Supplementary Information
Hydrogen storage properties of a new Ti-V-Cr-Zr-Nb high entropy alloy

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Figure SI-1. Structural analysis (phase fractions and corresponding lattice parameters) of the $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}H_x$ (x = 0.3; 0.8; 1.3) and the desorbed phase.

Table SI-1. Crystallographic information of the SR-XRD of the desorbed $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}$ sample.

Table SI-2. Crystallographic information of the SR-XRD of the $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}H_{0.3}$ hydride.

Table SI-3. Crystallographic information of the SR-XRD of the $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}H_{0.8}$ hydride.

Table SI-4. Crystallographic information of the SR-XRD of the $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}H_{1.3}$ hydride.

Figure SI-2. X-ray diffraction pattern after 20 absorption/desorption cycles (λ= 1.5406 Å) of the hydride $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}H_{1.53}$.

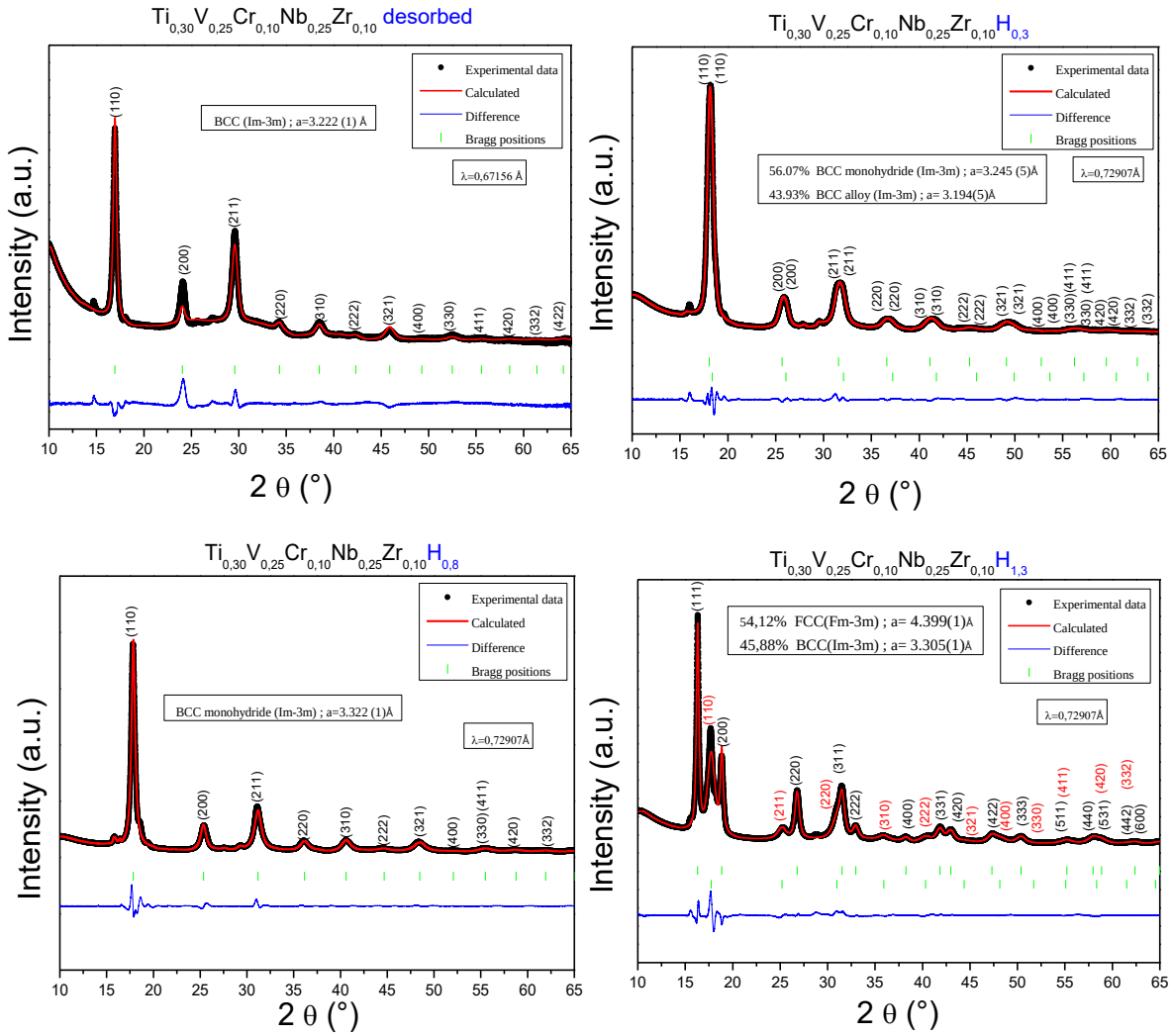

Figure SI-1. Structural analysis of the SR-XRD (phase fractions and corresponding lattice parameters) of the $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}H_x$ (x = 0.3; 0.8; 1.3) and the desorbed phase.

Composition	*fcc dihydride lattice parameter (Å)*	*phase fraction (%)*	*bcc monohydride lattice parameter (Å)*	*phase fraction (%)*	*bcc (desorbed) lattice parameter (Å)*	*phase fraction (%)*	R_B	χ^2
$Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}$ (Desorbed)	-	-	-	-	3.222 (2)	100	11.1	23.2
Position	-		-		(0 ; 0 ; 0)			
Elements	Ti	V	Cr		Nb	Zr		
Occupancy	30%	25%	10%		25%	10%		

Table SI-1. Crystallographic information of the SR-XRD of the desorbed $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}$ sample.

Composition	*fcc dihydride lattice parameter (Å)*	*phase fraction (%)*	*bcc monohydride lattice parameter (Å)*	*phase fraction (%)*	R_B	*bcc (desorbed) lattice parameter (Å)*	*phase fraction (%)*	R_B	χ^2
$Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}$ (H/M= 0.3)	-	-	3.245 (5)	56	1.82	3.194 (5)	44	1.31	15.6
Position	-		(0 ; 0 ; 0)			(0 ; 0 ; 0)			
Elements	Ti	V	Cr		Nb		Zr		
Occupancy	30%	25%	10%		25%		10%		

Table SI-2. Crystallographic information of the SR-XRD of the $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}H_{0.3}$ hydride.

Composition	*fcc dihydride lattice parameter (Å)*	*phase fraction (%)*	*bcc monohydride lattice parameter (Å)*	*phase fraction (%)*	R_B	*bcc (desorbed) lattice parameter (Å)*	*phase fraction (%)*	χ^2
$Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}$ (H/M= 0.8)	-	-	3.322 (1)	100	1.38	-	-	25.6
Position	-		(0 ; 0 ; 0)			-		
Elements	Ti	V	Cr		Nb		Zr	
Occupancy	30%	25%	10%		25%		10%	

Table SI-3. Crystallographic information of the SR-XRD of the $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}H_{0.8}$ hydride.

Composition	*fcc dihydride lattice parameter (Å)*	*phase fraction (%)*	R_B	*bcc monohydride lattice parameter (Å)*	*phase fraction (%)*	R_B	*bcc (desorbed) lattice parameter (Å)*	*phase fraction (%)*	χ^2
$Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}$ (H/M= 1.3)	4.399 (1)	54	2.71	3.305 (1)	46	4.09	-	-	23.4
Position	(0 ; 0 ; 0)			(0 ; 0 ; 0)			-		
Elements	Ti	V		Cr		Nb		Zr	
Occupancy	30%	25%		10%		25%		10%	

Table SI-4. Crystallographic information of the SR-XRD of the $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}H_{1.3}$ hydride.

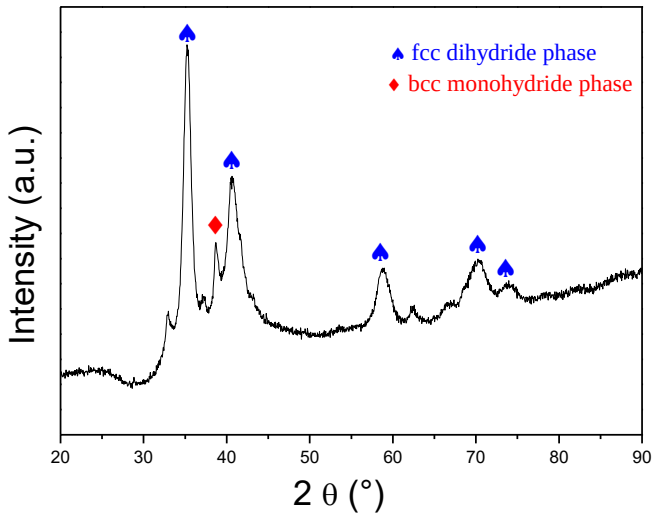

Figure SI-2. X-ray diffraction pattern after 20 absorption/desorption cycles (λ= 1.5406 Å) of the hydride $Ti_{0.30}V_{0.25}Cr_{0.10}Zr_{0.10}Nb_{0.25}H_{1.53}$.