Investigation of Entropy- Enthalpy Compensation effect in the Ti-V-Cr System.

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ABSTRACT

Selected composition of $Ti_xV_{70-x}Cr_{30}$ (x = 10, 20, 30, 40, 50) alloys doped with 4 wt.% of Zr_7Ni_{10} have been synthesized by arc melting. Crystal structure was characterized by X-ray diffraction pattern. Hydrogen storage properties were investigated using a Sievert- type apparatus. We found a strong discrepancy in the first hydrogenation curves of these samples. Maximum hydrogenation capacity was measured to be 4.0 wt.% for the $Ti_{50}V_{20}Cr_{30}$ alloy.

INTRODUCTION

Titanium-based alloys with a solid solutions Body Centered Cubic (BCC) crystal structure are well known to be good hydrogen storage materials because of their high volumetric hydrogen storage capacity.

We have recently found that in Ti-V-Cr system, the enthalpy of hydrogenation is linearly related to the entropy change[1,2,3] which is represented by the Fig.1. This is the so-called enthalpy-entropy compensation. The aim of the present work is to investigate the entropy-enthalpy compensation effect by varying the elemental concentration of the Ti-V-Cr system.

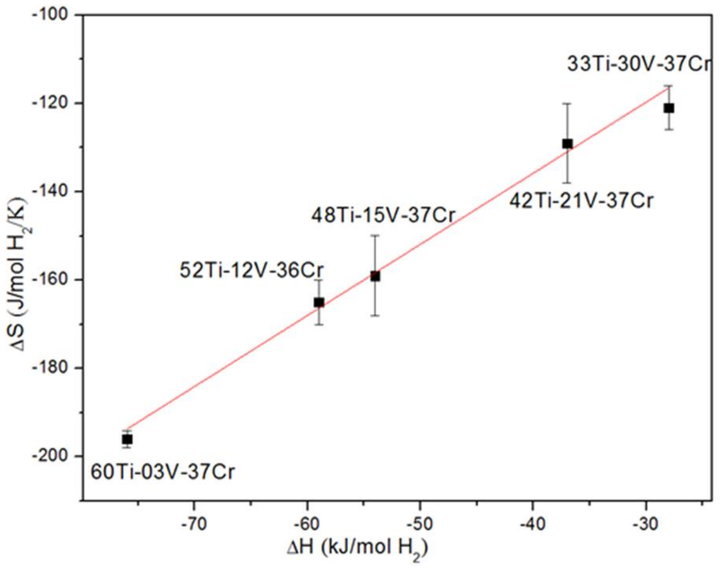


Fig.1:Enthalpy-Entropy plot of Ti-V-Cr system

OBJECTIVES

- Synthesis and structural characterization of the system $Ti_xV_{70-x}Cr_{30}$ (x = 10, 20, 30, 40, 50).
- Hydrogenation studies of these materials.
- Verify the Entropy-Enthalpy relationship and find the mechanism

METHODOLOGY

1. Material synthesis

- All samples were synthesized by arc melting.

2. Crystal structure

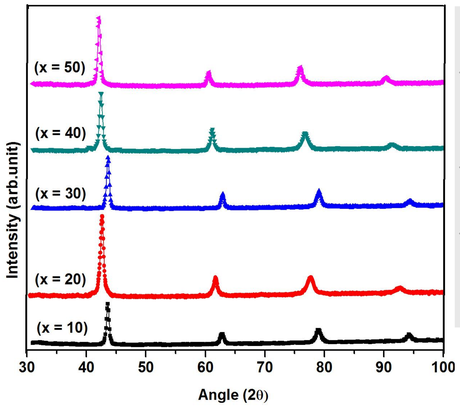
- The crystal structure was studied by X-Ray diffraction (XRD).

3. First hydrogenation properties

- Capacity of hydrogen absorption was determined with a Sievert-type apparatus.

RESULTS

Crystal Structure



- All samples have the BCC structure. Small peaks may indicate the
- Presence of a secondary phase.
- Crystal parameters of as cast samples are shown in Table. 1.

Fig. 2: X-Ray diffraction patterns of as-cast $Ti_xV_{70-x}Cr_{30}$ (x = 10, 20, 30, 40, 50) samples .

Table.1

Alloy	Lattice Parameter (Å)	Crystallite Size (nm)	Microstrain (%)
$Ti_{10}V_{60}Cr_{30}$	3.000(2)	18 (1)	0.43(9)
$Ti_{20}V_{50}Cr_{30}$	3.023(1)	12.5 (3)	0.62(4)
$Ti_{30}V_{40}Cr_{30}$	2.999(1)	16(1)	0.38(9)
$Ti_{40}V_{30}Cr_{30}$	3.069(1)	14.4(8)	0.47(9)
$Ti_{50}V_{20}Cr_{30}$	3.102(1)	15.6(6)	0.46(6)

First Hydrogenation

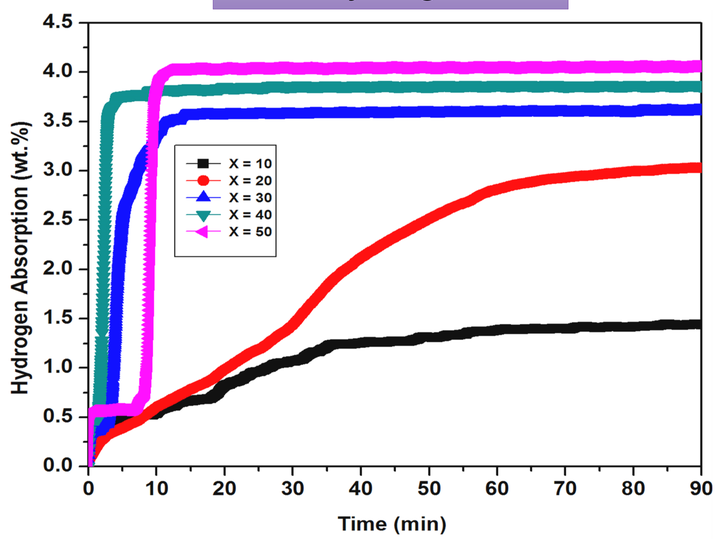


Fig. 3: First hydrogenation at 24°C and under 20 bar hydrogen pressure. As-cast samples: $Ti_xV_{70-x}Cr_{30}$ (x = 10, 20, 30, 40, 50) + 4 wt.% of Zr_7Ni_{10}.

- x = 50 has the highest capacity and an incubation time of less than 8 minutes.
- For x = 20, no incubation time but capacity is lowered.
- Sample x = 10 has shown low storage capacity.

CONCLUSION

- Five different compositions of Ti-V-Cr were investigated.
- All samples have the same crystal structure (BCC solid solution).
- Large discrepancies in the first hydrogenation behaviour are observed.
- Fast kinetics of first hydrogenation may be explained by the presence of a secondary phase.
- Microstructure and thermodynamic parameters are now being investigated.

REFERENCES

[1] Bibienne T and Huot J. Journal of Alloys and Compounds, 607 (2014) 251– 257.

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[3] Bibienne T and Huot J. To be published.

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