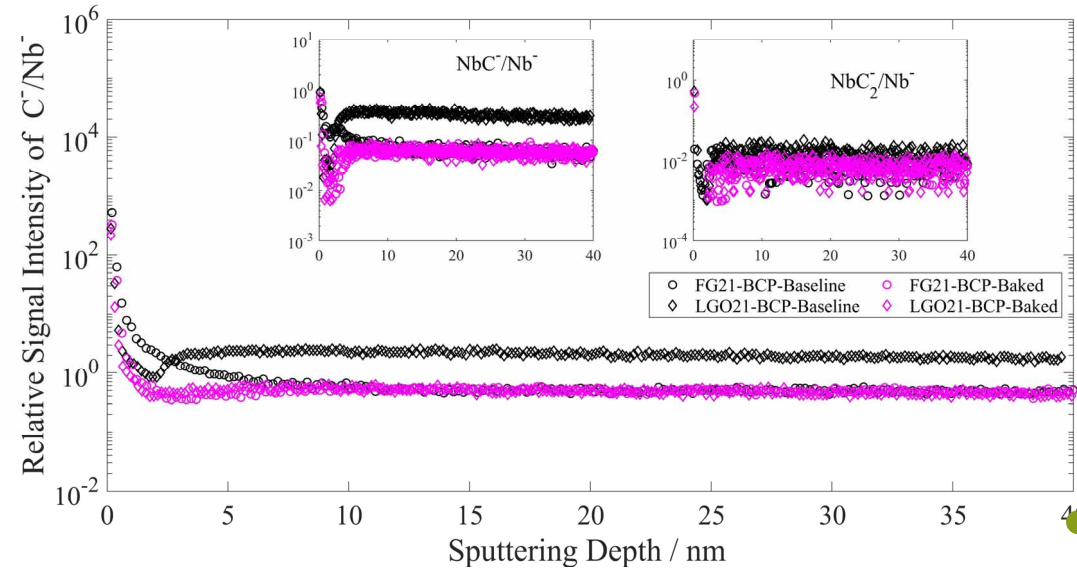
- Surface-Higher valence Nb
- Inner-Lower valence Nb

(b) 25, 400, 800°C - C Peaks



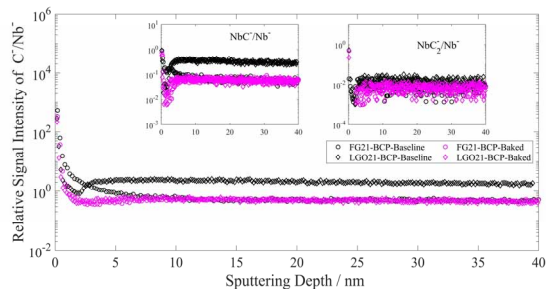
- Surface-Adventitious C
- Inner-Nb-C Compound

TOF-SIMS results  Before and after baking

TOF-SIMS results  Before and after bakingC: C, NbC, NbC₂

3.4

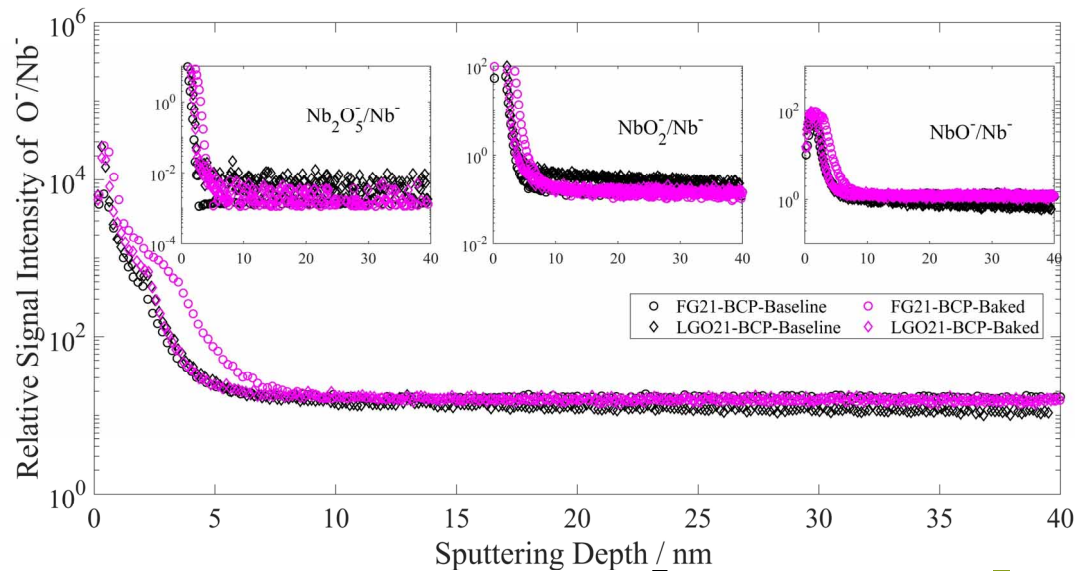
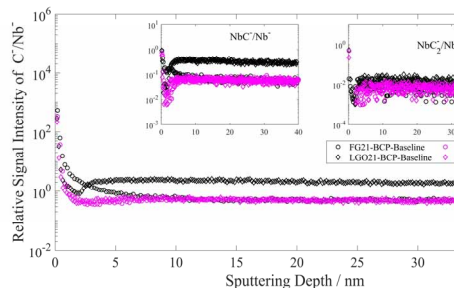
TOF-SIMS results Before and after baking



- C: C, NbC, NbC₂

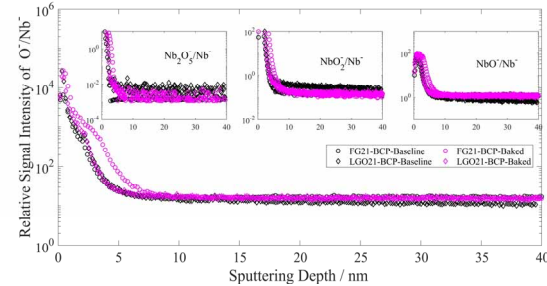
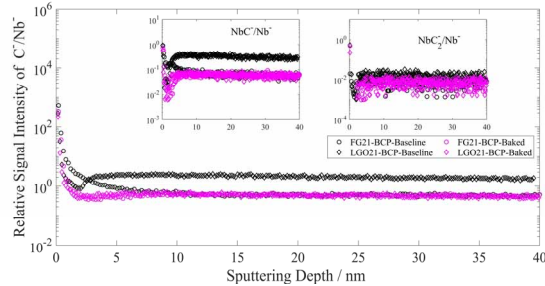
3.4

TOF-SIMS results Before and after baking



3.4

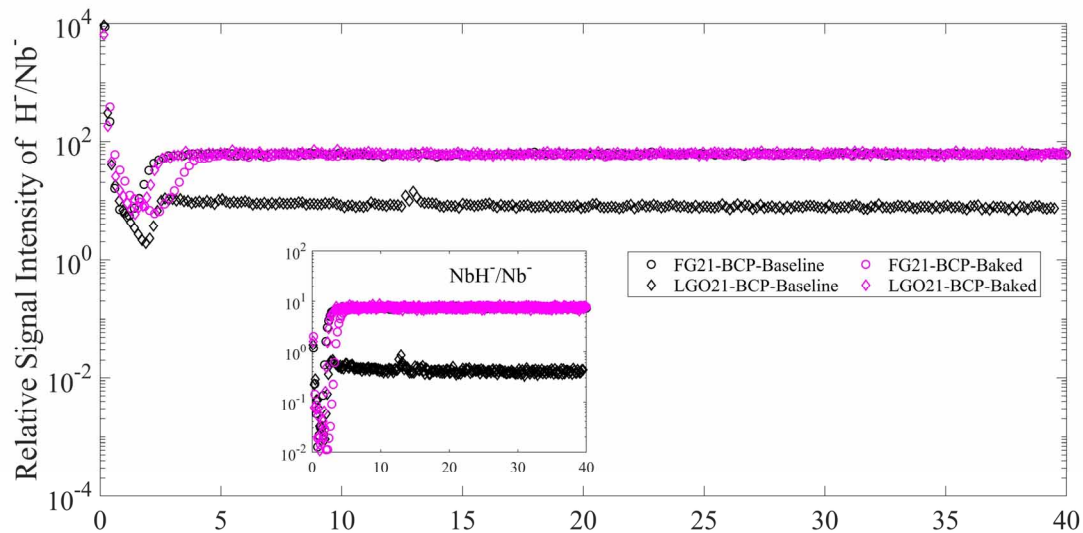
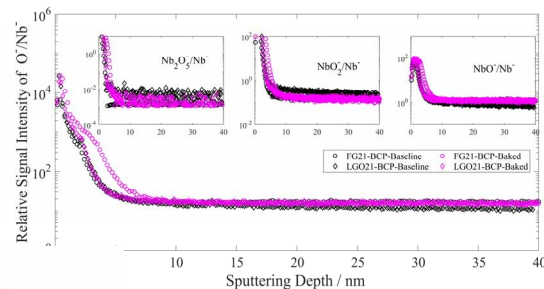
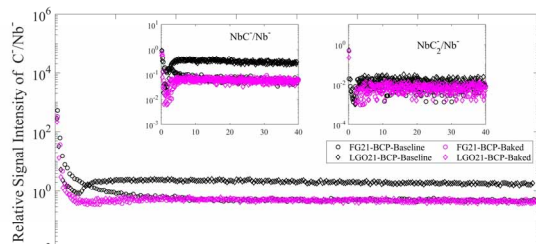
TOF-SIMS results Before and after baking



- C: C, NbC, NbC₂
- O: O, Nb₂O₅, NbO₂, NbO

3.4

TOF-SIMS results Before and after baking

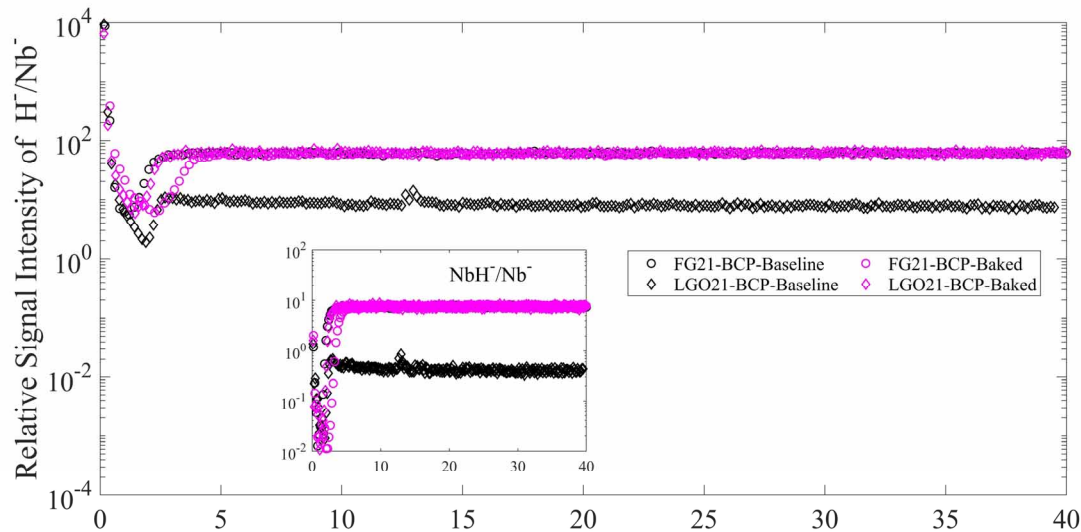
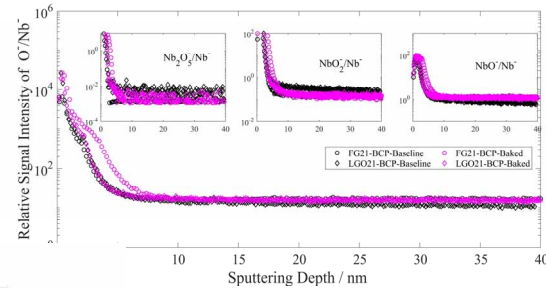
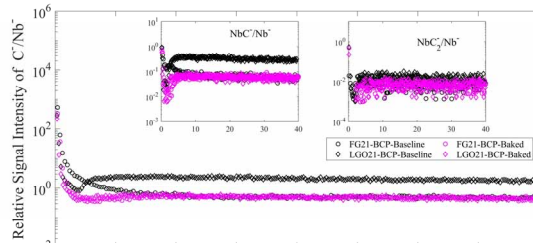


), NbC , NbC_2

), Nb_2O_5 , NbO_2 , NbO

3.4

TOF-SIMS results Before and after baking



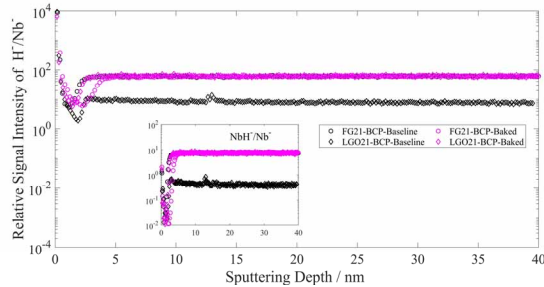
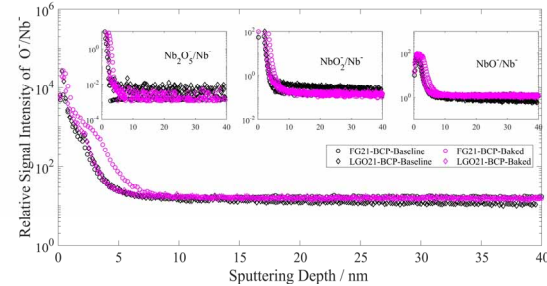
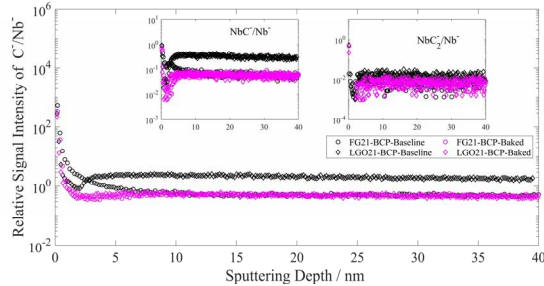
, NbC, NbC₂

, Nb₂O₅, NbO₂, NbO

t, NbH

3.4

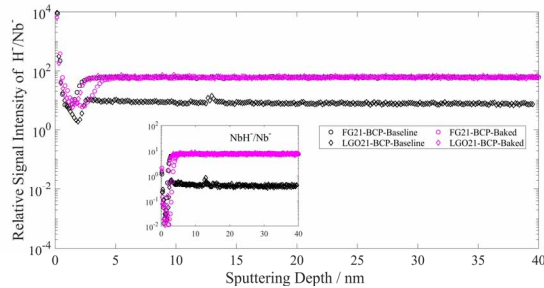
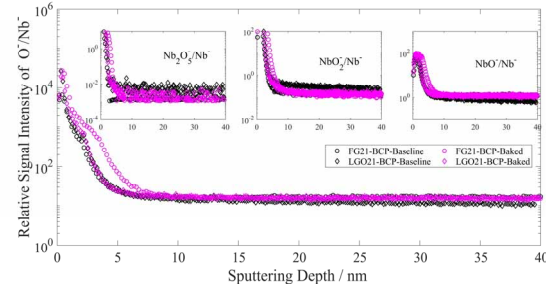
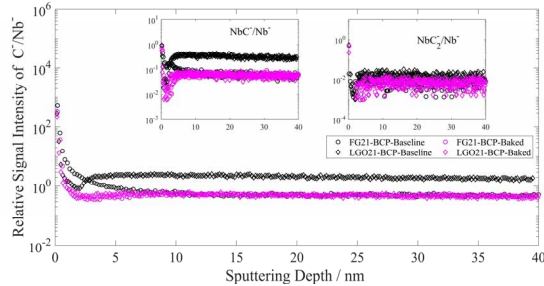
TOF-SIMS results Before and after baking



- C: C, NbC, NbC₂
- O: O, Nb₂O₅, NbO₂, NbO
- H: H, NbH

3.4

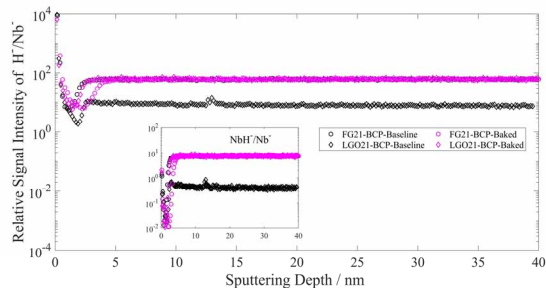
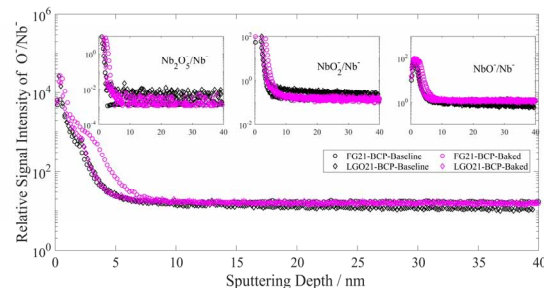
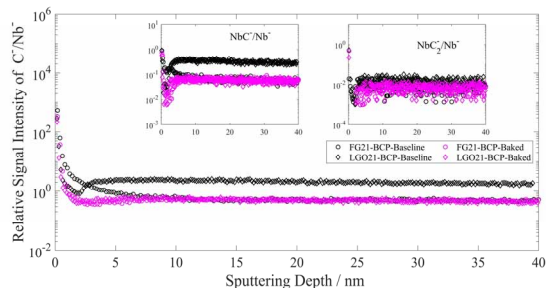
TOF-SIMS results Before and after baking



- C: C, NbC, NbC₂
- O: O, Nb₂O₅, NbO₂, NbO
- H: H, NbH
- Fine grain: C →, O →, H →

3.4

TOF-SIMS results Before and after baking



- C: C, NbC, NbC₂
- O: O, Nb₂O₅, NbO₂, NbO
- H: H, NbH
- Fine grain: C →, O →, H →
- Large Grain: C ↓, O →, H ↑

Conclusion



In-situ ARXPS



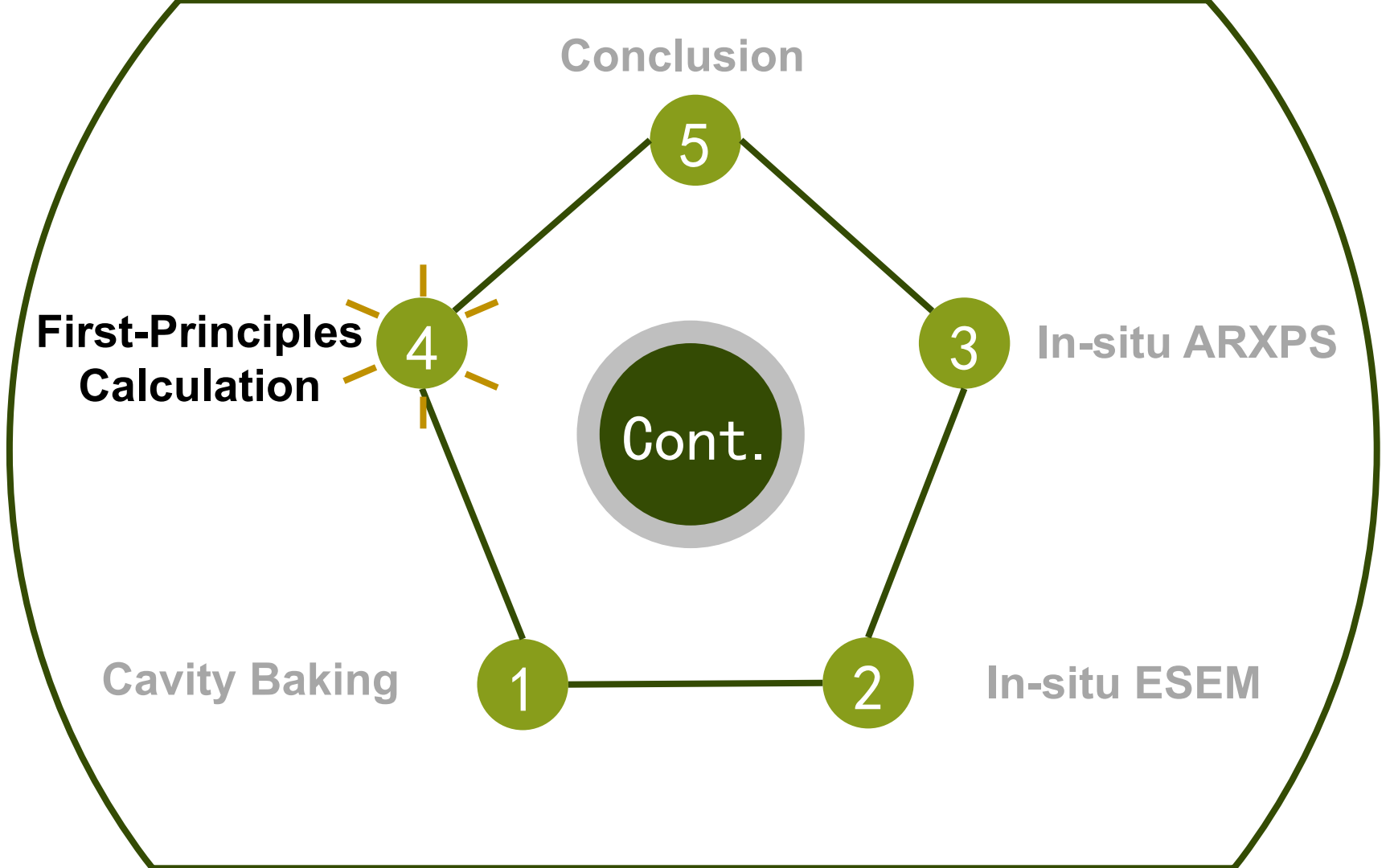
First-Principles
Calculation



Cavity Baking



In-situ ESEM



4.1

Interaction among interstitial atoms

A

H spatial distribution
WEPWB084



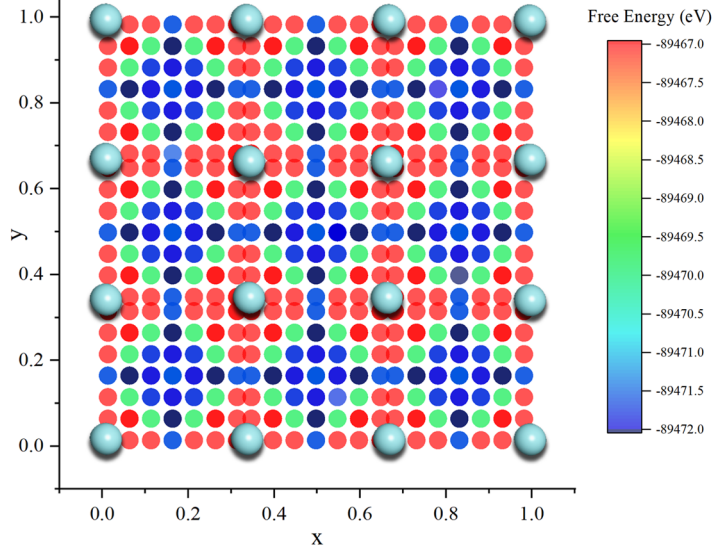
47



- First principles calculation & Density Function Theory

Interaction among

(a) Nb interstitial atoms



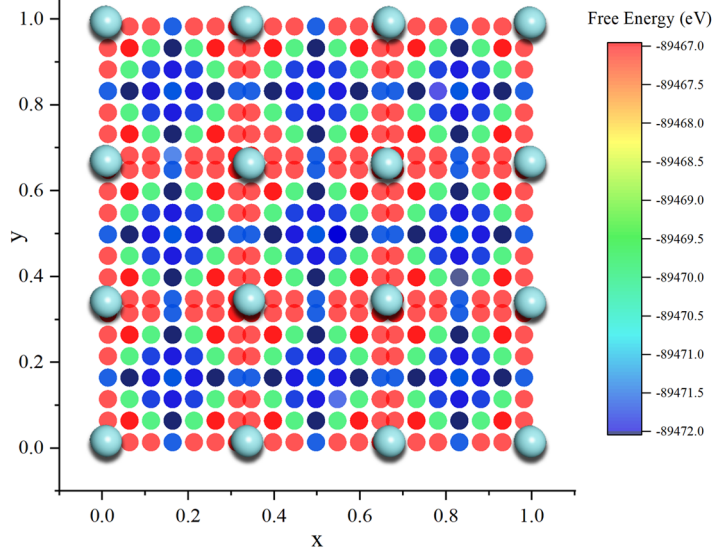
A H spatial distribution
WEPWB084



- First principles calculation & Density Function Theory

Interaction among

(a) Nb interstitial atoms

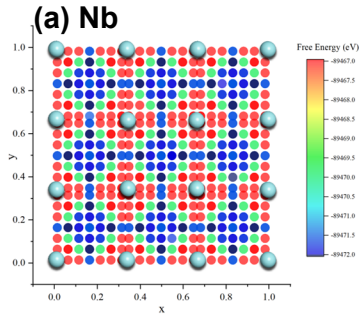


A H spatial distribution WEPWB084



- First principles calculation & Density Function Theory

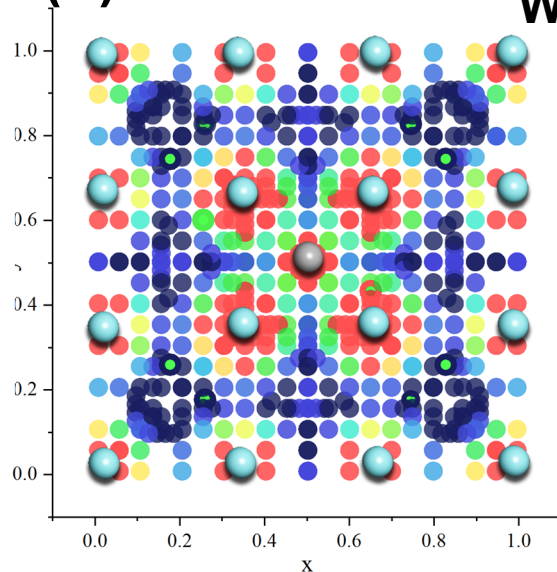
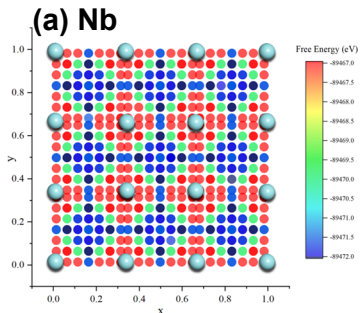
Light blue 3D sphere: Nb
Gray 3D sphere: C
Red 3D sphere: O
Dark blue 3D sphere: N
Colored 2D circles: H



- First principles calculation & Density Function Theory

Light blue 3D sphere: Nb
Gray 3D sphere: C
Red 3D sphere: O
Dark blue 3D sphere: N
Colored 2D circles: H

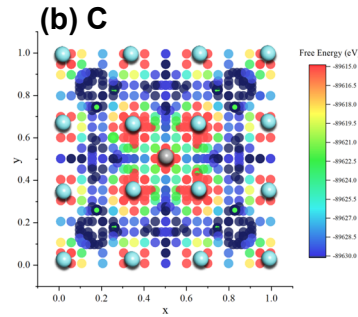
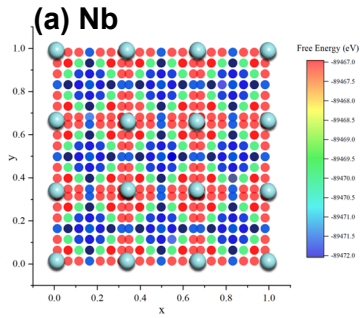
4.1

Interaction among
interstitial (b) CA H spatial distribution
WEPWB084

First principles
calculation & Density
Function Theory

Light blue 3D sphere: Nb
Gray 3D sphere: C
Red 3D sphere: O
Dark blue 3D sphere: N
Colored 2D circles: H





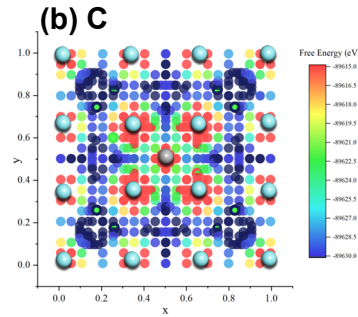
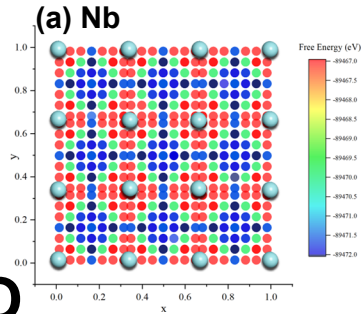
- First principles calculation & Density Function Theory

Light blue 3D sphere: Nb
 Gray 3D sphere: C
 Red 3D sphere: O
 Dark blue 3D sphere: N
 Colored 2D circles: H

4.4

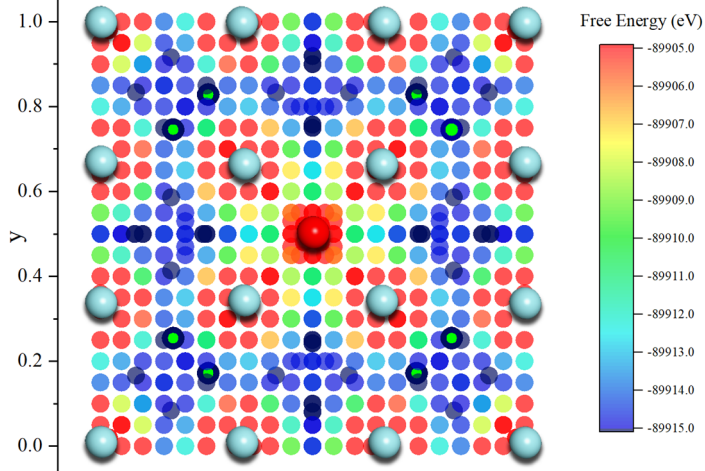
Interaction among interstitial atoms

A

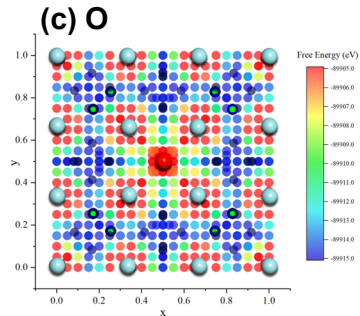
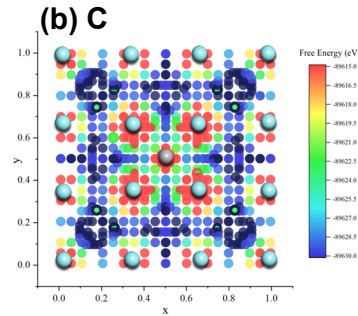
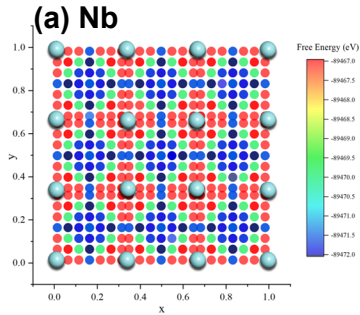
H spatial distribution
WEPWB084

- First principles calculation & Density Function Theory

(c) O



Light blue 3D sphere: Nb
 Gray 3D sphere: C
 Red 3D sphere: O
 Dark blue 3D sphere: N
 Colored 2D circles: H



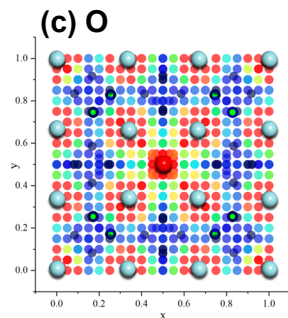
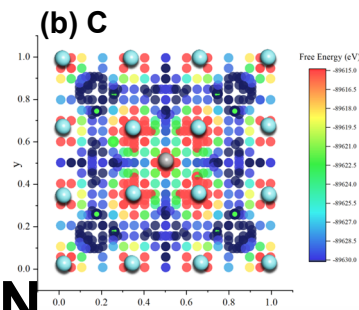
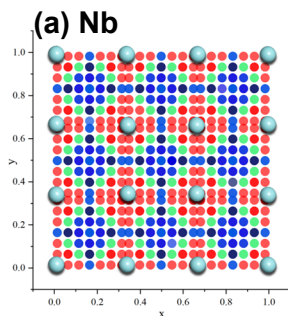
- First principles calculation & Density Function Theory

Light blue 3D sphere: Nb
 Gray 3D sphere: C
 Red 3D sphere: O
 Dark blue 3D sphere: N
 Colored 2D circles: H

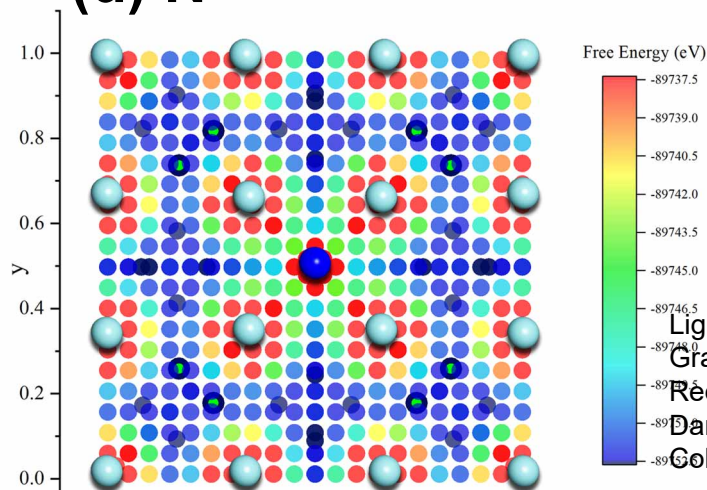
4.1

Interaction among interstitial atoms

A

H spatial distribution
WEPWB084

(d) N



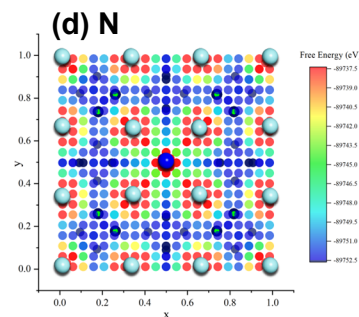
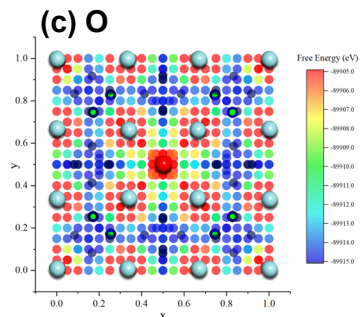
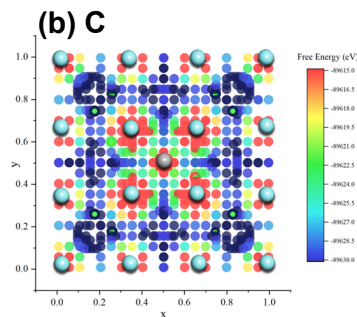
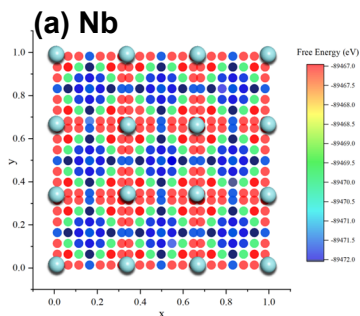
- First principles calculation & Density Function Theory

Light blue 3D sphere: Nb
 Gray 3D sphere: C
 Red 3D sphere: O
 Dark blue 3D sphere: N
 Colored 2D circles: H

4.1

Interaction among interstitial atoms

A

H spatial distribution
WEPWB084

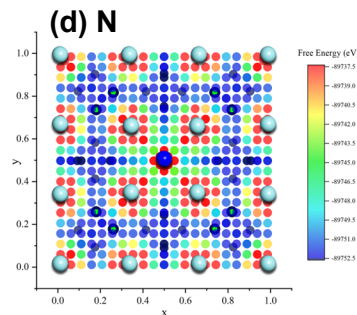
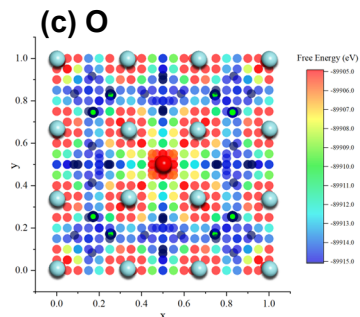
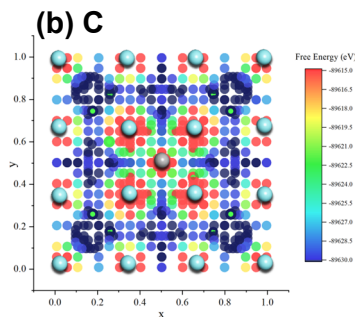
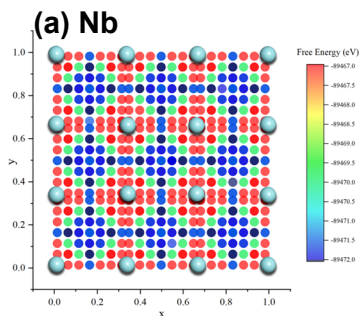
- First principles calculation & Density Function Theory

Light blue 3D sphere: Nb
 Gray 3D sphere: C
 Red 3D sphere: O
 Dark blue 3D sphere: N
 Colored 2D circles: H

4.1

Interaction among interstitial atoms

A

H spatial distribution
WEPWB084

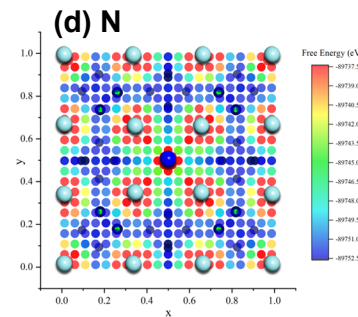
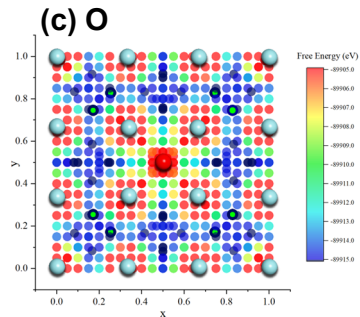
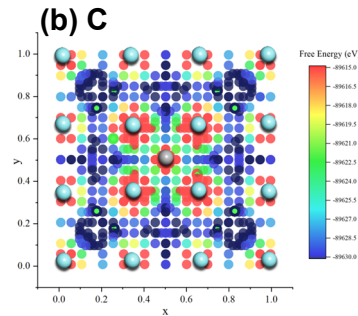
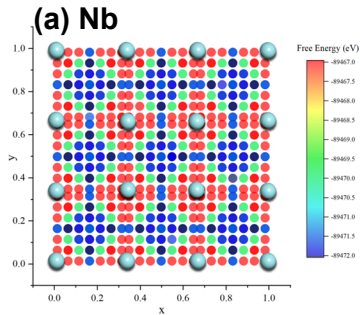
- First principles calculation & Density Function Theory
- Most stable positions: H-Tetrahedral sites, C/N/O-Octahedral sites

Light blue 3D sphere: Nb
 Gray 3D sphere: C
 Red 3D sphere: O
 Dark blue 3D sphere: N
 Colored 2D circles: H

4.1

Interaction among
interstitial atoms

A

H spatial distribution
WEPWB084

- First principles calculation & Density Function Theory
- Most stable positions: H-Tetrahedral sites, C/N/O-Octahedral sites
- C/N/O reduce the most stable sites of H, so as to diffusion routes of H

Light blue 3D sphere: Nb
 Gray 3D sphere: C
 Red 3D sphere: O
 Dark blue 3D sphere: N
 Colored 2D circles: H

4.1

Interaction among interstitial atoms

B

DOS distribution
WEPWB084



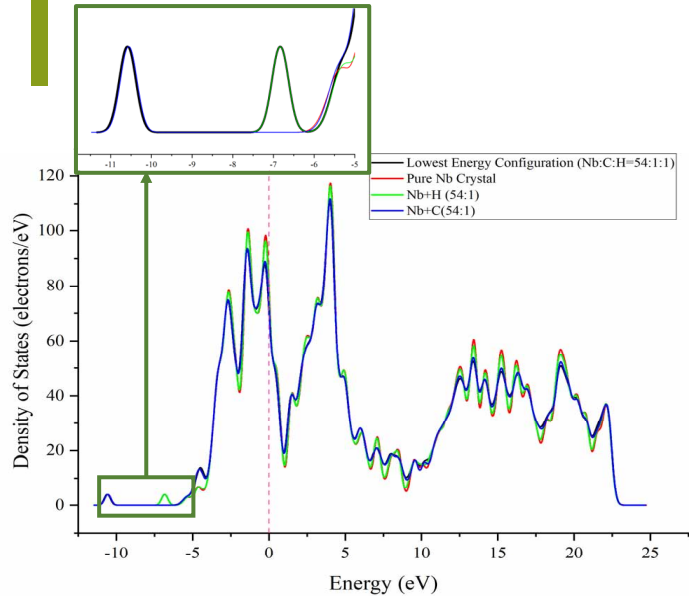
18

4

(a) Nb-C-H

Interaction among interstitial atoms

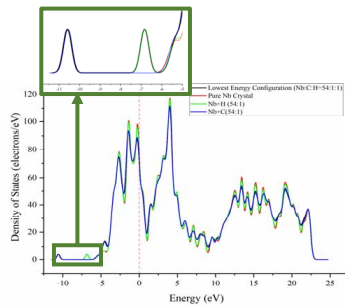
B

DOS distribution
WEPWB084

18



(a) Nb-C-H

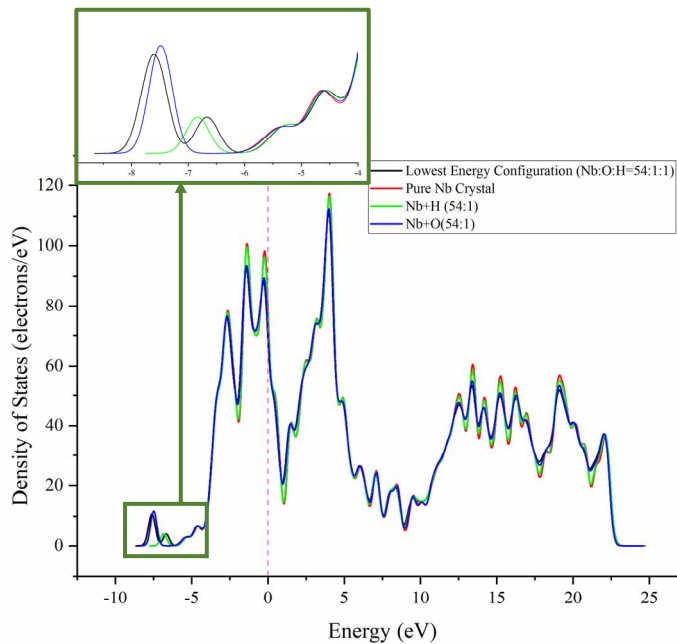
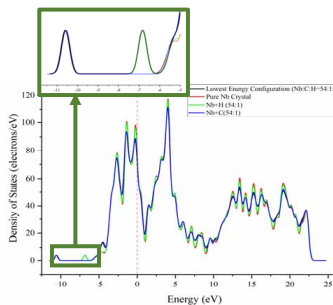


Interaction among interstitial atoms (B) Nb-O-H

B DOS distribution
WEPWB084

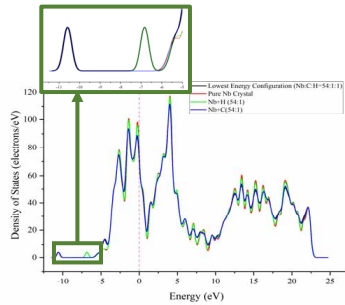


(a) Nb-C-H

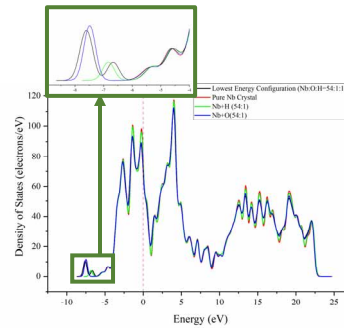




(a) Nb-C-H



(b) Nb-O-H

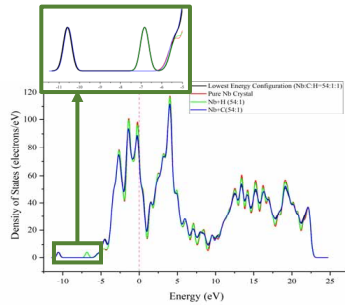


4.1

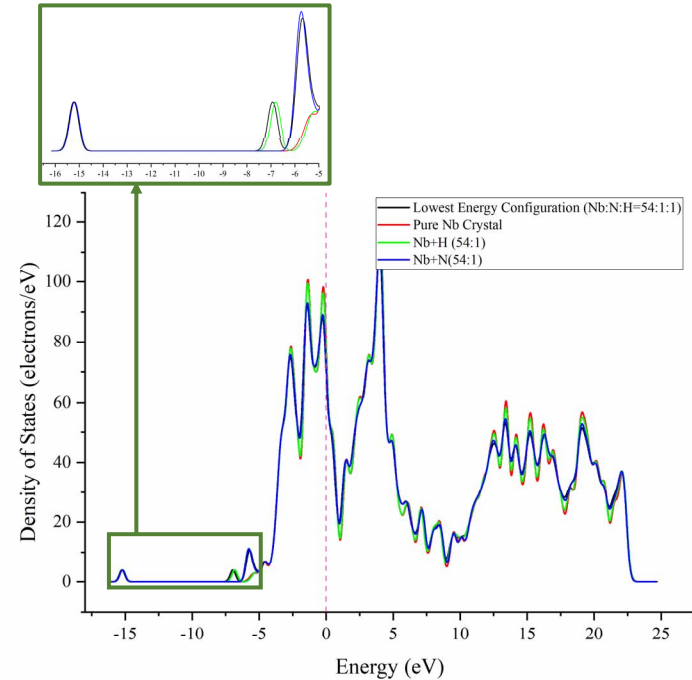
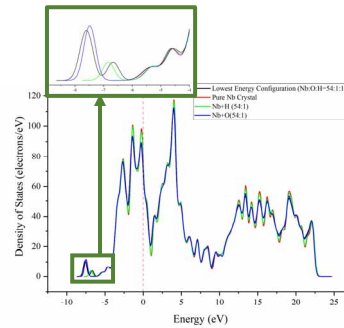
Interaction among interstitial atoms

B DOS distribution
w.r.t. Nb-N-H

(a) Nb-C-H

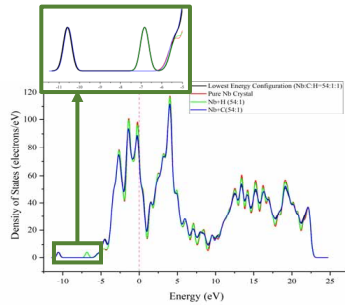


(b) Nb-O-H

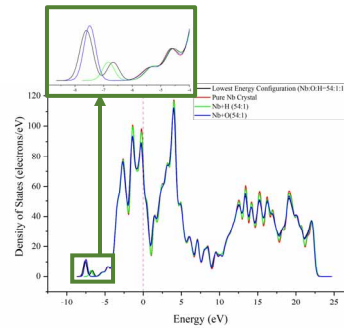




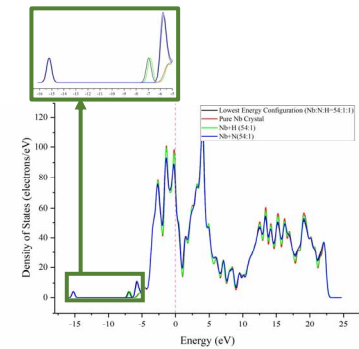
(a) Nb-C-H



(b) Nb-O-H

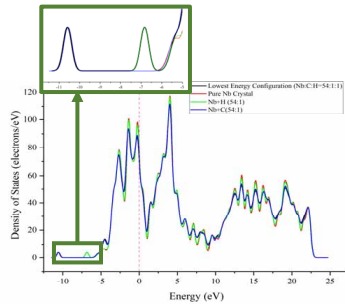


(c) Nb-N-H

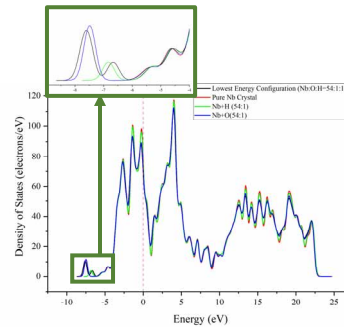




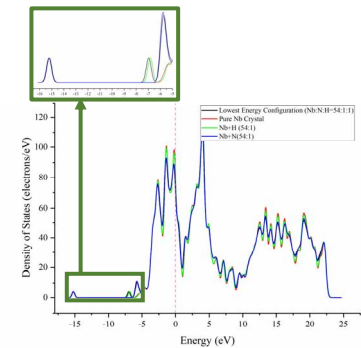
(a) Nb-C-H



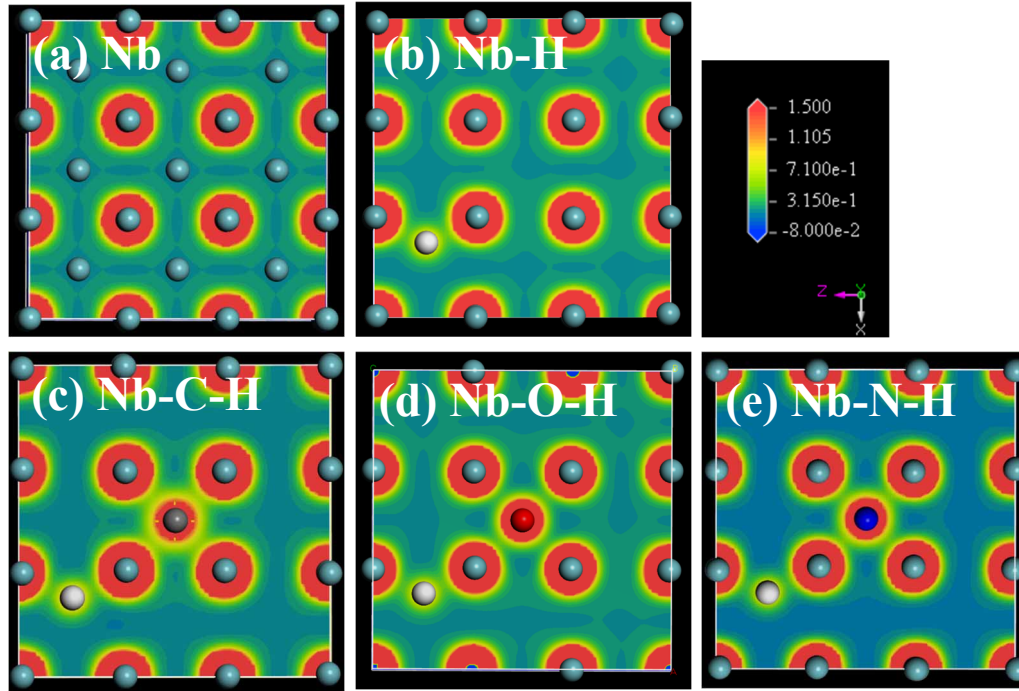
(b) Nb-O-H

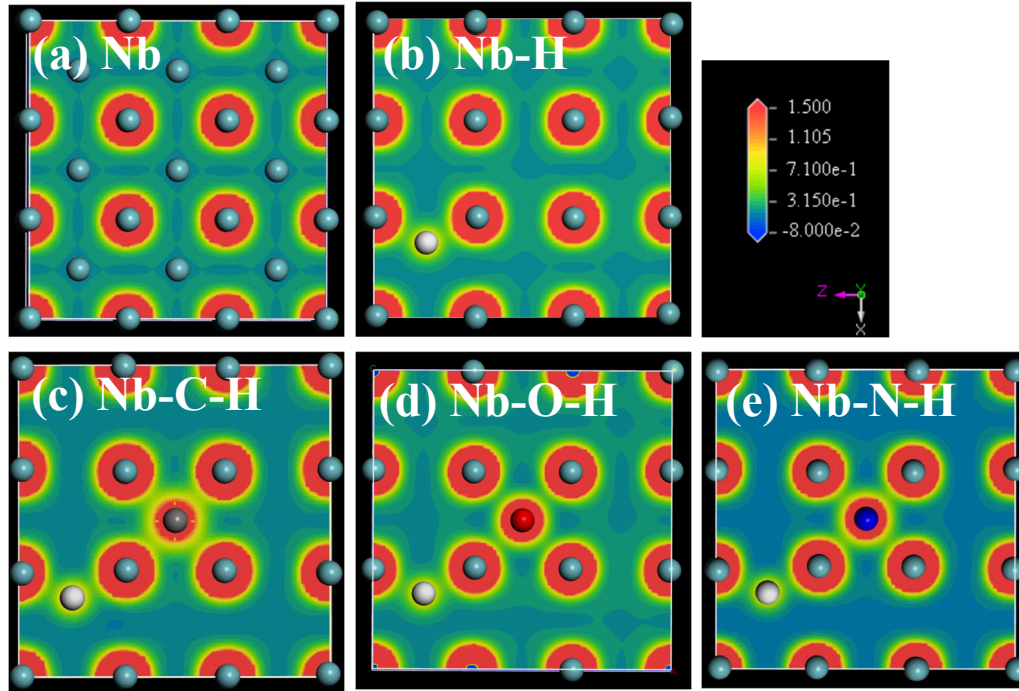


(c) Nb-N-H



- Nb-C, Nb-O, Nb-N, Nb-H Chemical Bonds
- C/N/O cannot destroy but slightly move Nb-H bond
- C/N/O/H can only slightly change DOS of Nb

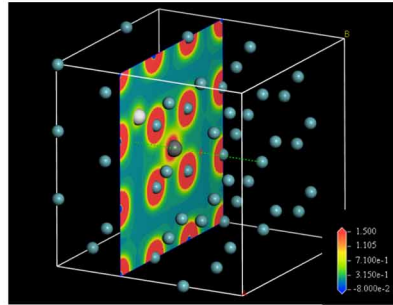




- C/N/O/H can attract free electron of Nb
- C/N/O have stronger attractive effects of electron than H
- C have similar interaction with H as N and O in the aspects of stable sites of H, Nb DOS and system electron density

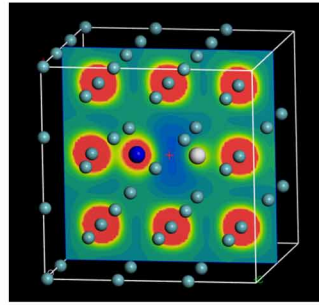


Lowest Energy Structure
Nb-V-C-H

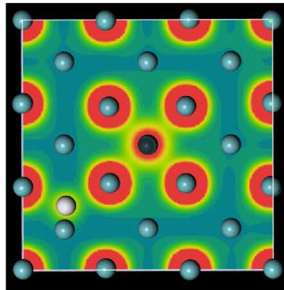


(a)

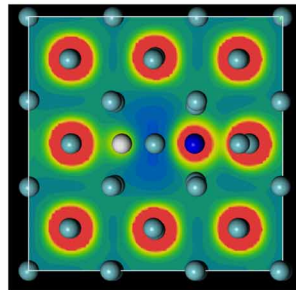
Lowest Energy Structure
Nb-V-N/O-H



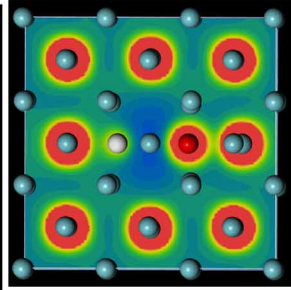
(b)



(c)

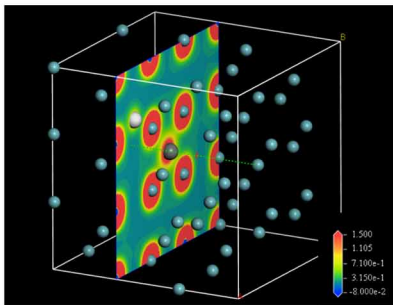


(d)

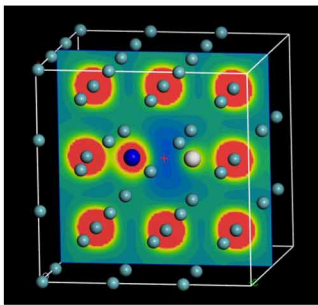


(e)

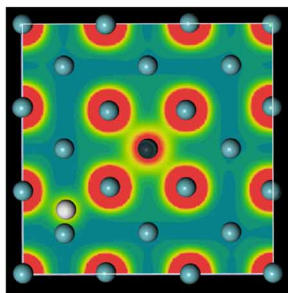
Electron density Nb-V-C-H Electron density Nb-V-N-H Electron density Nb-V-O-H

Lowest Energy Structure
Nb-V-C-H

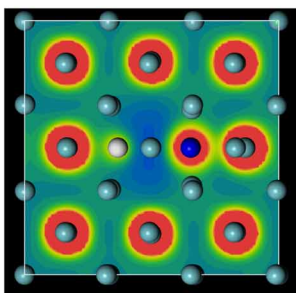
(a)

Lowest Energy Structure
Nb-V-N/O-H

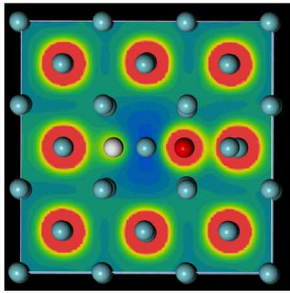
(b)



(c)



(d)



(e)

Electron density Nb-V-C-H Electron density Nb-V-N-H Electron density Nb-V-O-H

- In the lowest energy structure Nb-V-C-H, H locates at a tetrahedral site near the vacancy, similarly to the situation without vacancy.
- In the lowest energy structure Nb-V-N-H and Nb-V-O-H, H locates at the octahedral site near the vacancy

4.2

Interaction between
vacancy and C/N/O/H

B

Peak searching of DOS
WEPWB084

System	Element	Peak 1		Peak 2		Peak 3		Peak 4	
		Center (eV)	Area(e)	Center (eV)	Area(e)	Center (eV)	Area(e)	Center (eV)	Area(e)
C+H+ V+Nb	C	-10.892	1.383	-7.536	1.120	-4.022	2.890		
	H	-	-	-7.536	1.120				
	Nb	10.892	0.513	-7.536	0.581	?	?		
N+H+ V+Nb	N	-14.678	1.616	-6.081	0.893	-5.334	2.463	-4.671	3.732
	H	-	-	-6.081	0.893			-4.524	1.052
	Nb	14.678	0.415	-6.071	0.544	-5.334	1.819	-4.608	1.238
O+H+ V+Nb	O	19.98156	1.75907	-6.72451	3.74937			-5.66185	2.35442
	H	-	-	-6.72451	3.74937	-6.44043	0.42456	-5.61976	1.52196
	Nb	19.98156	0.27757	-6.70347	1.67848	?	?	-5.6408	0.73405

Note: '?' means that the peaks are so close to the Fermi surface that one cannot deduct the background signal properly.

Conclusion

5

First-Principles
Calculation

4

In-situ ARXPS

3

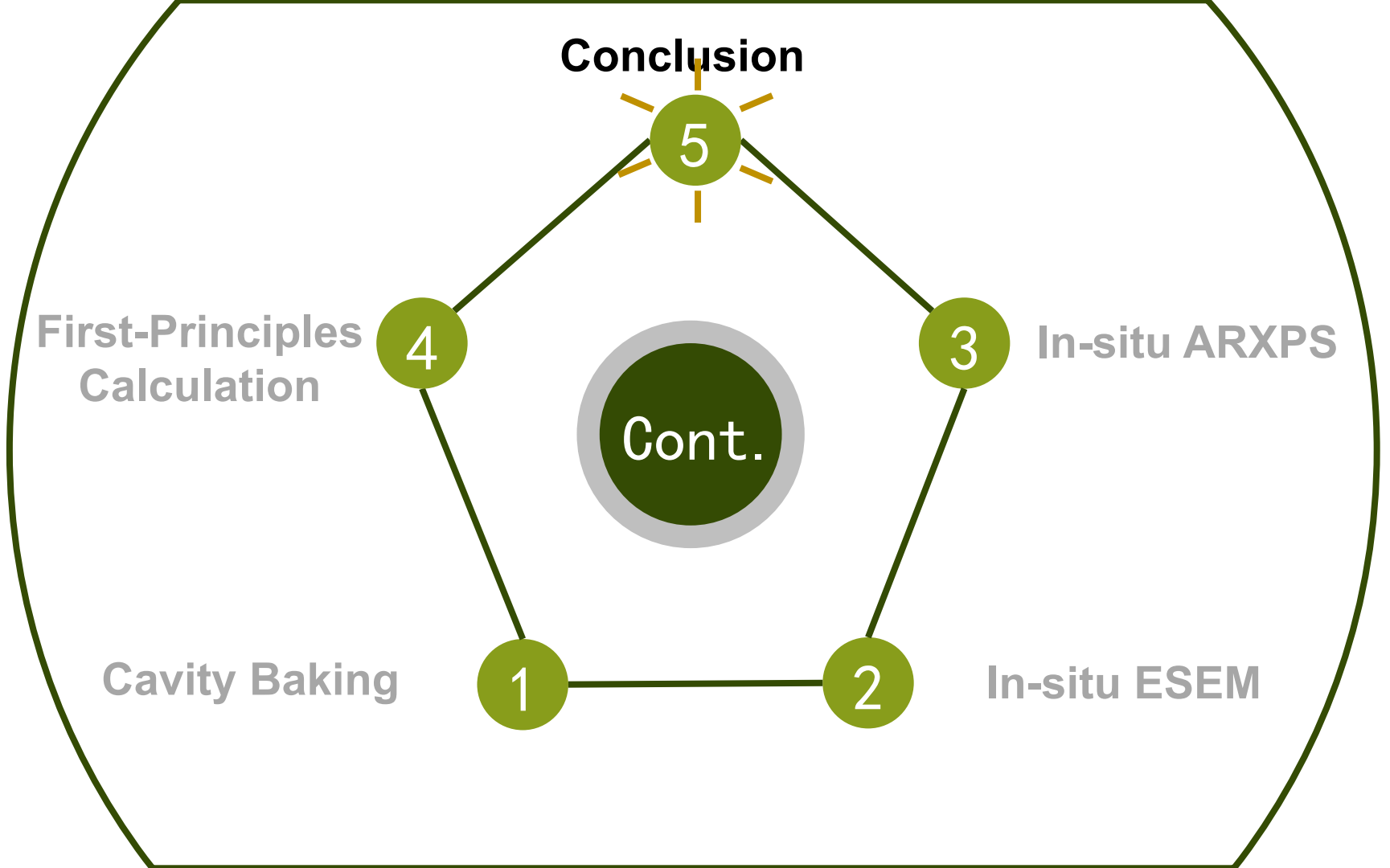
Cont.

Cavity Baking

1

In-situ ESEM

2







400°C can decompose Nb-O and form Nb-C compounds, maybe C-doping effect



800°C decompose Nb-O and Nb-C, only pure Nb left



400°C can decompose Nb-O and form Nb-C compounds, maybe C-doping effect

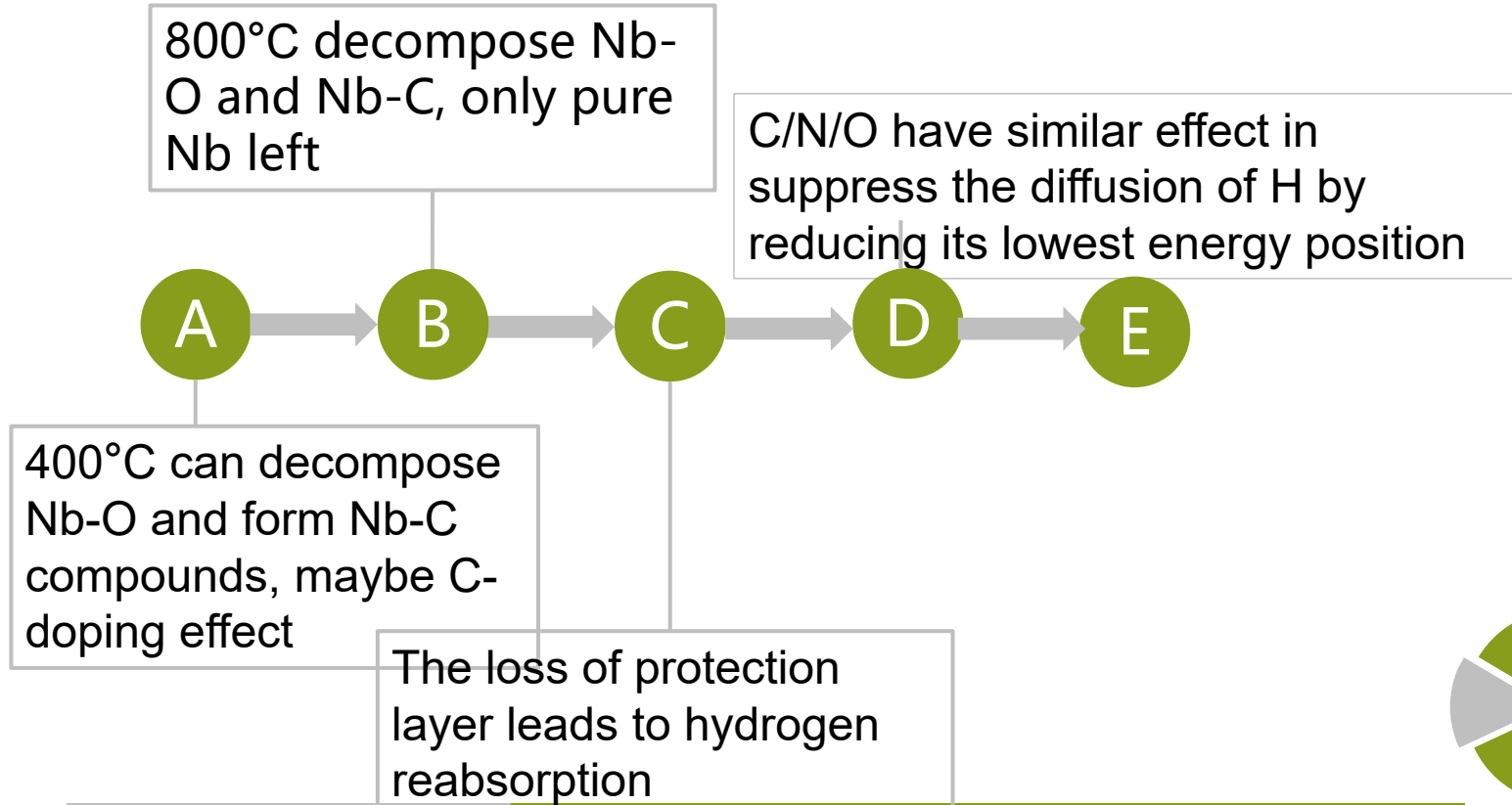


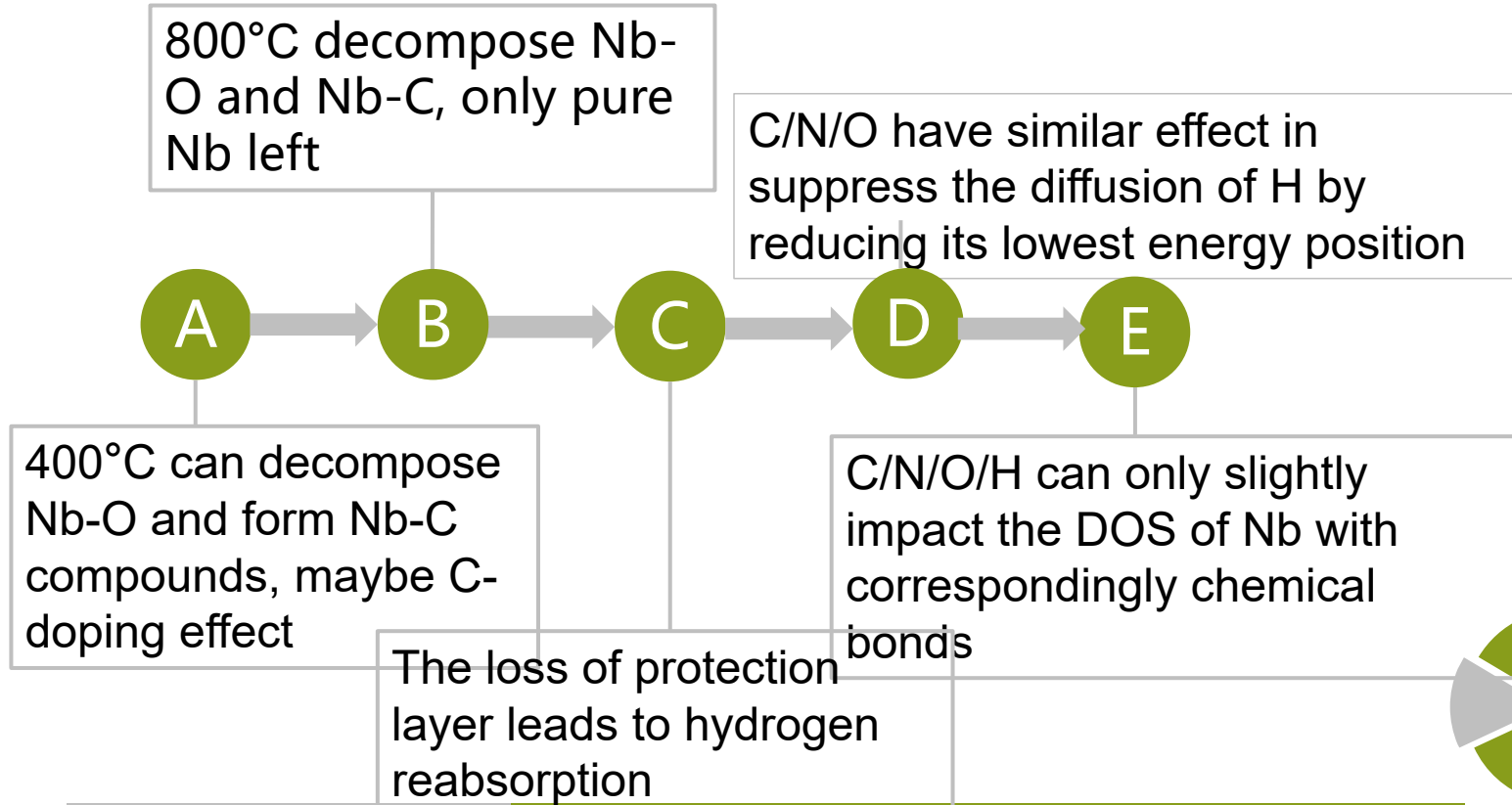
800°C decompose Nb-O and Nb-C, only pure Nb left



400°C can decompose Nb-O and form Nb-C compounds, maybe C-doping effect

The loss of protection layer leads to hydrogen reabsorption





5.2

Future work



24



Experiment

- In-situ ARPES experiment on superconducting niobium: observe the baking temperature responses of the electron pair behavior in momentum space
- Medium temperature baking of Niobium cavity with more accurate temperature controlling and pre-oxidization (**WEPWB045**)





Experiment

- In-situ ARPES experiment on superconducting niobium: observe the baking temperature responses of the electron pair behavior in momentum space
- Medium temperature baking of Niobium cavity with more accurate temperature controlling and pre-oxidization (**WEPWB045**)



Simulation

- Interaction among vacancy, dislocation and grain boundaries
- Temperature responses of the interaction between interstitial C/N/O and H
- Temperature responses of the interaction between vacancy and H
- Nb-H precipitation, cooling



FOREVER MEMORY

Thanks for your attention

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