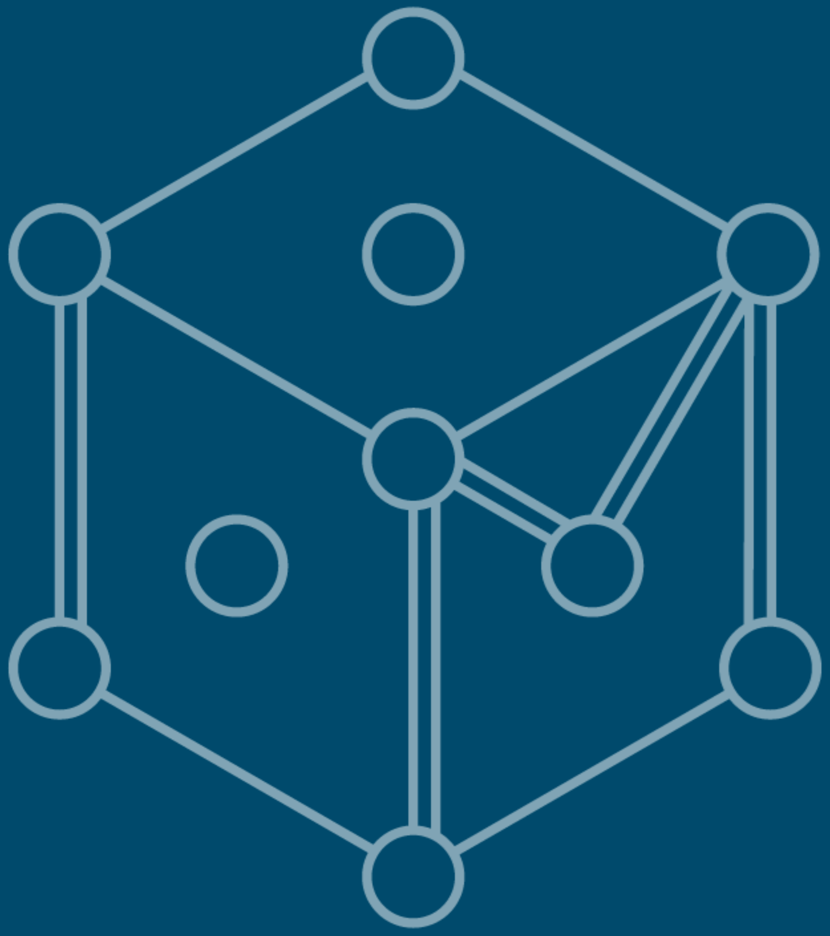

Faculty of Materials Science and Engineering
Warsaw University of Technology

Characterization of Ti-containing HEAs as Emerging Materials for Solid-State Hydrogen Storage

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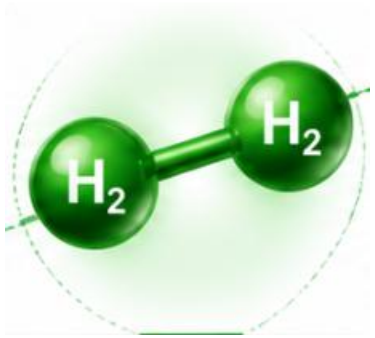
From hydrogen economy to advanced materials: Why HEAs?

Hydrogen Economy



Clean energy carrier for industrial and transport decarbonization

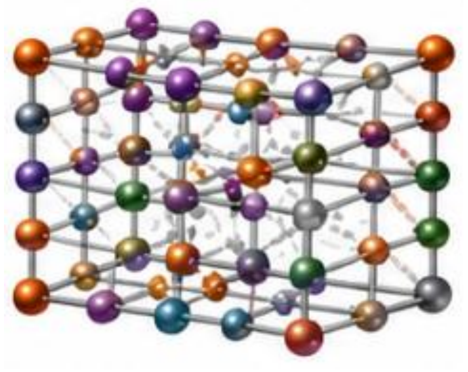
High gravimetric energy density (120 MJ/kg)

The Storage Bottleneck

High compression (350–700 bar) and cryogenic cooling (−253°C) carry large energy penalties and safety challenges

Strong demand for safe, compact solid-state metal hydrides

Ti-containing HEAs



BCC solid solutions formed by multi-principal elements (Ti,V,Cr,Nb,Ta,Zr)

Severe lattice distortion and cocktail effect enhance interstitial hydrogen uptake and phase stability

Research Objective & Scope

To evaluate and compare phase transformation, hydrogen storage capacity, and particle stability in BCC-structured **TiTaNbZr** and **$(TiVNb)_{85}Cr_{15}$** high-entropy alloys.

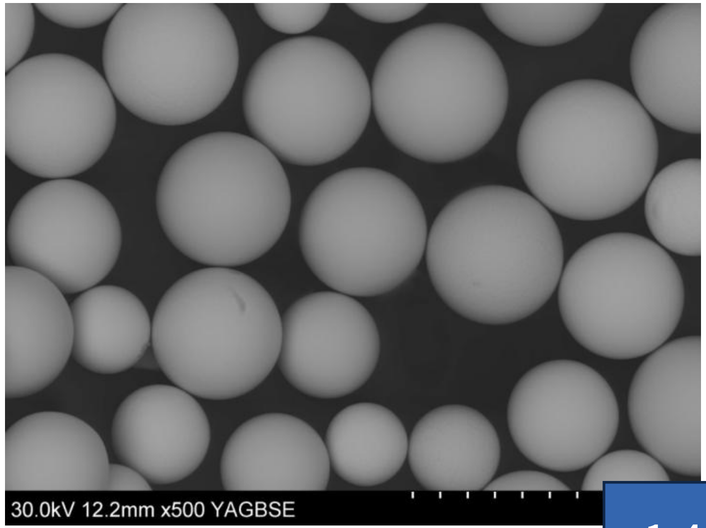
Characterization of TiTaNbZr before and after hydrogenation

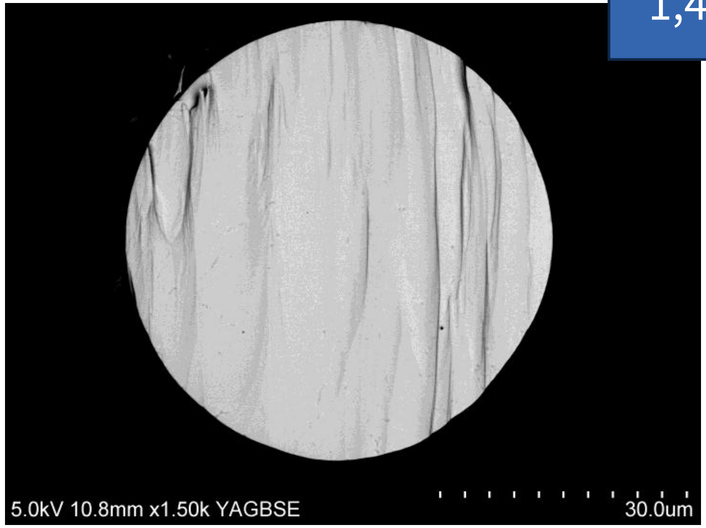
SEM

Homogeneous structure of spherical particles

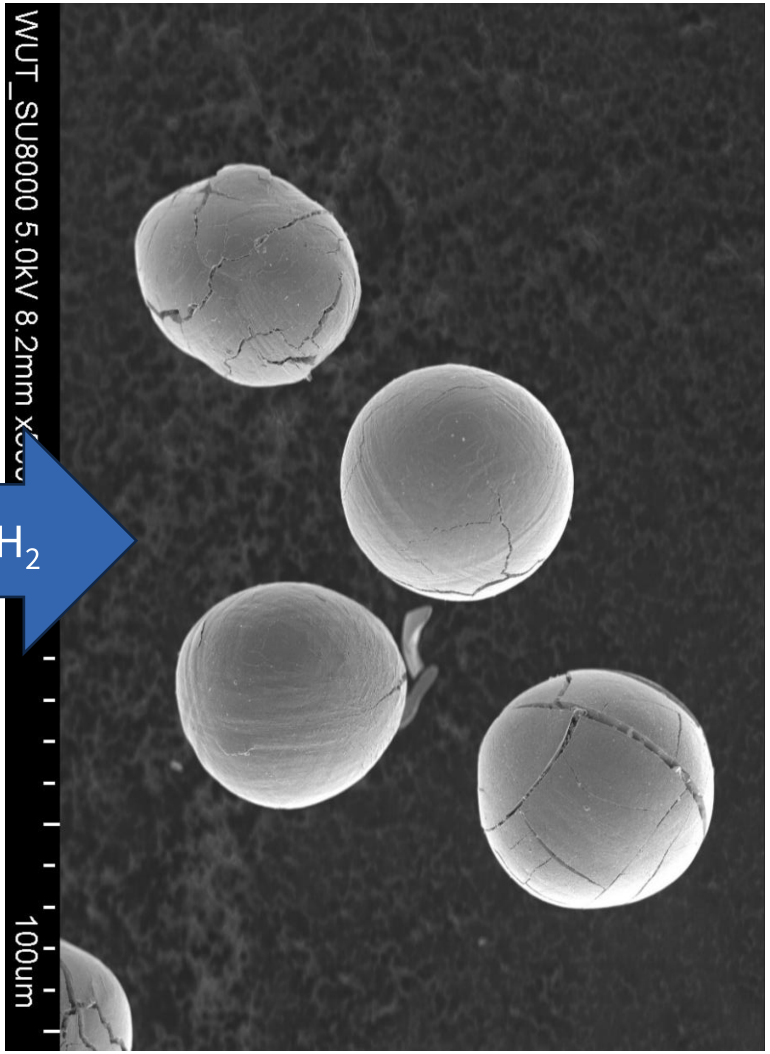
surface cracking

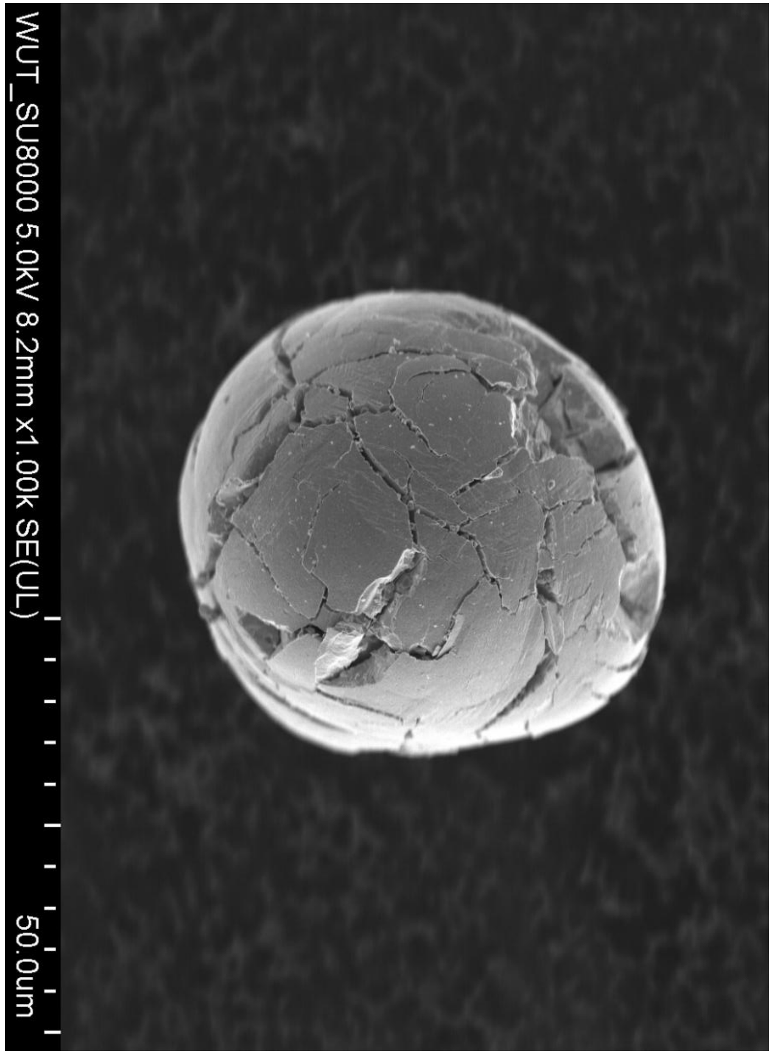
the overall spherical particle integrity and grain size distribution are preserved





1,4wt%H_2

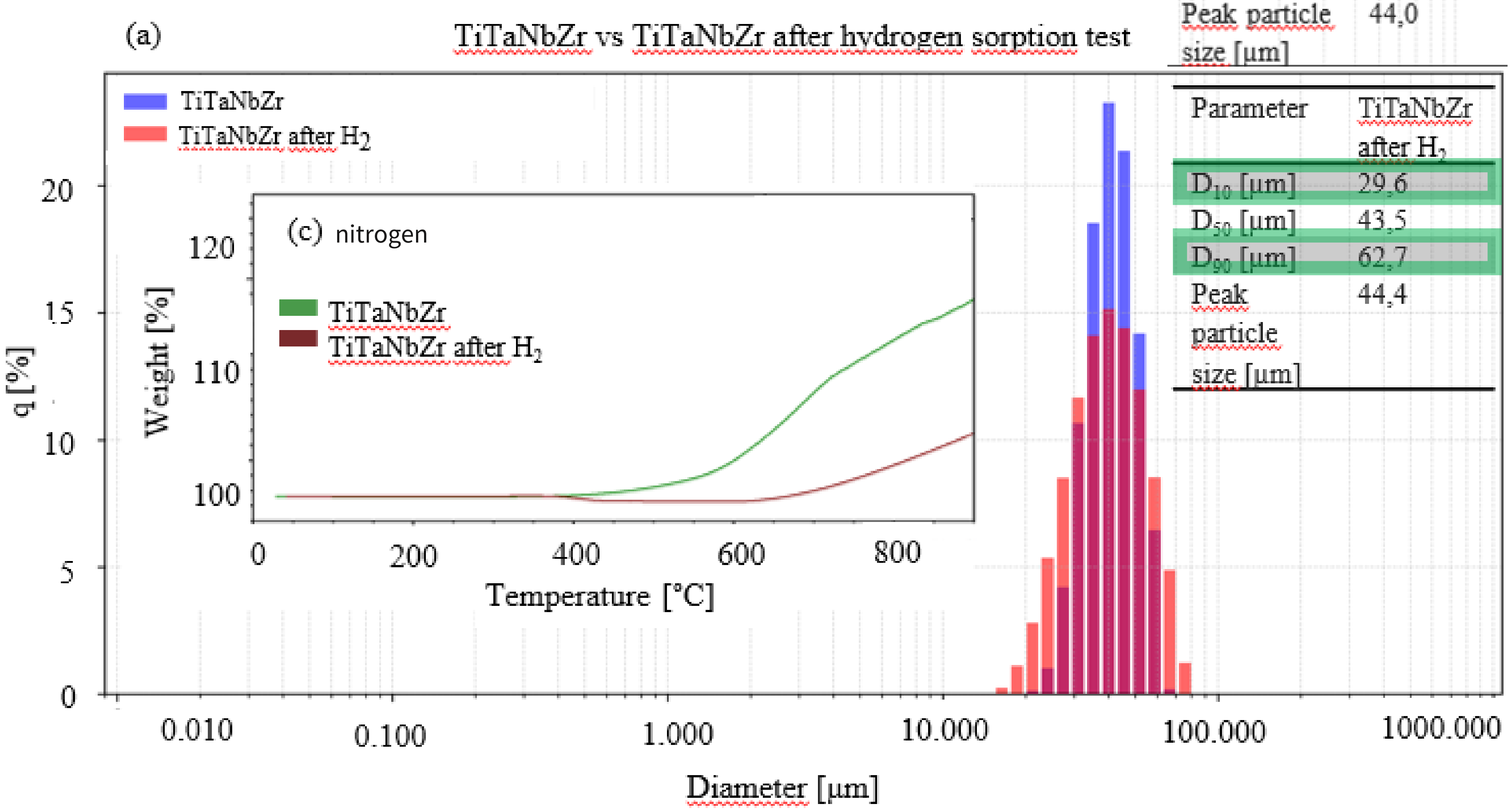




TGA and particle size distibution

Parameter	TiTaNbZr
D_{10} [µm]	32,9
D_{50} [µm]	43,7
D_{90} [µm]	57,1
Peak particle size [µm]	44,0

Parameter	TiTaNbZr after H_2
D_{10} [µm]	29,6
D_{50} [µm]	43,5
D_{90} [µm]	62,7
Peak particle size [µm]	44,4



For the hydrogenated alloy (~1.4 wt.% H2) - Between 380°C and 450°C, a mass loss of approximately 0.4 wt.%

Above 600 °C - weight gain exceeding 105% at 900 °C - nitrogenation

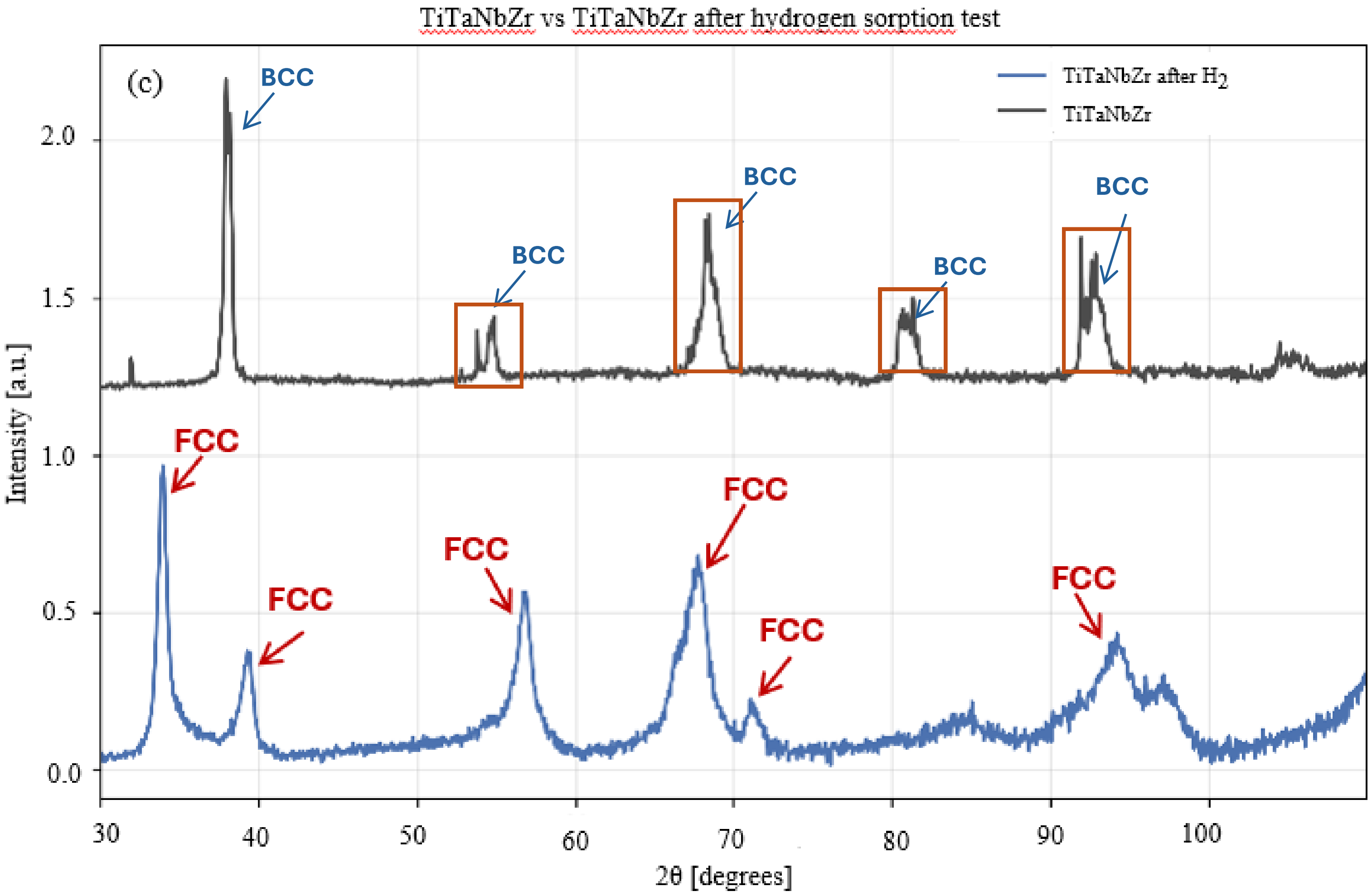
Following hydrogenation, D_{50} and peak - virtually unchanged

D_{10} decreased from 32.9 µm to 29.6 µm, while D_{90} increased from 57.1 µm to 62.7 µm

XRD

TiTaNbZr before H_2

BCC-dominated



TiTaNbZr after H_2

the hydrogenated TiTaNbZr alloy (1.4 wt.% H2) can be described by FCC dihydride lattice

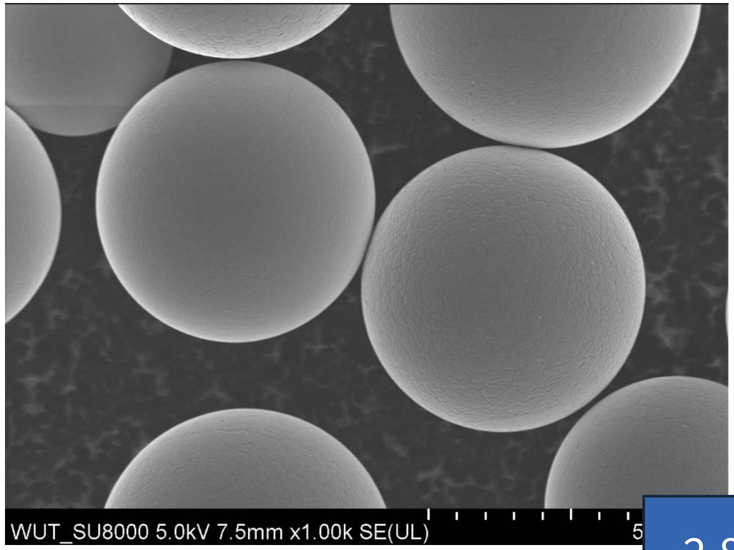
Characterization of (TiVNb)85Cr15 before and after hydrogenation

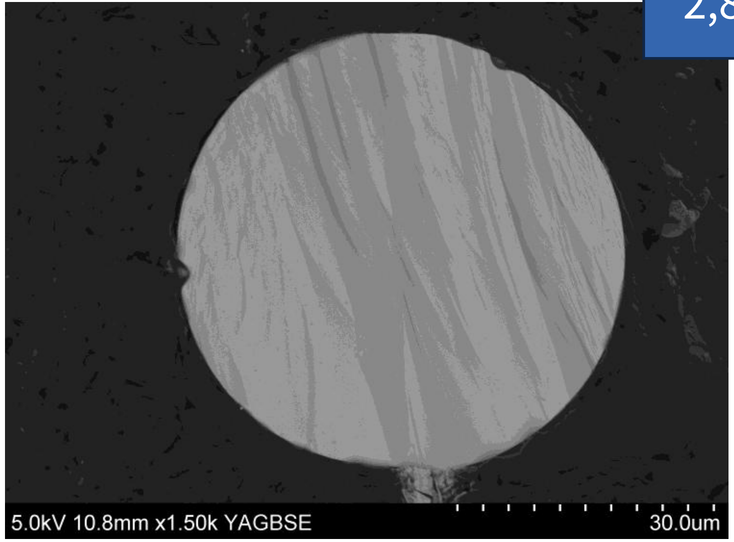
SEM

Homogeneous structure of spherical particles

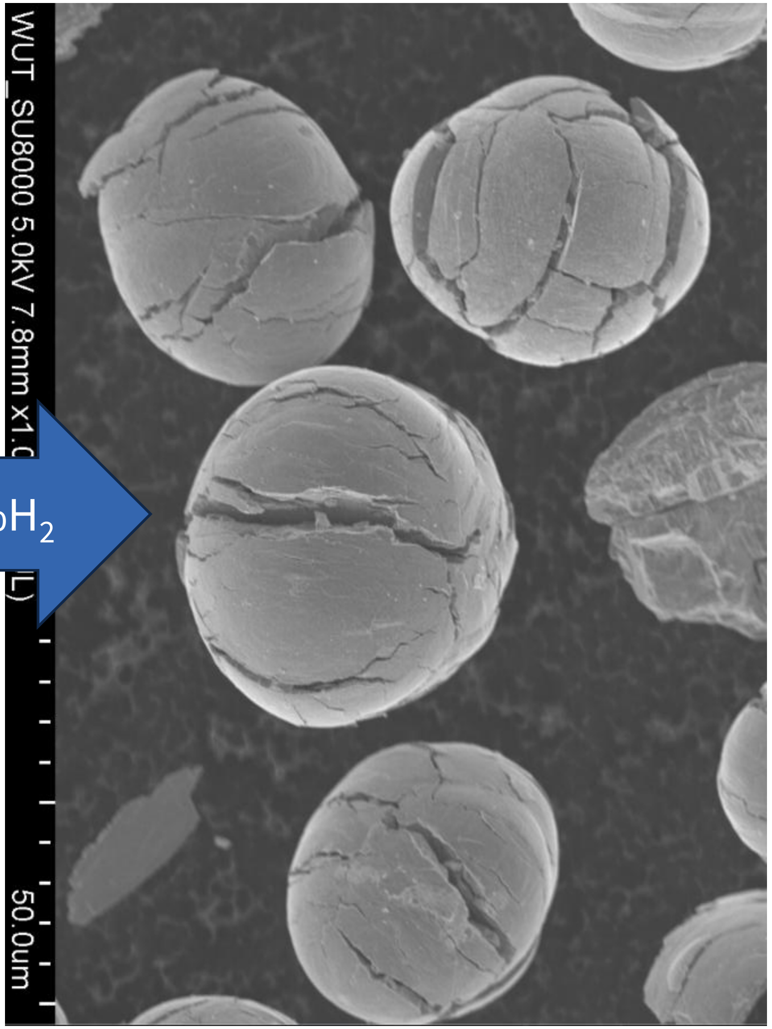
surface cracking

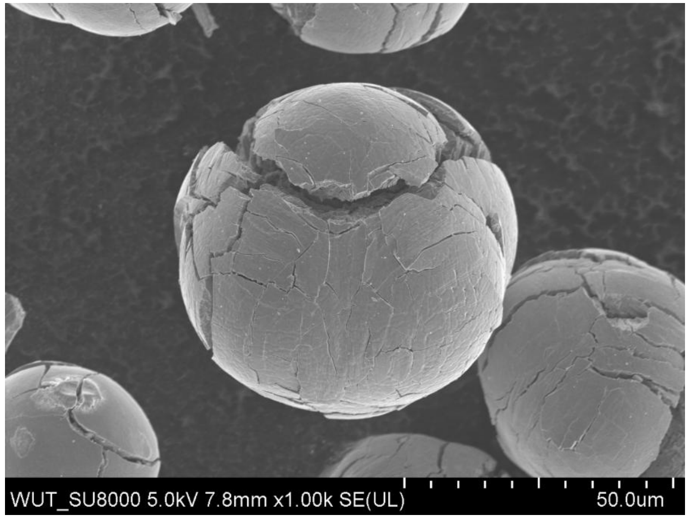
the overall spherical particle integrity is preserved

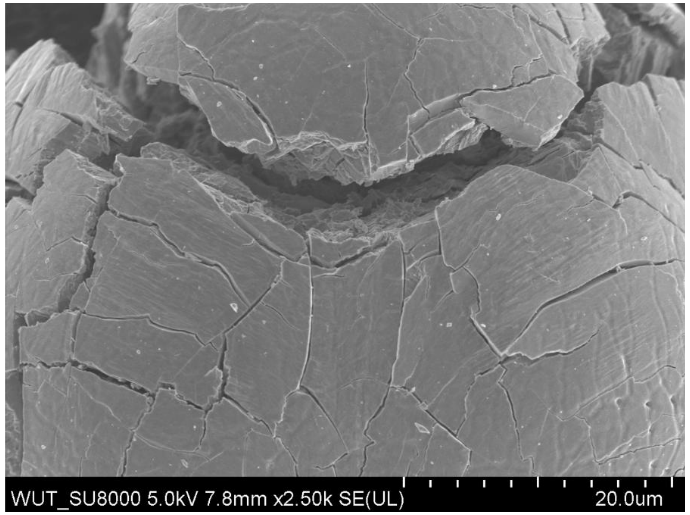




2,8wt%H_2



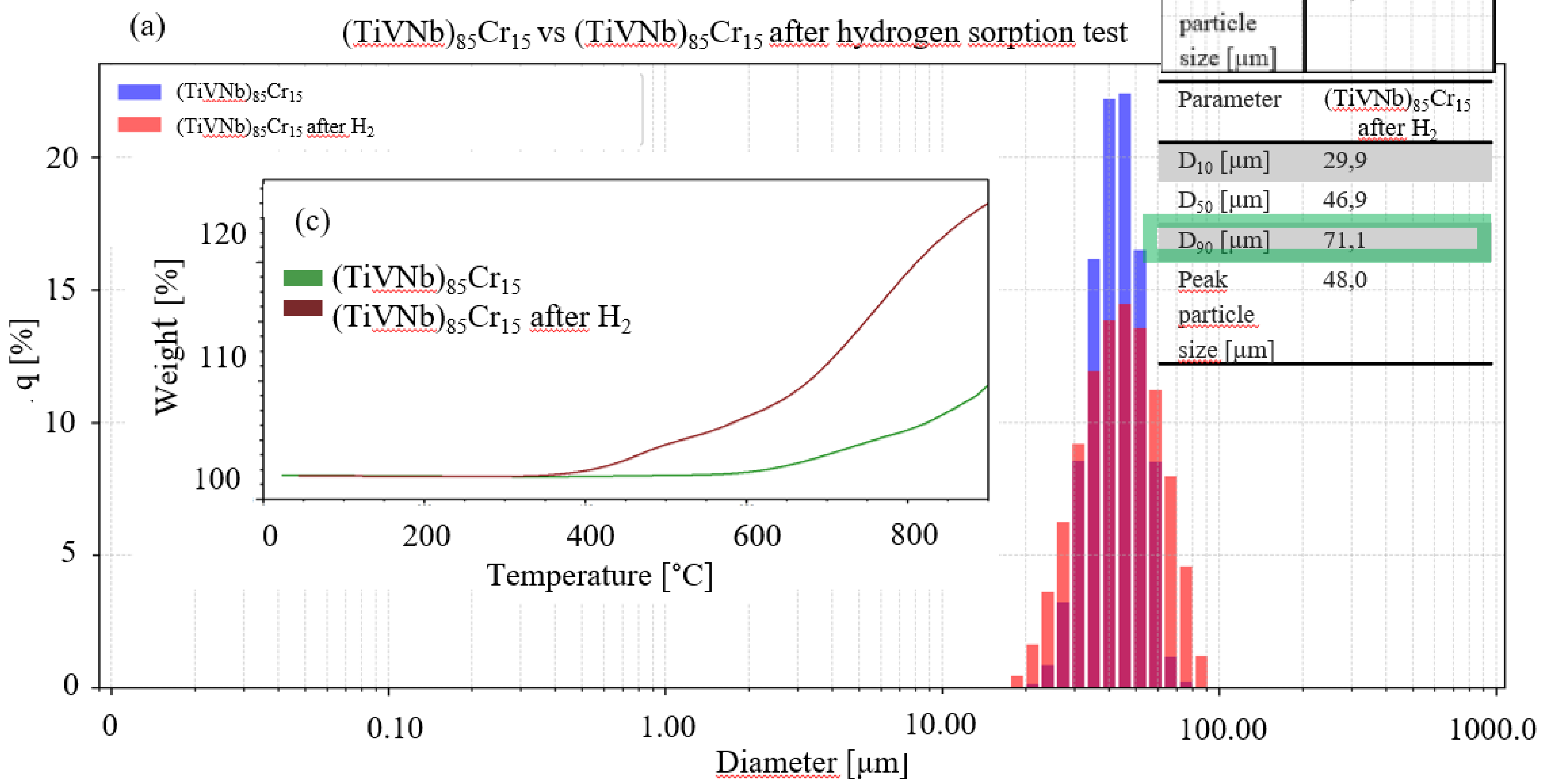




TGA and particle size distibution

Parameter	$(TiVNb)_{85}Cr_{15}$
D_{10} [µm]	33,9
D_{50} [µm]	45,3
D_{90} [µm]	58,8
Peak particle size [µm]	45,8

Parameter	$(TiVNb)_{85}Cr_{15}$ after H_2
D_{10} [µm]	29,9
D_{50} [µm]	46,9
D_{90} [µm]	71,1
Peak particle size [µm]	48,0



changes in the distribution width, particularly for D_{10}=29.9 µm and D_{90}=71.1 µm, where the peak becomes slightly broader and higher

the hydrogenated $(TiVNb)_{85}Cr_{15}$ powder exhibits thermal stability up to approximately 380 °C, above - nitrogenation

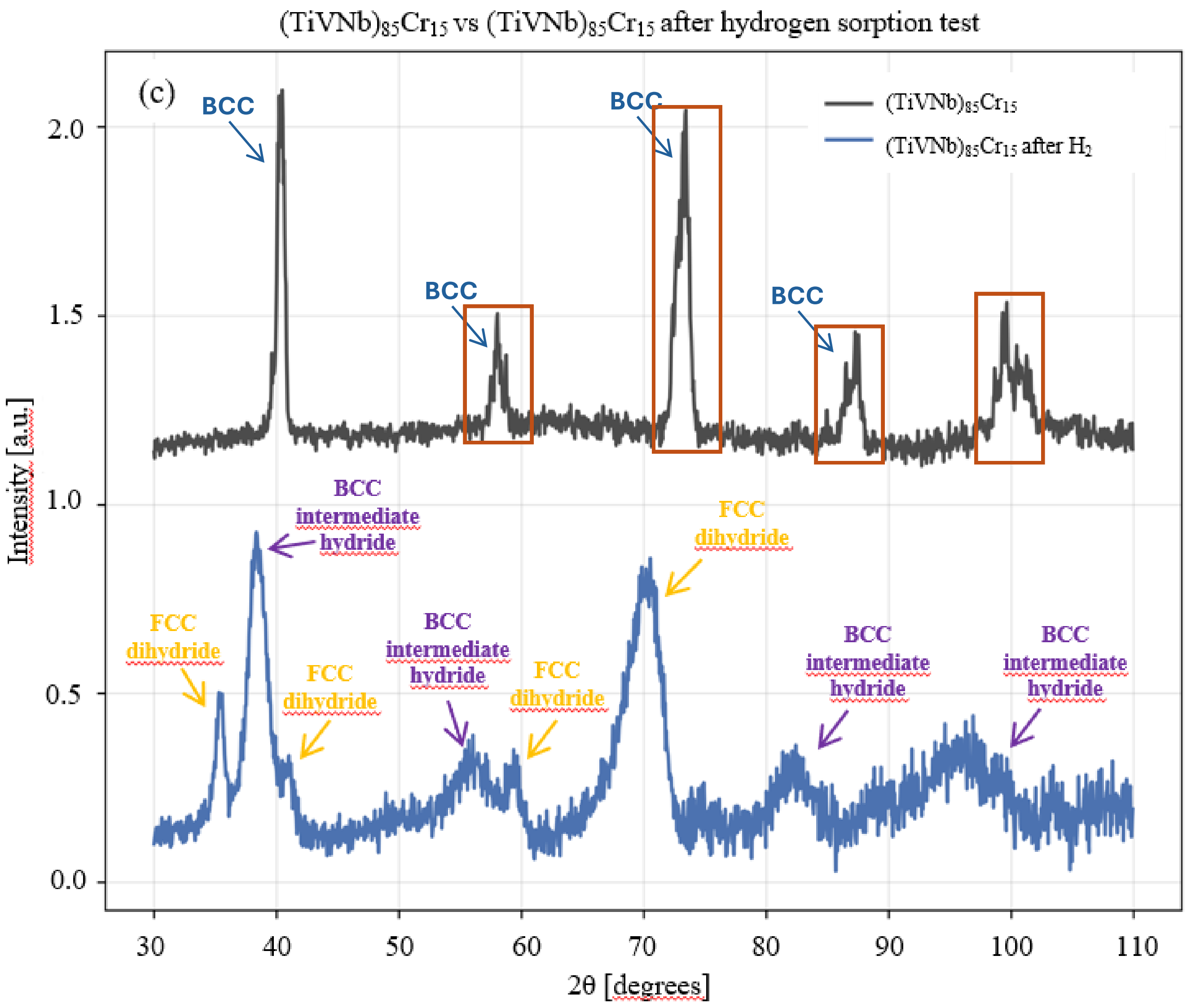
The hydrogenated sample is notably more sensitive to elevated temperature and the nitrogen environment than the as-synthesized alloy

Characterization of (TiVNb)85Cr15 before and after hydrogenation

XRD

(TiVNb)85Cr15 before H_2

a predominantly BCC solid solution



(TiVNb)85Cr15 after H_2

Upon hydrogen absorption (~2.8wt%) the diffraction pattern reveals a dual-phase hydride mixture

Conclusions

Feature	TiTaNbZr	(TiVNb)85Cr15
Initial Structure	Predominantly BCC solid solution	Predominantly BCC solid solution
H_2 Absorption Capacity	≈1.4 wt.% H_2	≈2.8 wt.% H_2
Hydride Phase Evolution	FCC dihydride	Dual-phase hydride mixture
Particle Integrity	Spherical shape preserved, surface cracking	Spherical shape preserved, surface cracking
Particle Size Distribution (PSD)	D_{50} virtually unchanged;, slight span broadening	span broadening , D_{90}, D_{50} and peak increased, D_{10}decreased

Ti-containing BCC high-entropy alloys prove to be versatile, robust candidates for solid-state hydrogen storage.

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Thank you

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NCBR
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