hydrogen

MDPI

Supplementary Materials

Hydrogen Sorption Properties of a Novel Refractory Ti-V-Zr-Nb-Mo High Entropy Alloy

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Part SI-1: Thermodynamic modelling of the Pressure-Composition-Isotherm for the $Ti_{0.30}V_{0.25}Zr_{0.10}Nb_{0.25}Mo_{0.10}$ composition at 25 °C.

Figure SI-2: SR-XRD pattern together with the corresponding Rietveld refinement for $Ti_{0.325}V_{0.275}Zr_{0.125}Nb_{0.275}H_{1.7}$.

Figure SI-3: nD pattern and related Rietveld refinement for $Ti_{0.325}V_{0.275}Zr_{0.125}Nb_{0.275}D_{1.7}$.

Part SI-1: The enthalpy and entropy of the *bcc* and *fcc* phases of the Ti-V-Zr-Nb-Mo alloys were calculated according to the thermodynamic model proposed in [1]. Table SI-1 presents the values of partial molar enthalpy (h_i) of the different alloying element *i* for the *bcc* and *fcc* phases. The values for Ti, V, Zr and Nb were reported in [1]. The value for Mo-*bcc* was taken from reference [1] and for Mo-*fcc* was calculated by DFT using the same method described in [1]. Table SI-2 presents the *bcc* and *fcc* bond energies (ε_{ij}) for the atomic pairs of the Ti-V-Zr-Nb-Mo. These values were obtained by DFT calculation using the same method described in [1]. The configurational entropy parameters for the *bcc* and *fcc* phases are presented in Table SI-3.

Table SI-**1.** Partial molar enthalpy (h_i) of the different alloying element i for the bcc and fcc phases. Values in kJ/mol of H.

	h_i^{bcc}	h_i^{fcc}
Ti	−58	−64.22
V	−29.5	−31.75
Zr	−64	−74.39
Nb	−35.3	−40.82
Mo	15	0.79

Table SI-2. ε_{i-j}^{bcc} and ε_{i-j}^{fcc} bond energies in kJ/mol for the atomic pairs considered in this work.

ε_{i-j}^{bcc}	**Ti**	**V**	**Zr**	**Nb**	**Mo**	ε_{i-j}^{bcc}
	−560421.1	−591764.2	−1461425.9	−1534040.5	−1609236.0	**Ti**
ε_{i-j}^{fcc}		−623110.6	−1492766.4	−1565384.6	−1640581.3	**V**
Ti	−373615.0		−2362431.4	−2435044.2	−2510238.4	**Zr**
V	−394508.8	−415403.3		−2507661.1	−2582856.8	**Nb**
Zr	−974285.1	−995177.5	−1574955.1		−2658046.5	**Mo**
Nb	−1022693.3	−1043586.6	−1623361.7	−1671769.0		ε_{i-j}^{bcc}
Mo	−1072820.8	−1093714.4	−1673489.3	−1721896.4	−1772024.5	
ε_{i-j}^{fcc}	**Ti**	**V**	**Zr**	**Nb**	**Mo**	ε_{i-j}^{fcc}

Table SI-**3.** Entropy parameters for describing the configurational entropy of the bcc and fcc phases used in this work.

	$\boldsymbol{\theta}$	$\boldsymbol{r}$
$\boldsymbol{bcc}$	6	5
$\boldsymbol{fcc}$	2	1

Table SI-**4.** Plateau enthalpies and plateau entropies for the nominal composition. ΔH_{plat} and ΔS_{plat} are given in kJ/mol of H and J/K.mol of H, respectively.

Temperature (°C)	**Nominal**	
	$\boldsymbol{\Delta H_{plat}}$	$\boldsymbol{\Delta S_{plat}}$
25	−38.5	−76.0
75	−38.4	−77.9
100	−38.3	−78.8
200	−38.1	−81.7
250	−38.0	−82.9
300	−37.8	−84.0

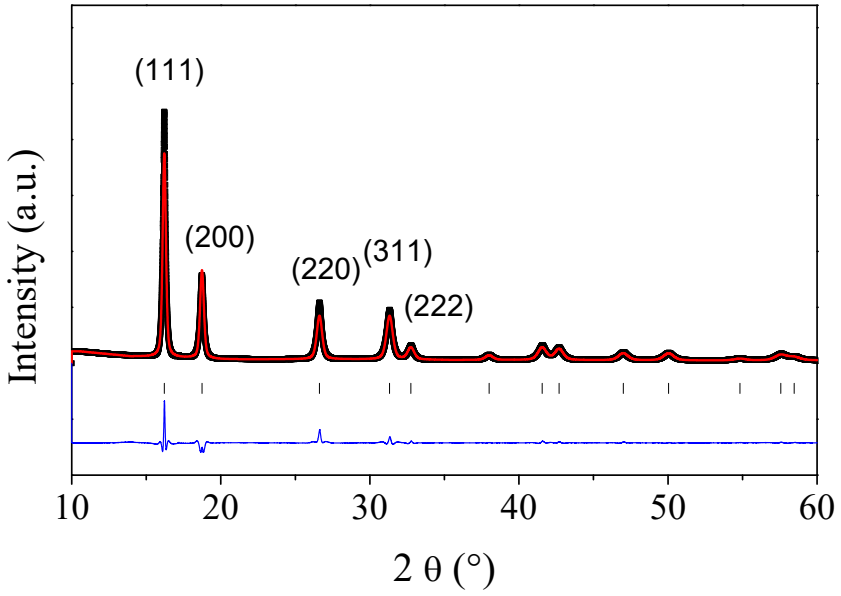

Figure SI-2. SR-XRD pattern together with the corresponding Rietveld refinements for $Ti_{0.325}V_{0.275}Zr_{0.125}Nb_{0.275}H_{1.7}$.

The refinement structural model is a *fcc* structure ($Fm\bar{3}m$) with the four types of metal atoms randomly distributed on the crystallographic sites. The lattice parameter is 4.478(1) Å.

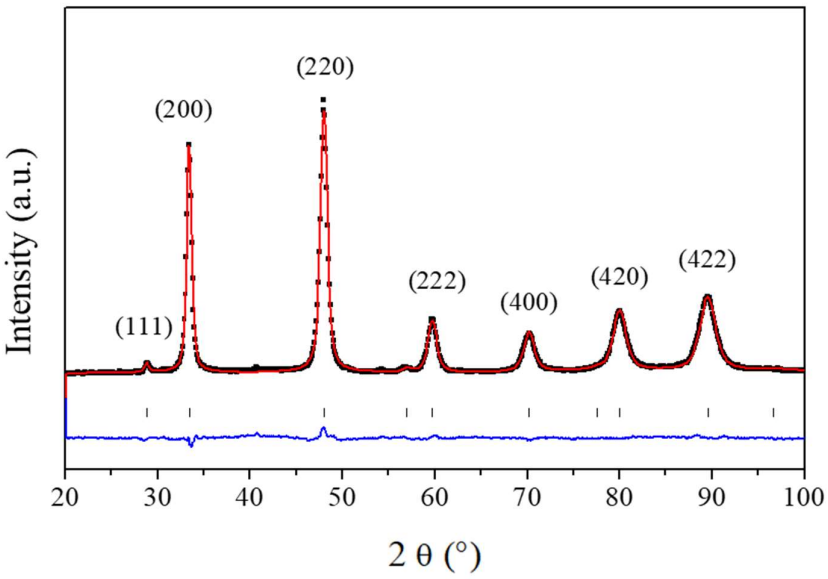

Figure SI-3. nD pattern and related Rietveld refinements for $Ti_{0.325}V_{0.275}Zr_{0.125}Nb_{0.275}D_{1.7.}$

The refinement structural model is a *fcc* structure ($Fm\bar{3}m$) with the four types of metal atoms randomly distributed on the specific crystallographic sites. The lattice parameter is 4.475(1) Å and the deuterium atoms are determined to occupy the tetrahedral interstitial sites of the *fcc* lattice.

Reference:

1. Zepon, G.; Silva, B.H.; Zlotea, C.; Botta, W.J.; Champion, Y. Thermodynamic Modelling of Hydrogen-Multicomponent Alloy Systems: Calculating Pressure-Composition-Temperature Diagrams. *Acta Mater.* **2021**, *215*, 117070, doi:10.1016/j.actamat.2021.117070.