



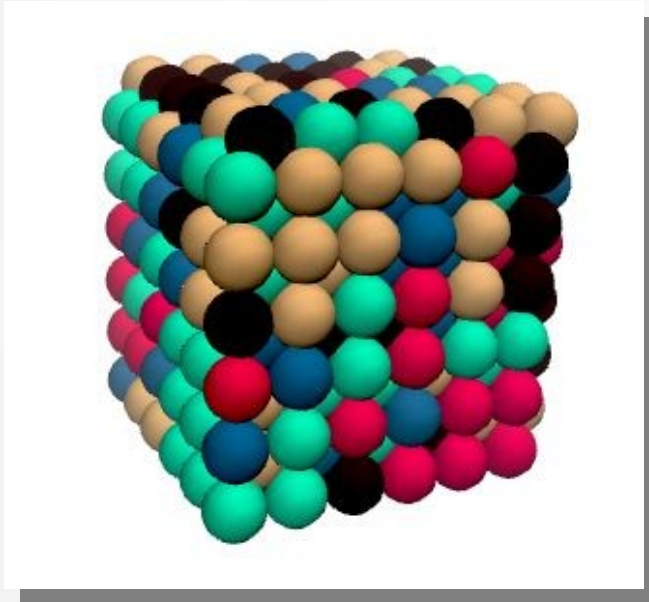
Deuterium in WMoTaNbV high-entropy alloy

Anna Liski, Marianna Kemell, Guanying Wei, Jesper Byggmästar, Flyura Djurabekova, Kai Nordlund, Tomi Vuoriheimo, Tommy Ahlgren, Kalle Heinola, Jouni Heino, Yevgen Zayachuk, Anna Widdowson, Ko-Kai Tseng, Ting-En Shen, Che-Wei Tsai, Jien-Wei Yeh, Kenichiro Mizohata





WMoTaNbV high-entropy alloy



W Mo Ta Nb V

High-entropy alloy

- ≥ 5 components
- Random
- Equimolar

Refractory metals

- High melting point
- Hardness
- Creep resistance
- Corrosion resistant
- Irradiation tolerant

REFRACTORY METALS

s, d, p, f - blocks
Blocks are sets of elements having the same orbital

s												p					He									
H												B	C	N	O	F	Ne									
Li	Be											Al	Si	P	S	Cl	Ar									
Na	Mg	d										Ga	Ge	As	Se	Br	Kr									
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	In	Sn	Sb	Te	I	Xe									
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Cs	Ba	67-71	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn									
Fr	Ra	89-103	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og									
		f																								
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu										
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr										

Extreme environments

→ Fusion first wall
Interaction with hydrogen



WMoTaNbV samples



Manufacturing

Powder

→ Vacuum arc melting

Impurities of N, C and O

→ from the process

Sample preparation

Polishing

→ mirror surface

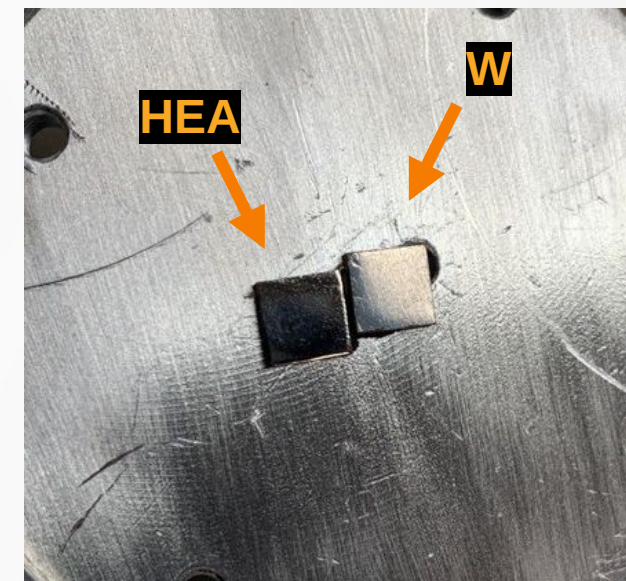
Annealing

→ 1000 C° 24 h

→ remove H, N, O and C
(partially as CO and CO₂)

→ no recrystallization at T < 1400 C°

→ elemental segregation?



Samples on holder for D implantation



WMoTaNbV samples



Manufacturing

Powder

→ Vacuum arc melting

Impurities of N, C and O

→ from the process

Sample preparation

Polishing

→ mirror surface

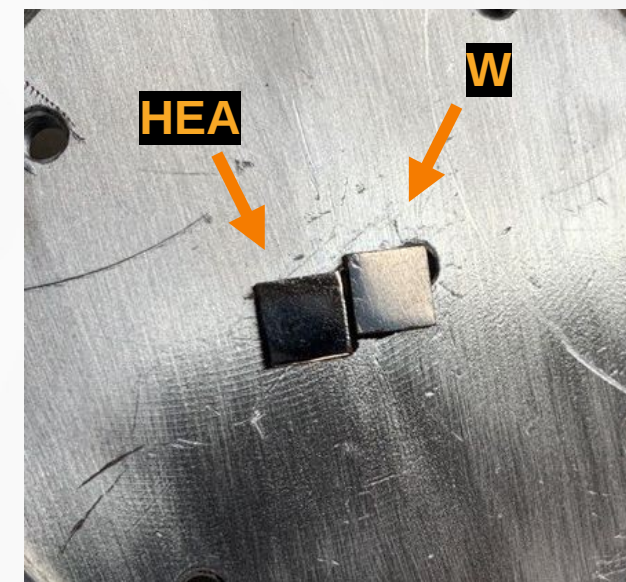
Annealing

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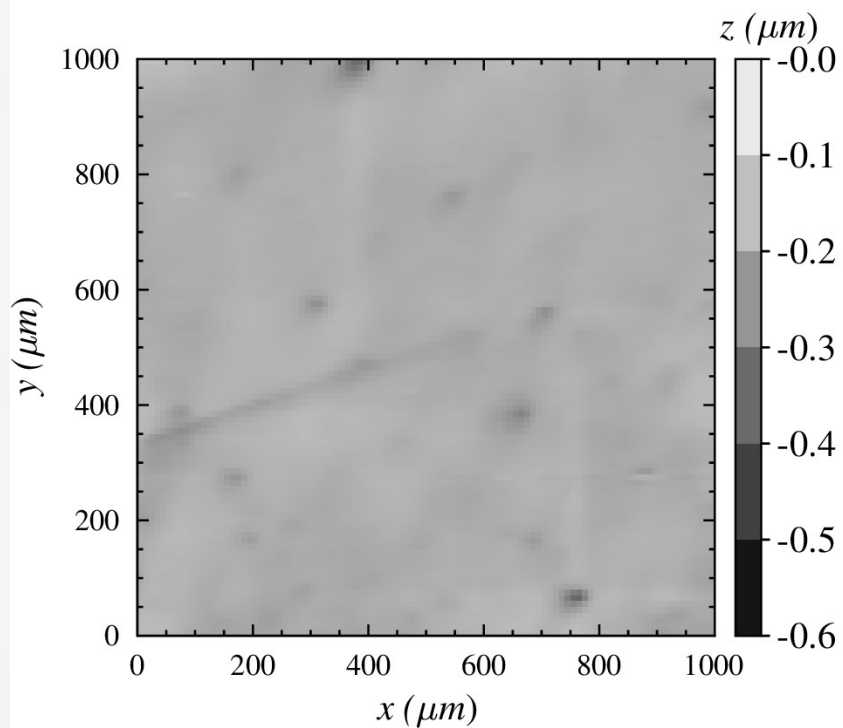
C°



Samples on holder for D implantation

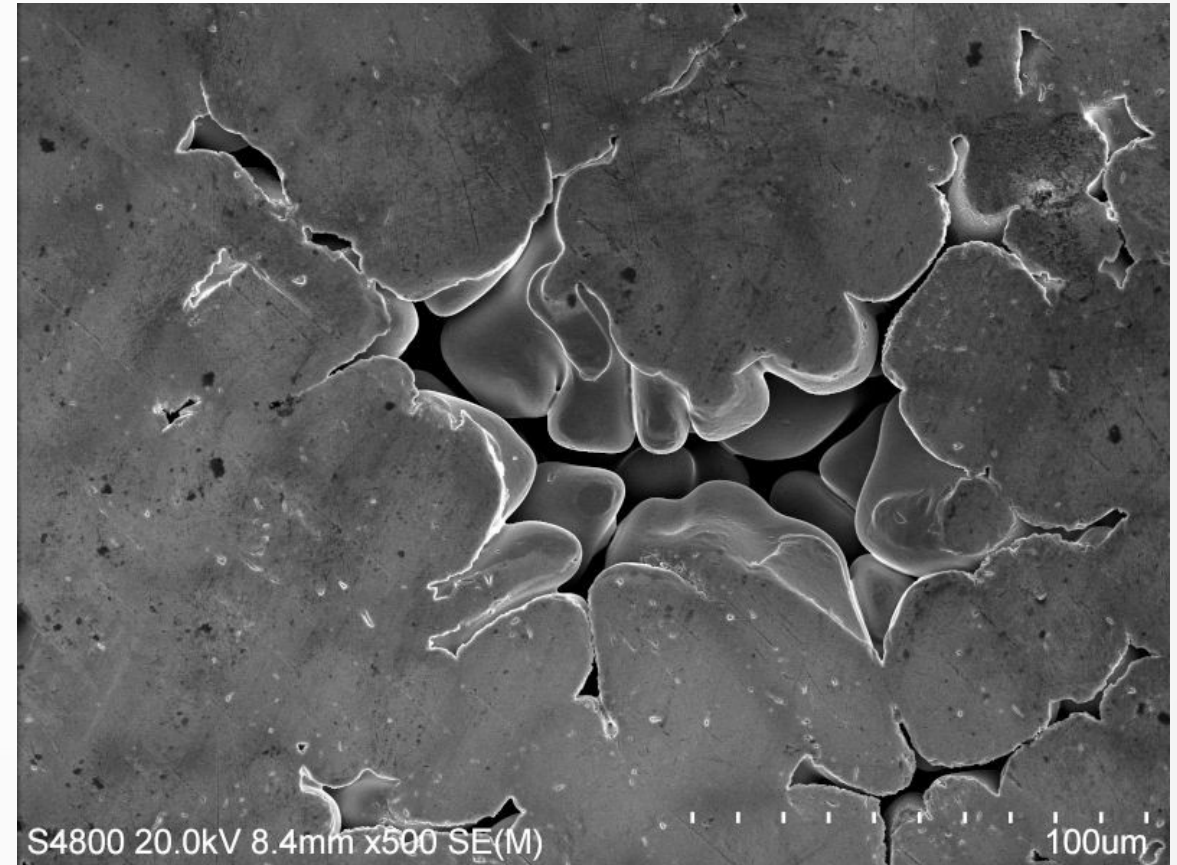
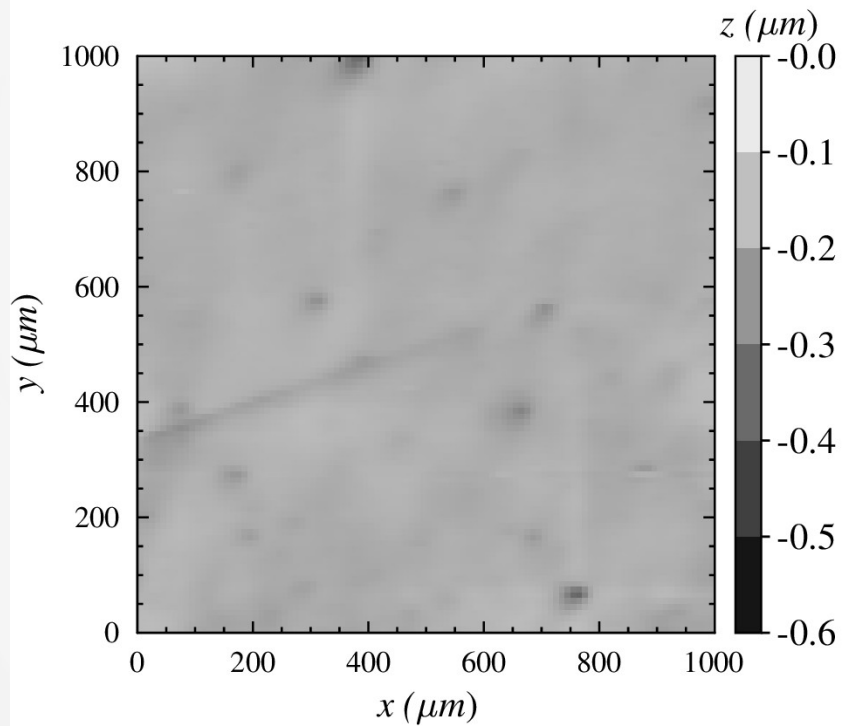


WMoTaNbV samples



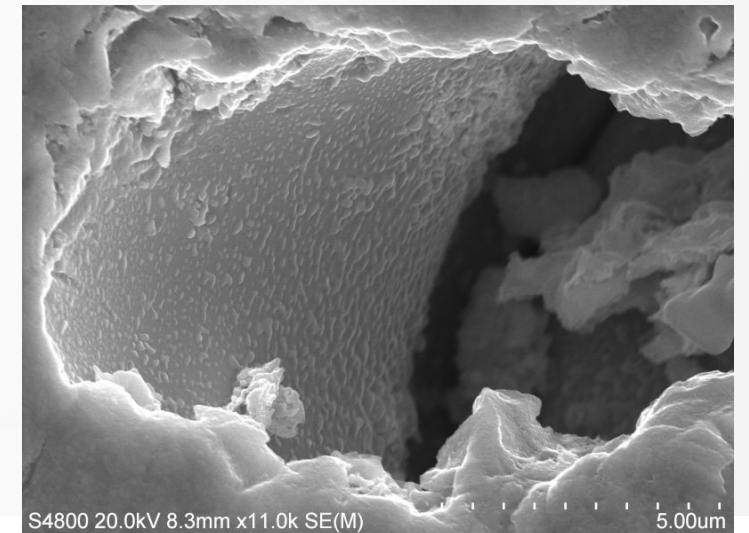
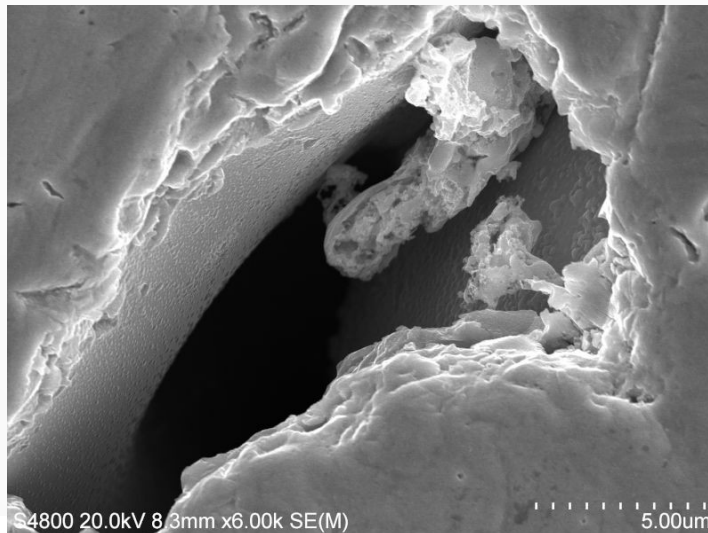
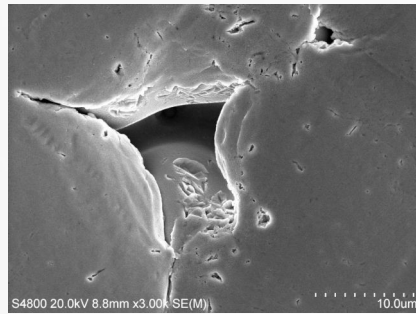
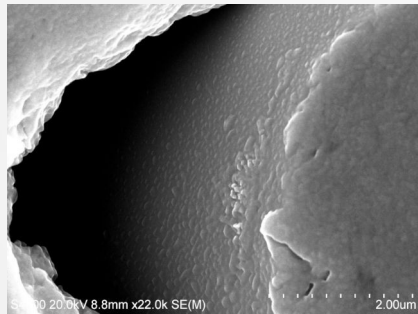
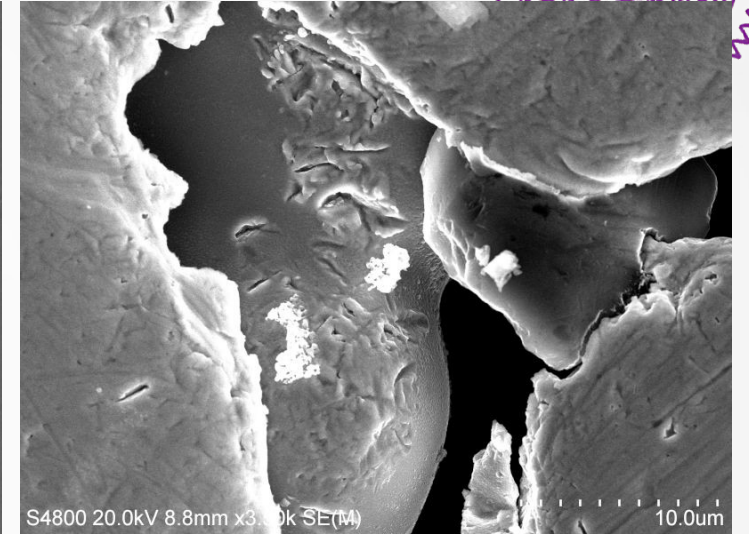
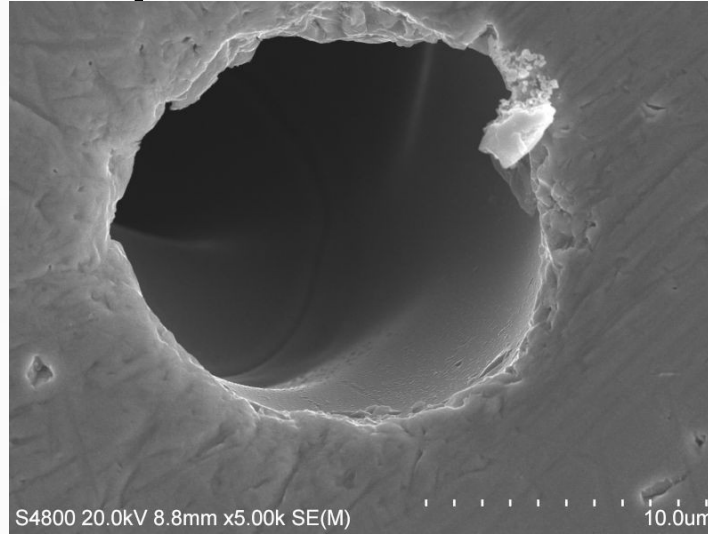
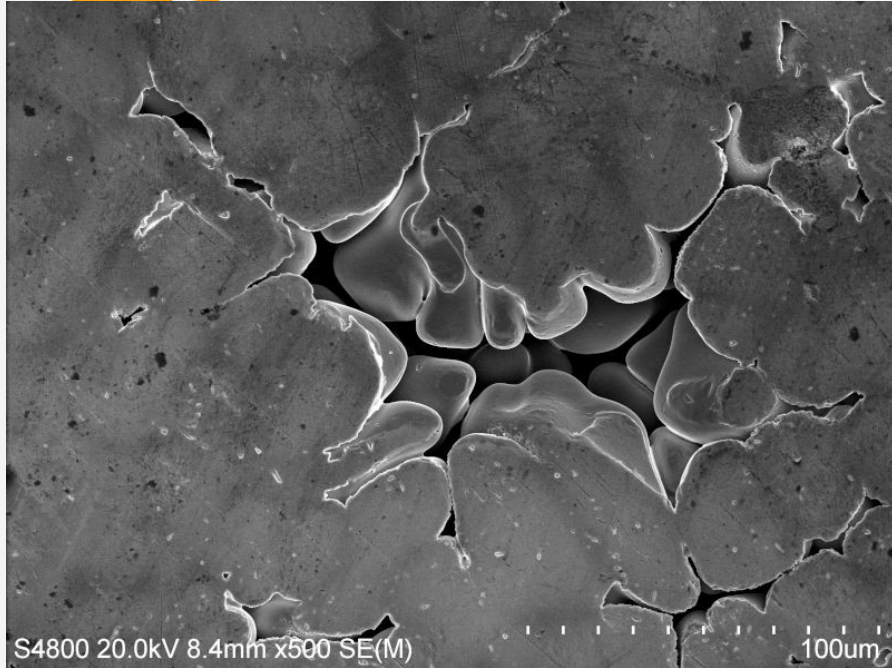


WMoTaNbV samples



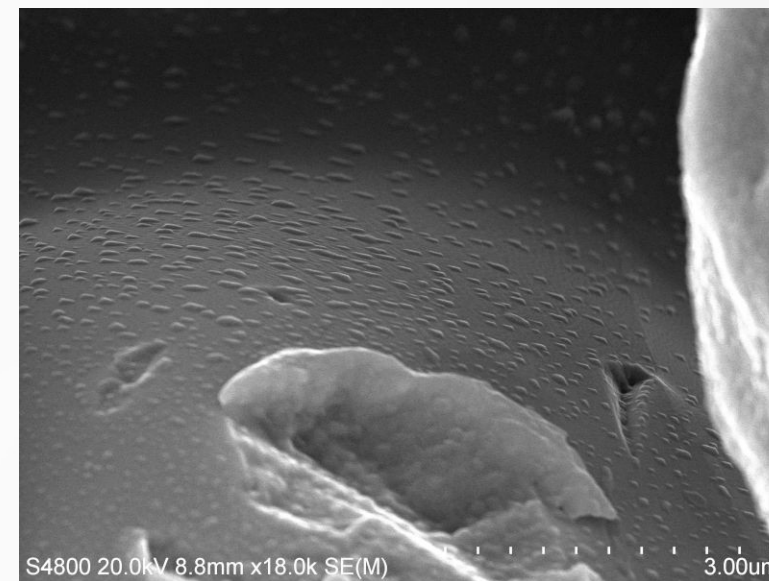
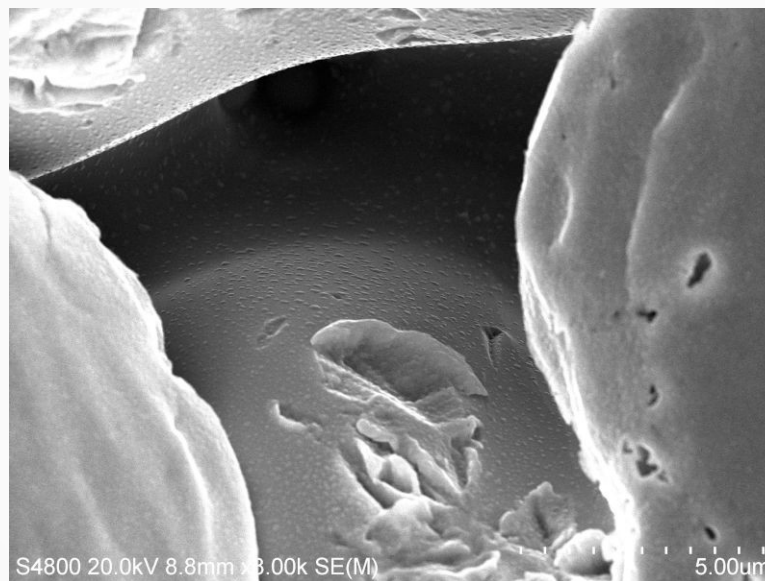
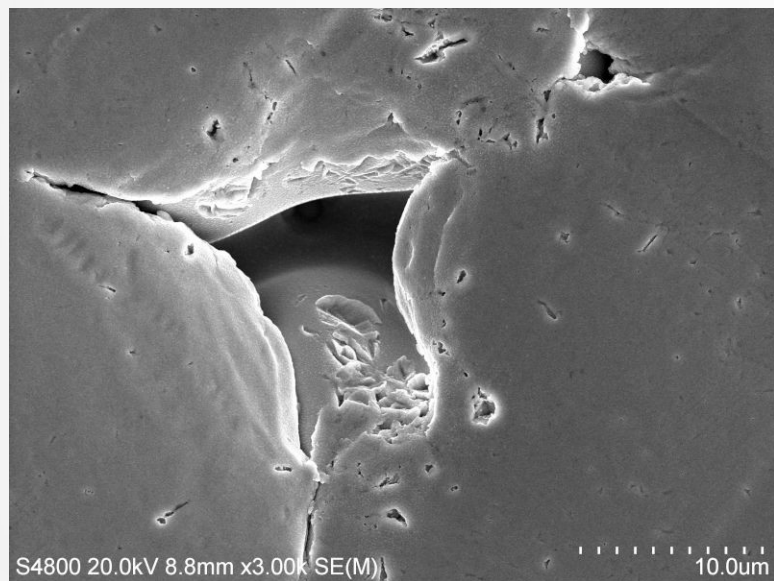


WMoTaNbV samples





WMoTaNbV samples

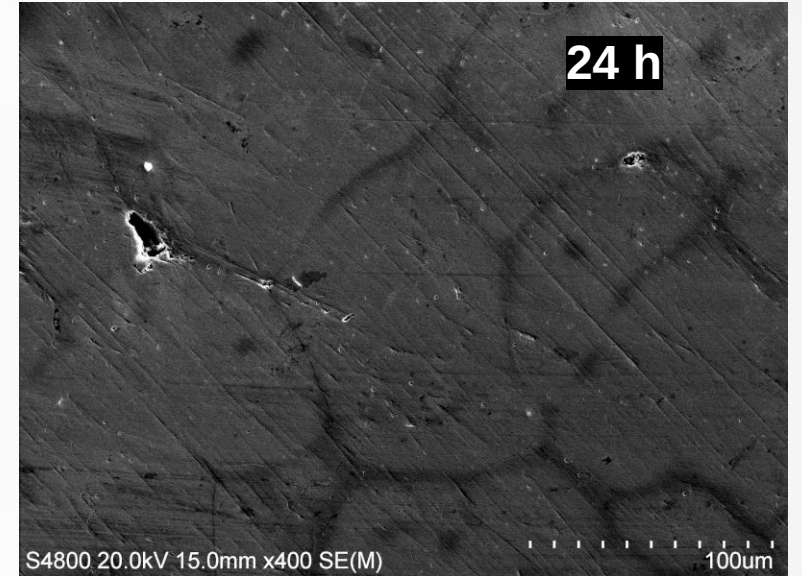
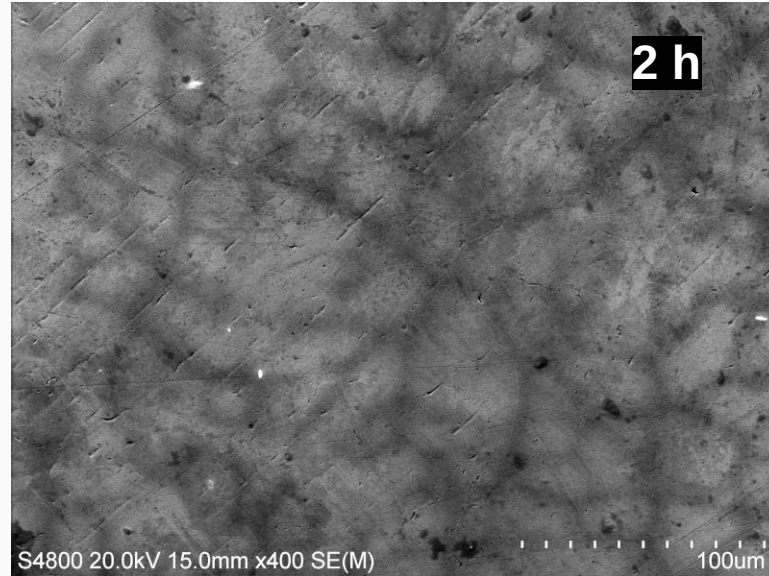
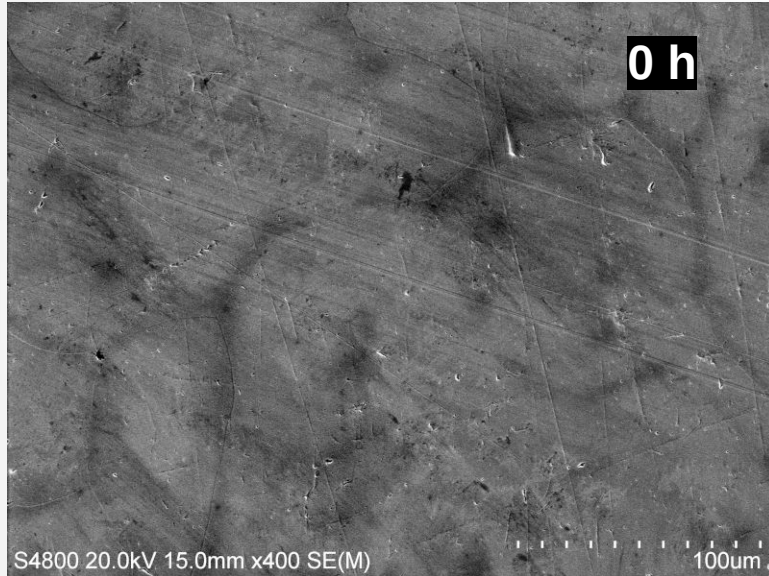




WMoTaNbV hydrogen concentration



1000 C°

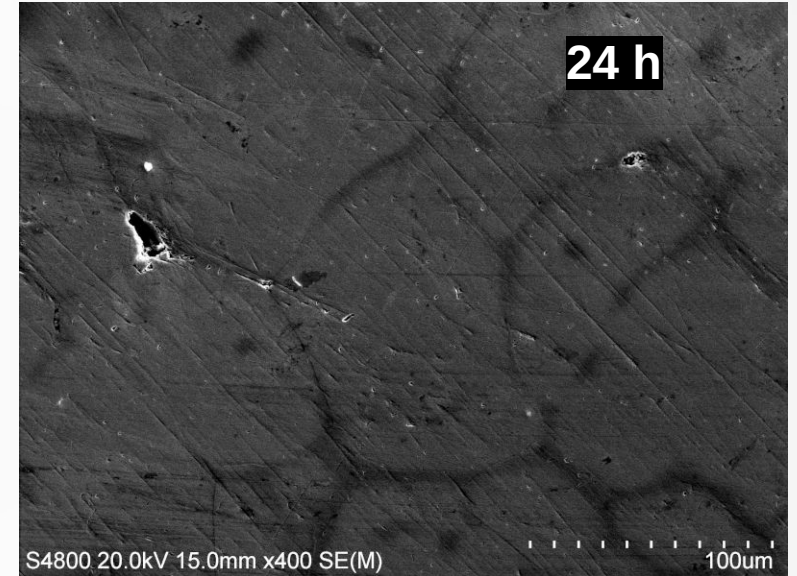
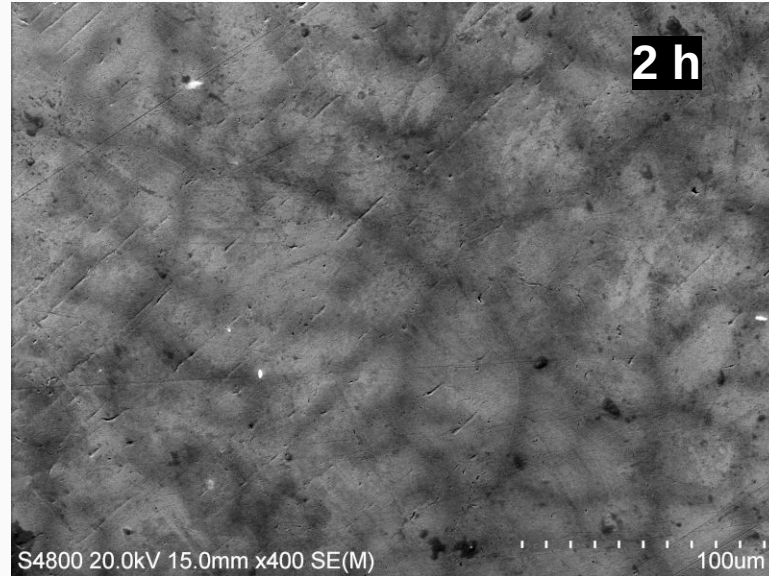
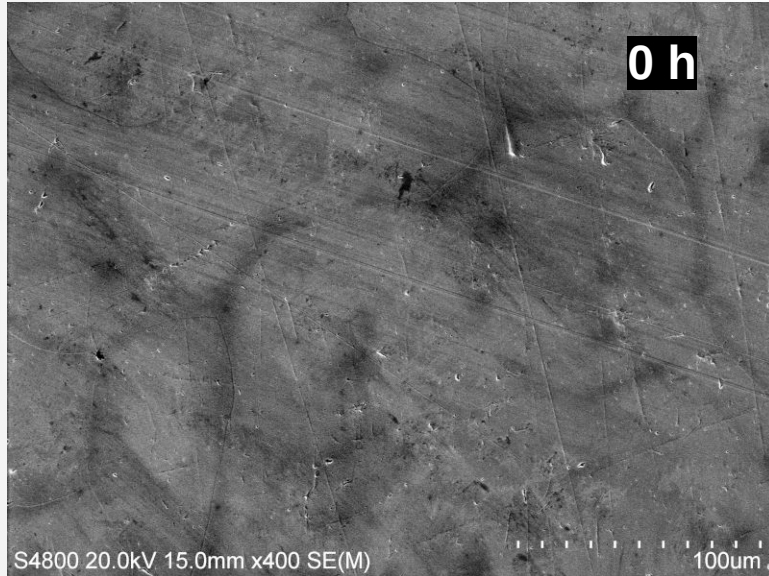




WMoTaNbV hydrogen concentration



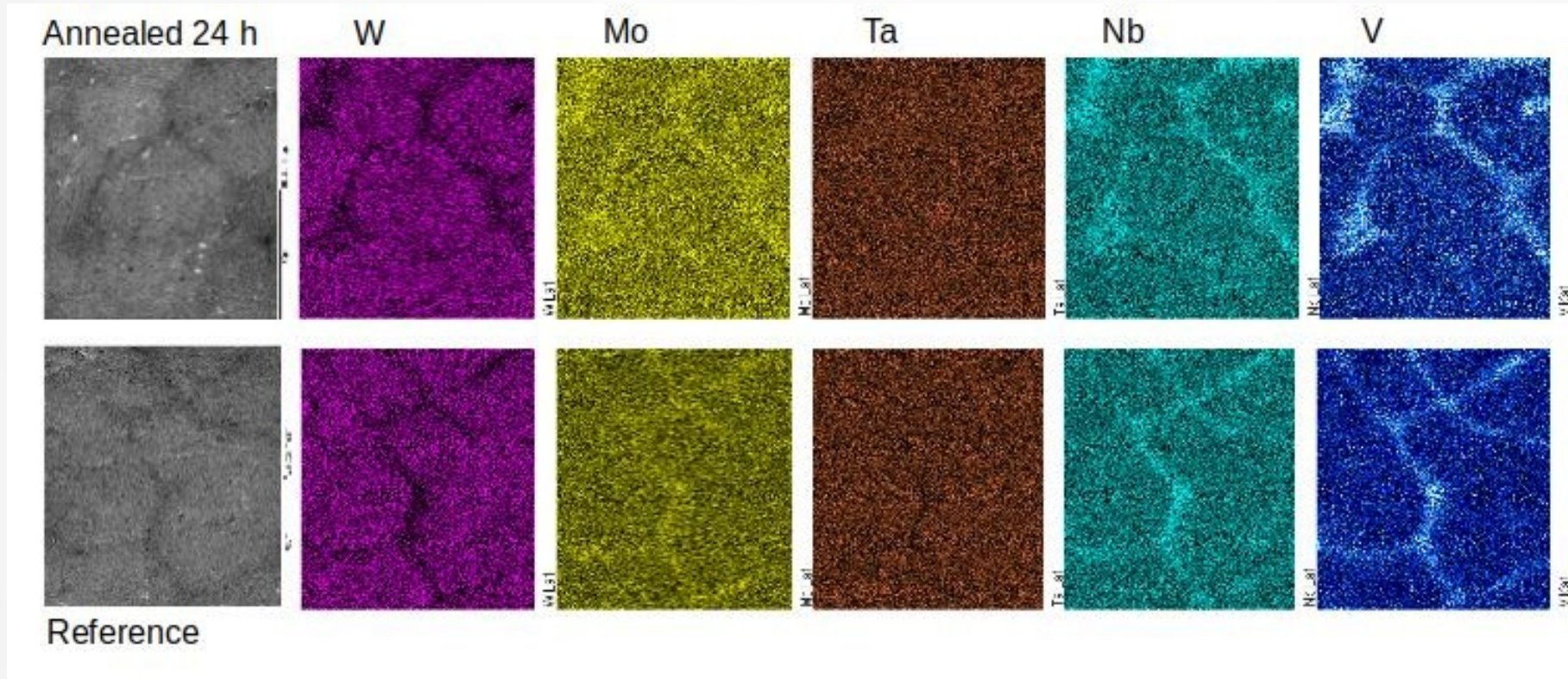
1000 C°



	Grainsize (μm)	Hydrogen concentration (10^{16} H/cm ²)
0 h	120 ± 25	0.42 ± 0.02
2 h	25 ± 7	1.78 ± 0.02
24 h	90 ± 12	0.76 ± 0.03

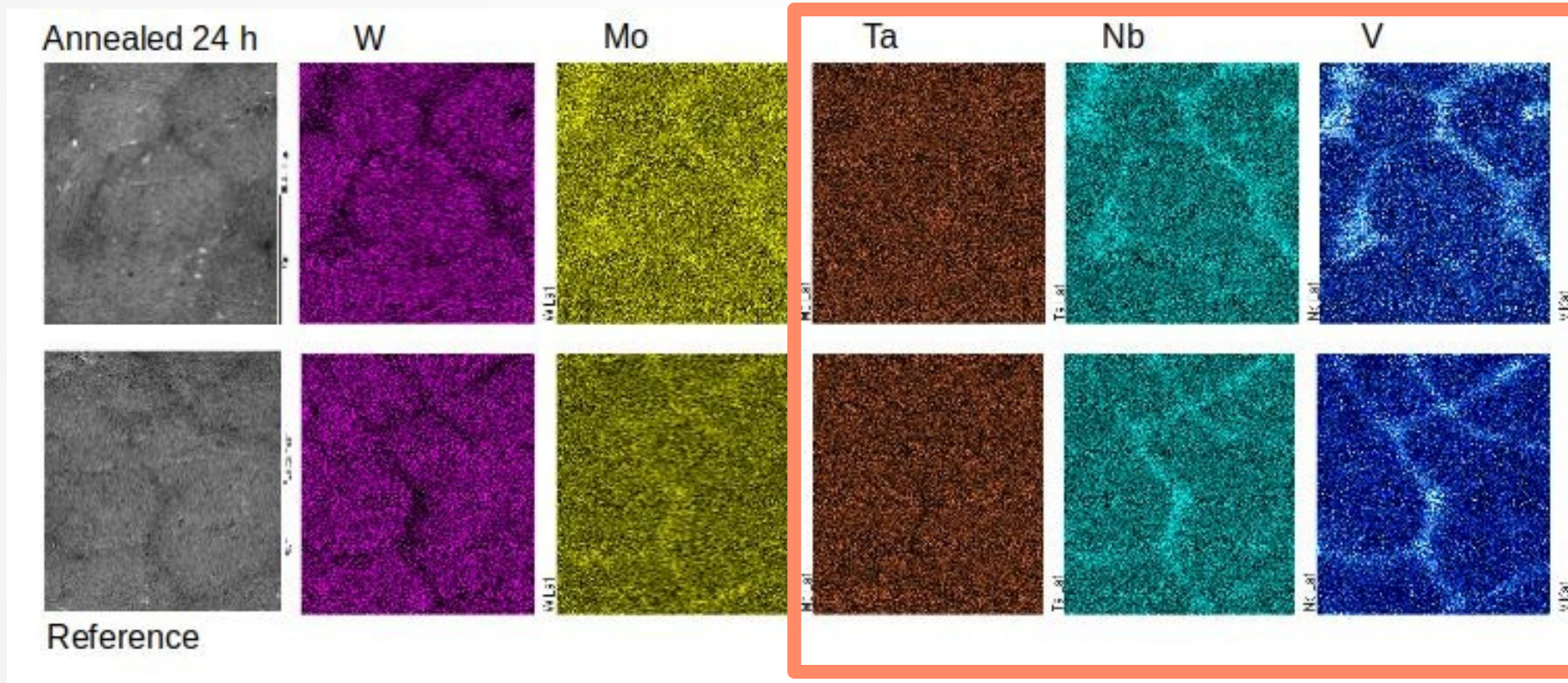


WMoTaNbV elemental segregation



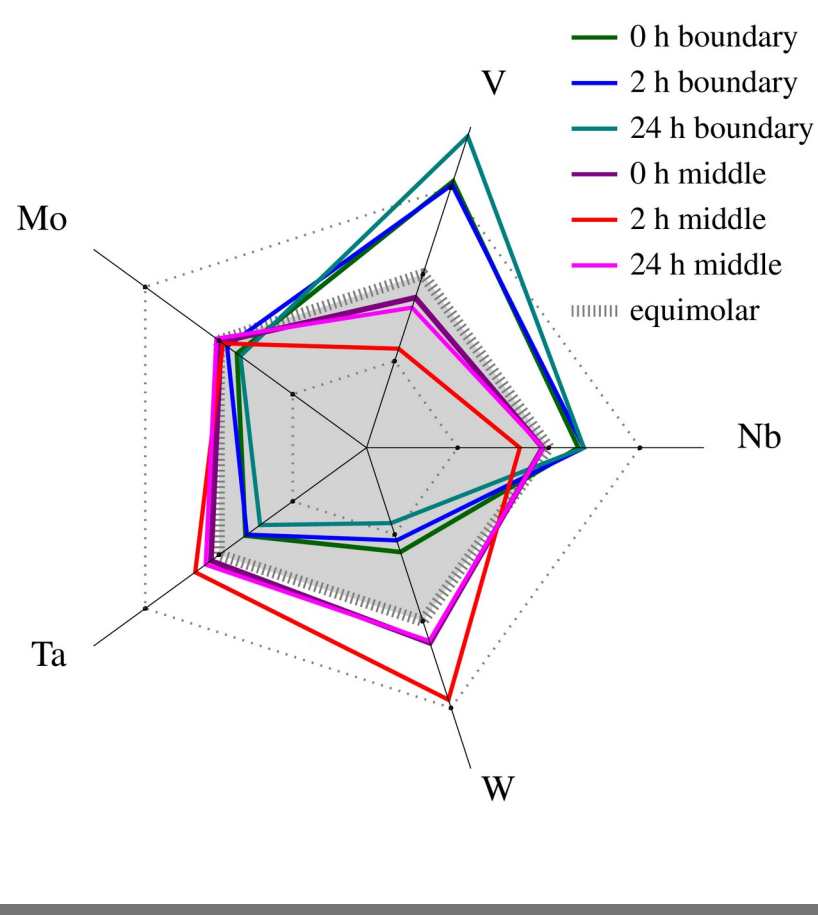


WMoTaNbV elemental segregation





WMoTaNbV elemental segregation



Middle

Relatively even composition

+ W
- V

Boundary

Clear differences

+ V
+ Nb
- Ta
- W

Annealing time has no effect on the segregation



WMoTaNbV hydrogen concentration



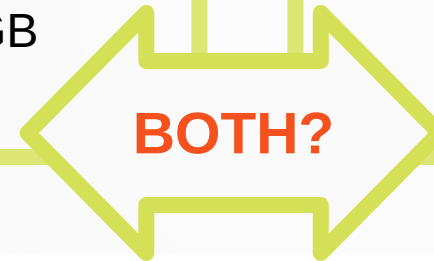
Option #1

Hydrogen absorbed by the elements with negative solution energy

→ Nb and V more prominent at GB

Option #2

Hydrogen attaching to the GB
→ structural defect



	Grainsize (μm)	Hydrogen concentration (10^{16} H/cm ²)
0 h	120 ± 25	0.42 ± 0.02
2 h	25 ± 7	1.78 ± 0.02
24 h	90 ± 12	0.76 ± 0.03



Deuterium implantations to W-irradiated samples



TAMIA – 5 MV electrostatic tandem accelerator

All elements (excluding noble gases)

HEA and W

pre-irradiated with W

→ 0, 0.007, 0.03, 0.07, 0.3, 0.7 dpa



KIIA – 500 keV ion implanter

Energy range ~ 50 eV – 500 keV

Beam current max 100 μA

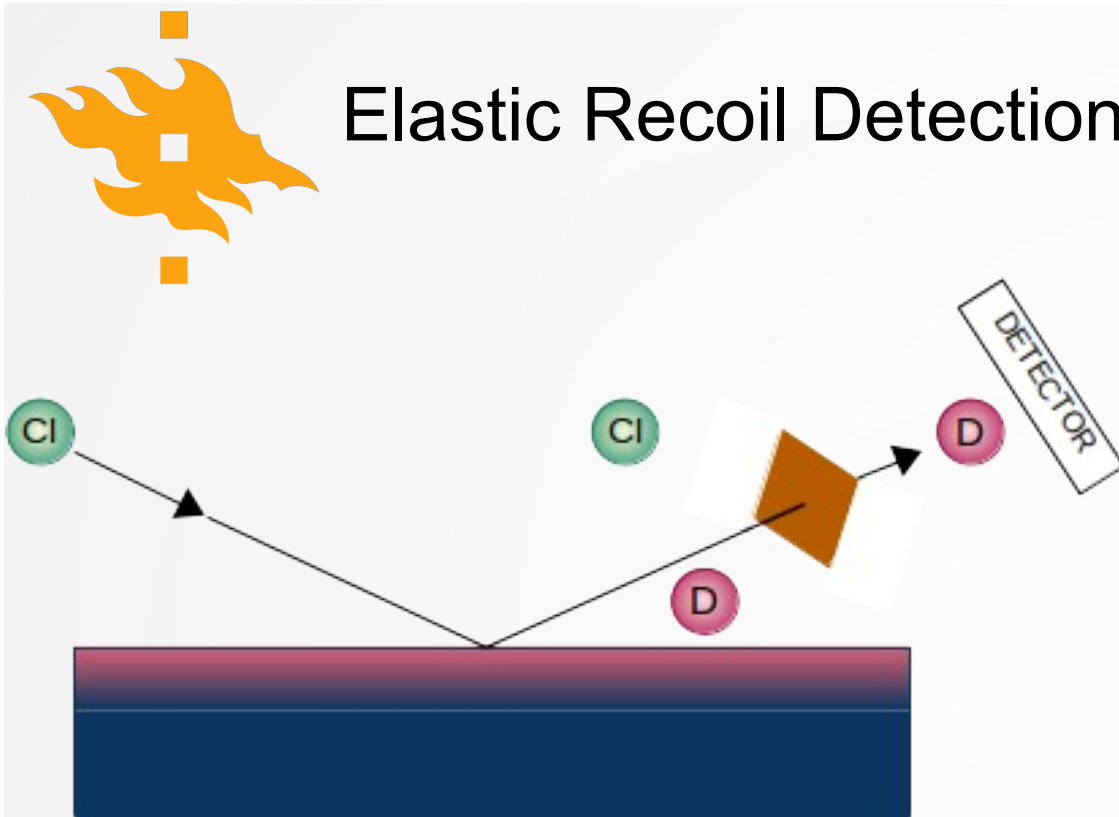
All elements (including noble gases)

Deuterium implantation

Energy → 1 keV/D

Dose → 10^{17} D/cm²

Elastic Recoil Detection Analysis



Heavy projectile (Cl, Si)

Foil-ERDA

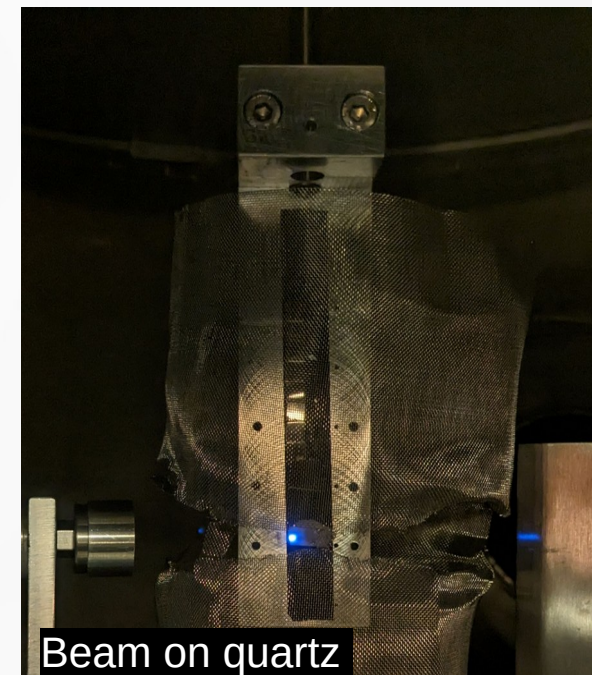
Light recoils H and D (He possible)

→ Stopping foil for heavier recoils (havar 4 μm)

TOF-ERDA → All elements

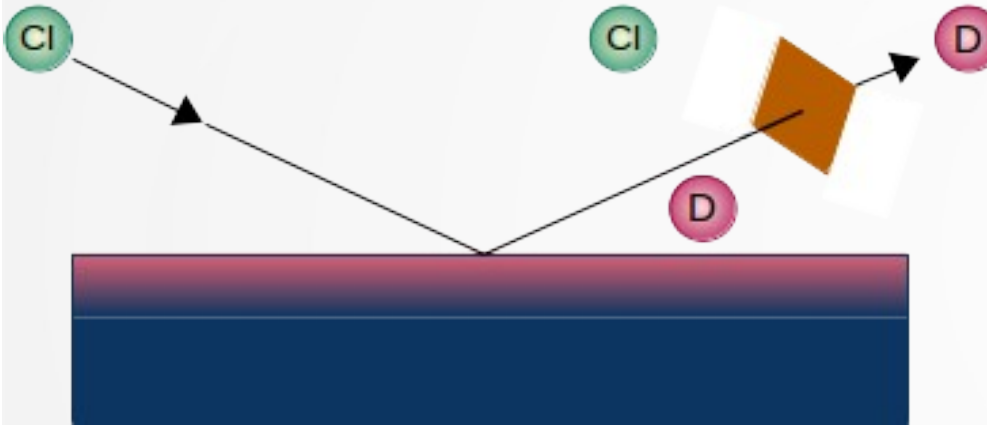
Depth profiling

→ Analysis depth: max 300 – 500 nm

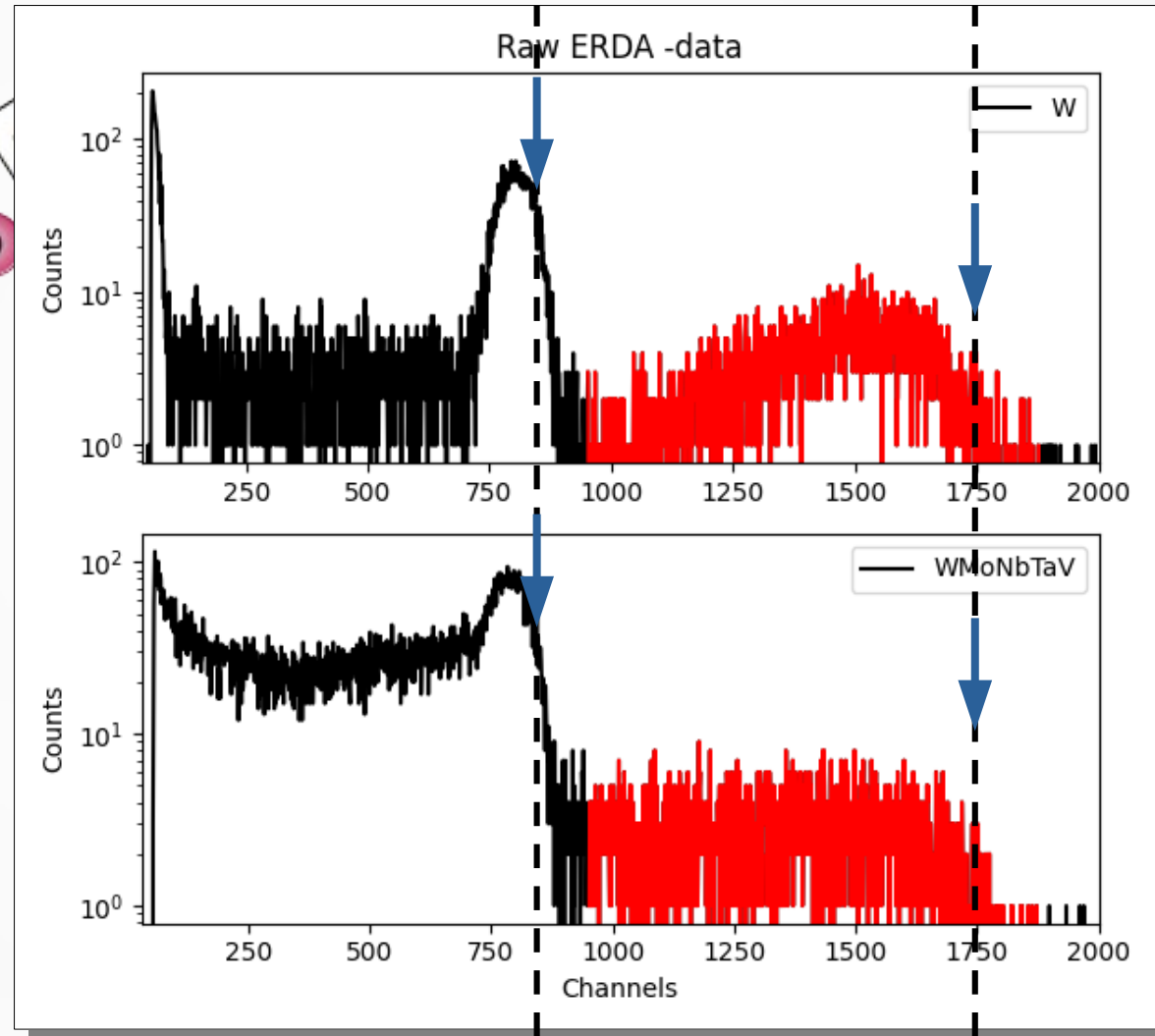




Elastic Recoil Detection Analysis



Placement of samples on a holder





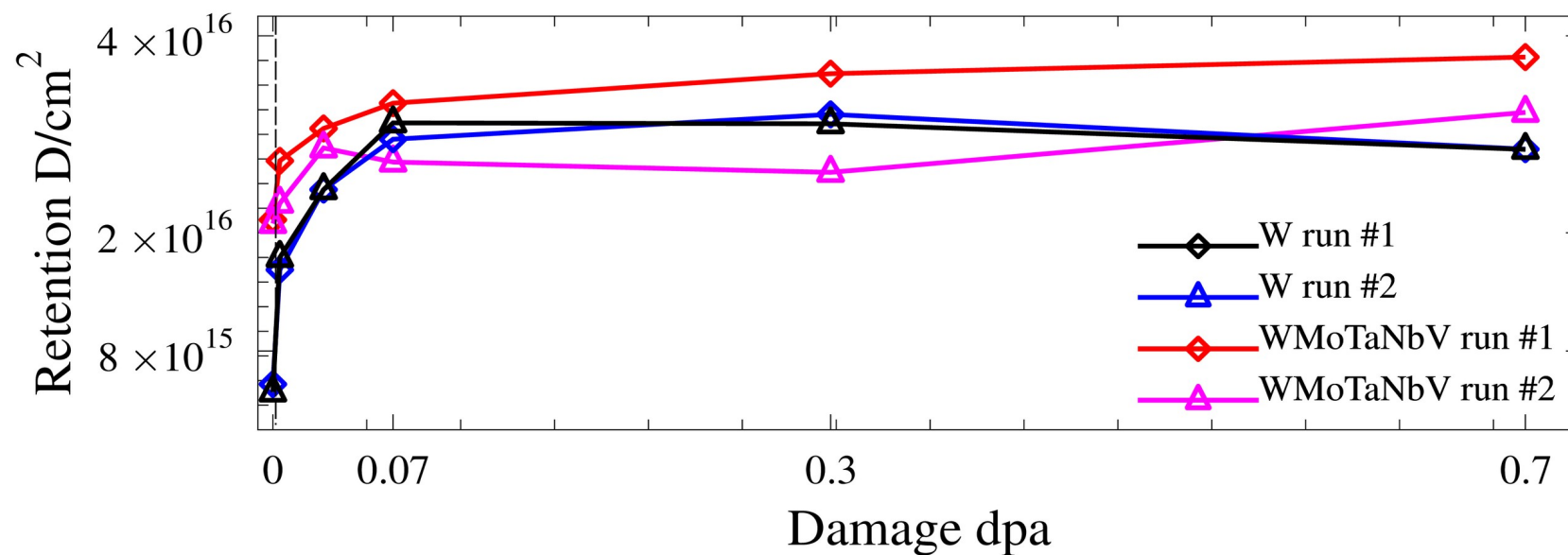
Foil-ERDA

HEA and W

pre-irradiated with W

→ 0, 0.007, 0.03, 0.07, 0.3, 0.7 dpa

D implanted 1 keV/D

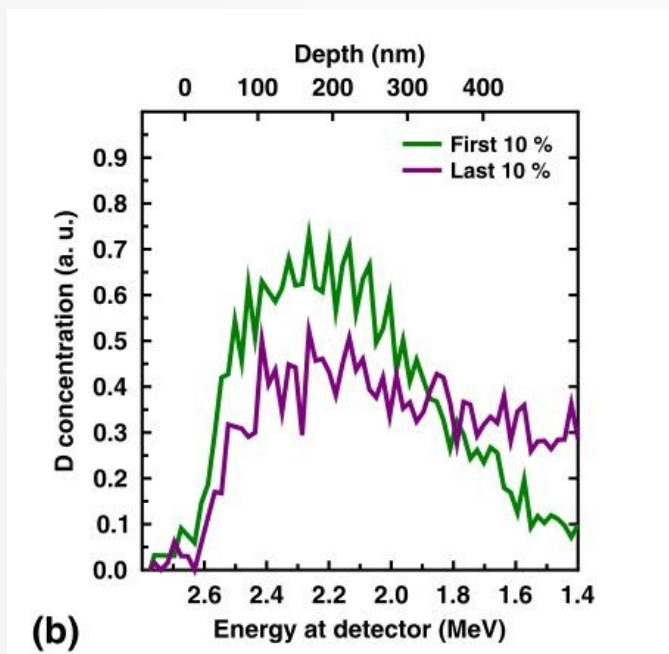




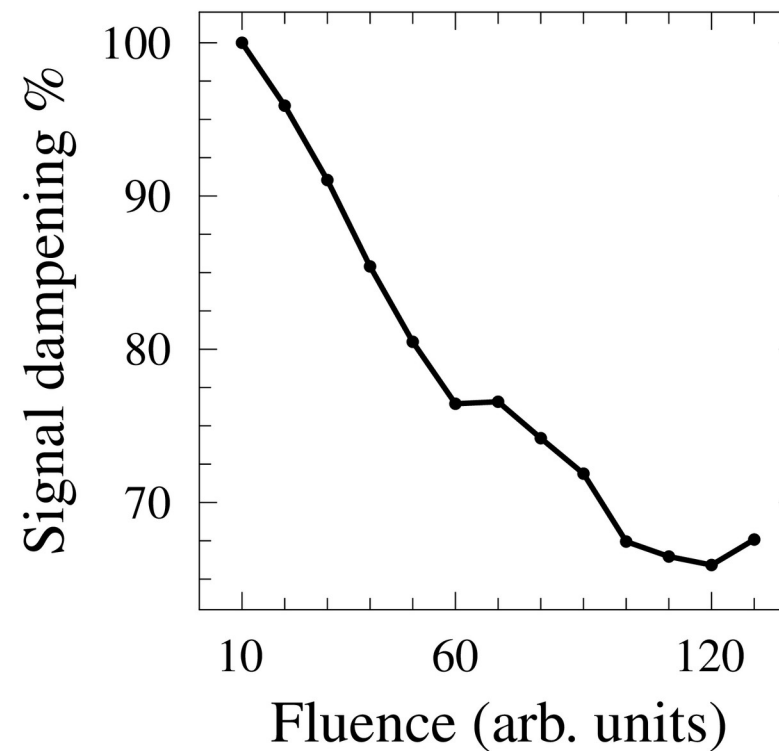
Foil-ERDA

Mobility of D

- Not trapping
- Hydrogen absorbing elements



T. Vuoriheimo, et. al., Nuclear Materials and Energy 34 (2023) 101348.





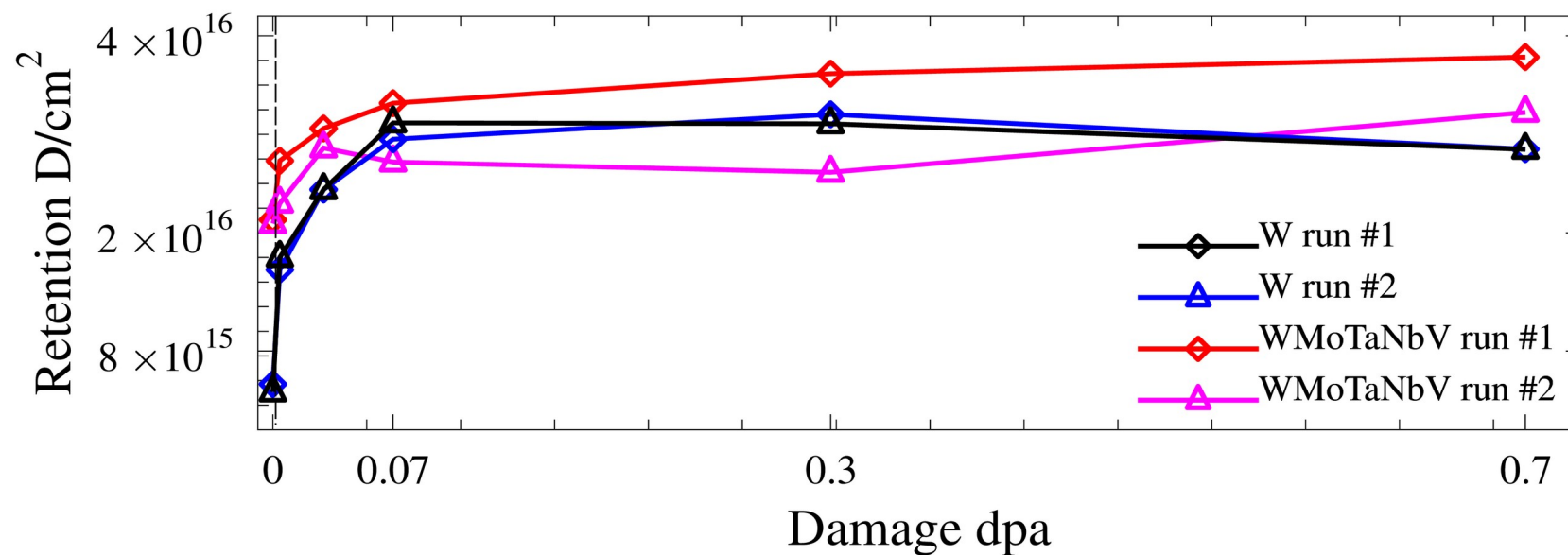
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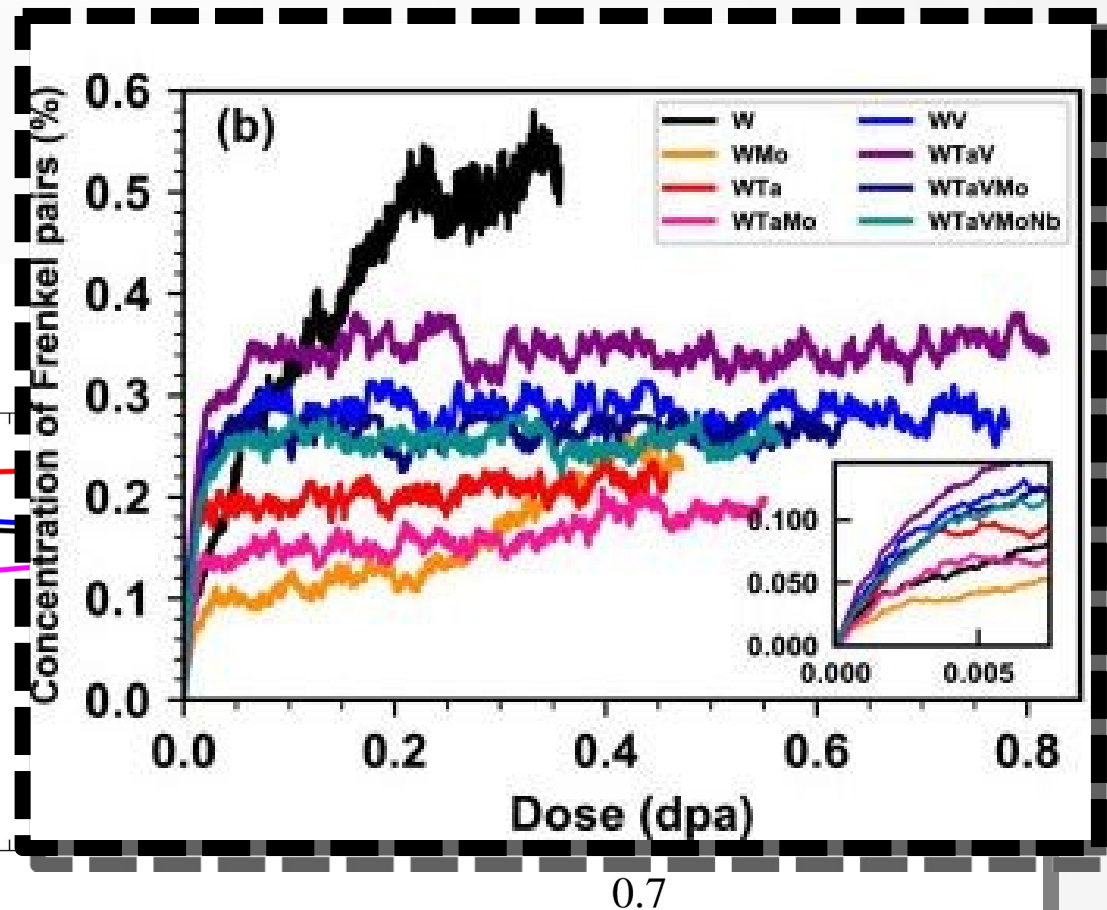
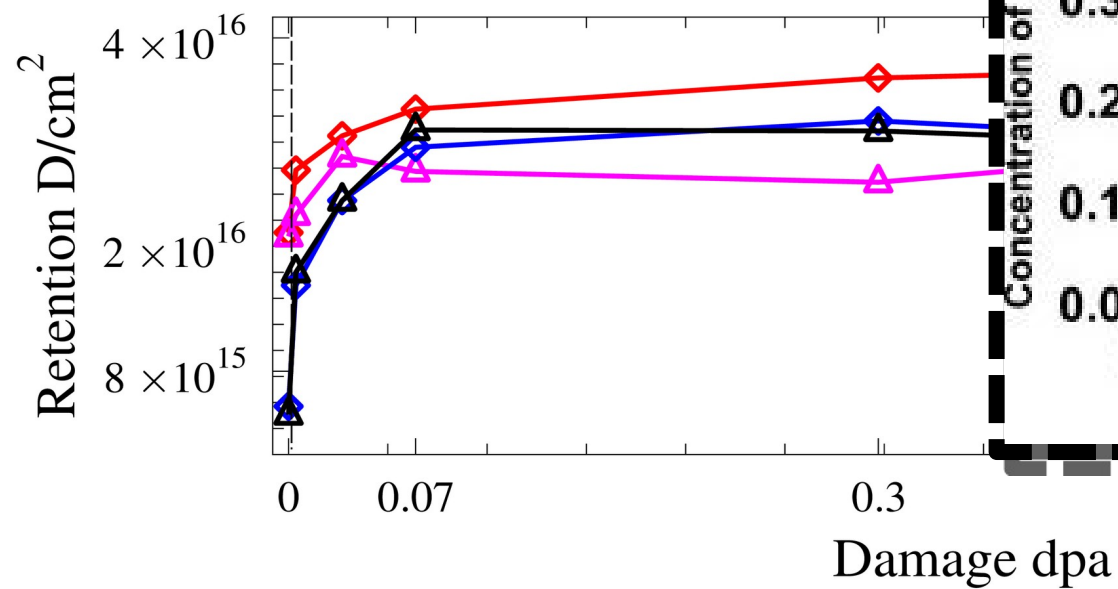
D implanted 1 keV/D





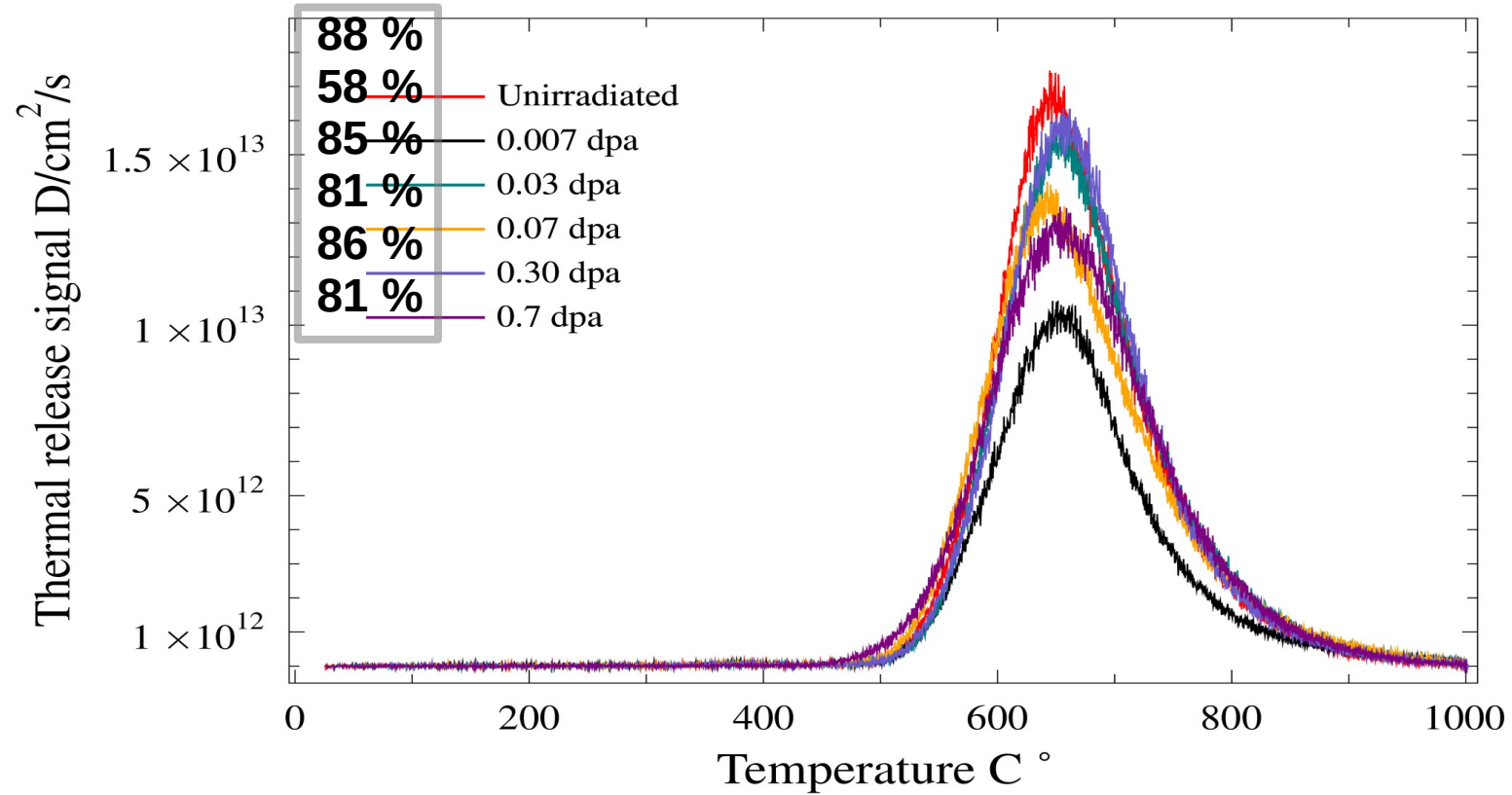
Foil-ERDA

G. Wei, et. al., *Acta Materialia*, 274 (2024) 119991.



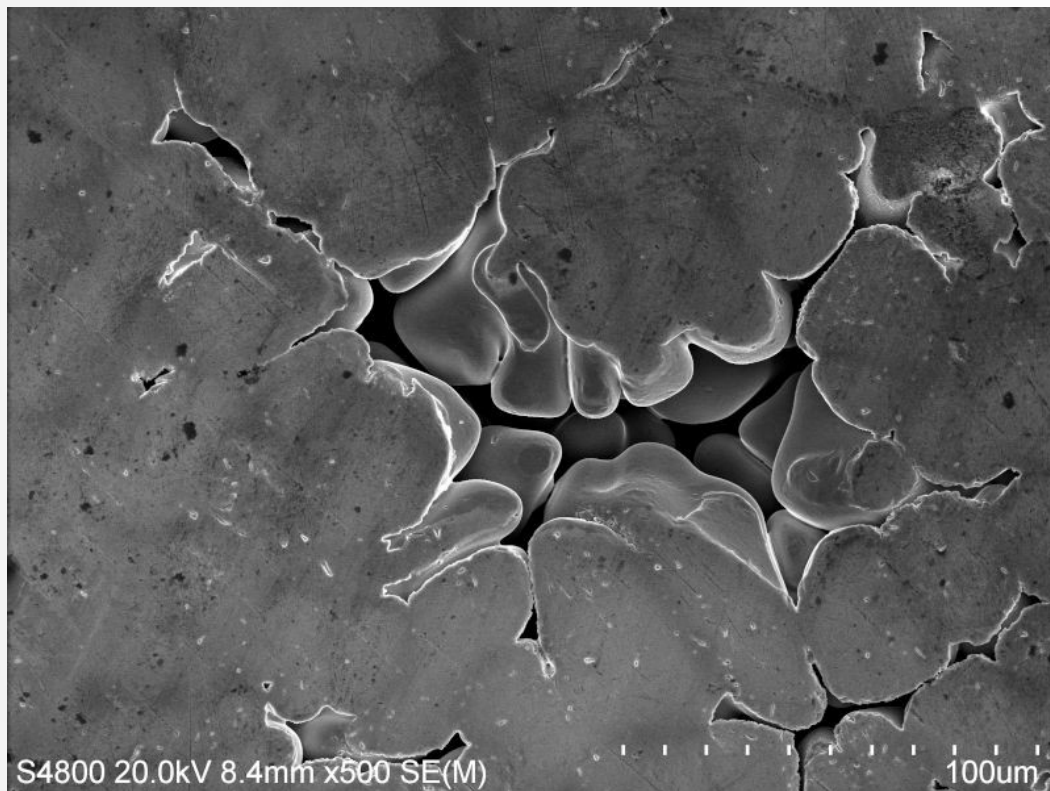


Thermal Desorption Spectrometry





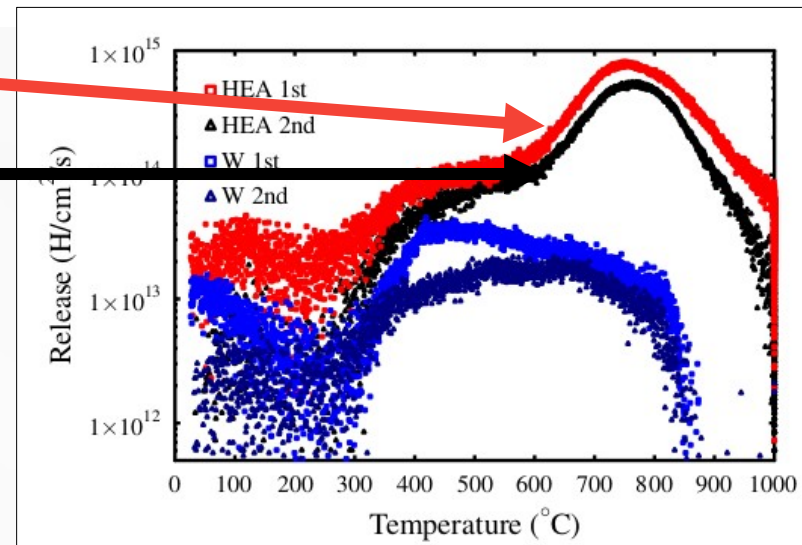
Summary



H in HEA (TDS)

H in HEA (TDS)

- same sample
- many weeks in atmospheric conditions.



WMoTaNbV alloy retains plenty of H
→ Absorbs from atmosphere

Microstructure important for H/D retention
→ H/D trapped in structural defects (GB, vacancies, voids)
→ More defects, more H/D

Quality of samples is crucial.



Thank you!

