cbecimat26
26° Congresso Brasileiro de Engenharia e Ciência dos Materiais
22 a 26 de novembro de 2026
Costão do Santinho
Florianópolis-SC

Metallurgical Aspects and Their Impacts on the Hydrogen Storage Properties of BCC Multicomponent Alloys

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Introduction

A para-equilibrium kinetic model is proposed for the two-step hydrogenation of BCC alloys [α → β (H/M~1) → δ (H/M~2)] considering the displacive phase transformation mechanism with growth velocity controlled by the H diffusion from the parent phase to the growing hydride.

Structural Characterization

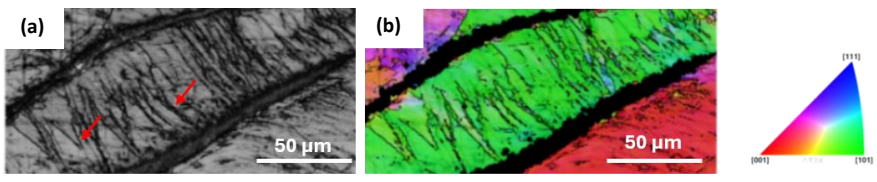


Figure 1: BSE-SEM and EBSD images of coexisting α- and β-phase for **(a)** and **(b)** TiVNbCr alloy.

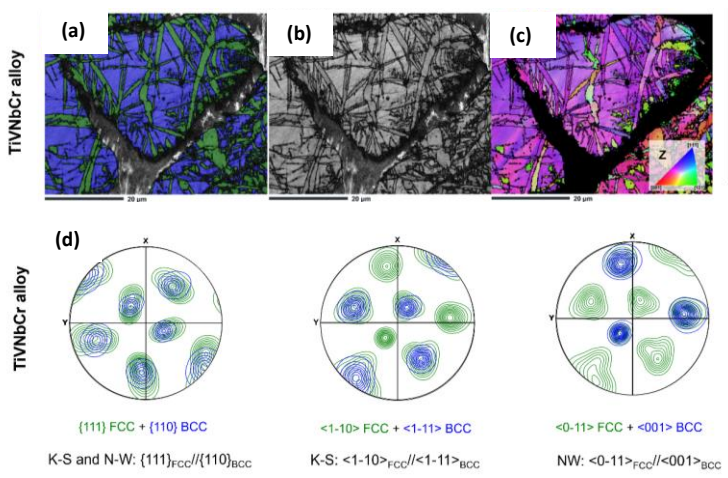


Figure 2: (a) EBSD Phase Map, **(b)** Band Contrast, and **(c)** IPF of a partially hydrogenated TiVNbCr alloys with approximately 1.3 H/M showing the coexistence of δ- (FCC) and β-phase (BCC). **d)** Pole Figure showing the ORs between β-phase (BCC) and δ-phase (FCC) of the TiVNbCr alloy.

Hydride Formation Mechanism

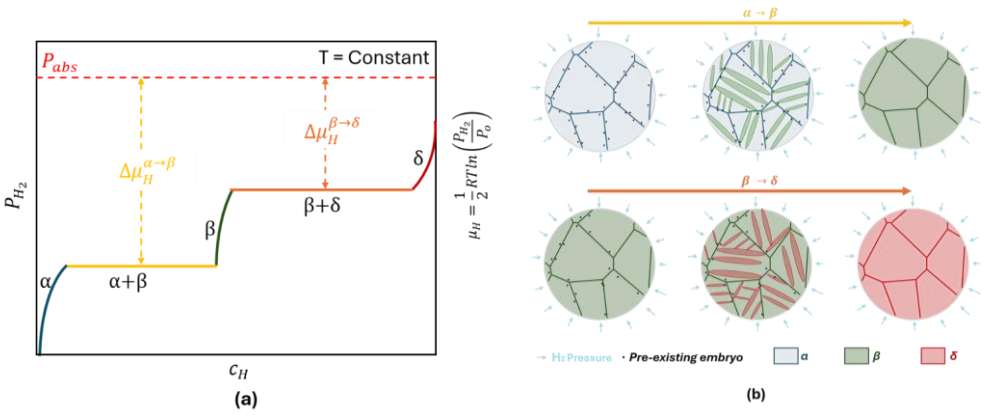
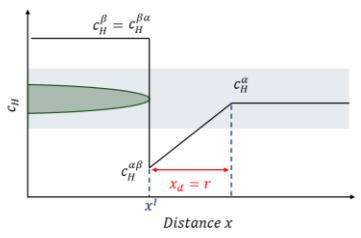
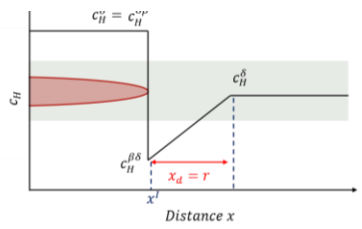


Figure 3: (a) Schematic representation of a PCI diagram for BCC metal and alloys. **(b)** Schematic representation of the formation mechanism of β-phase into the α-phase matrix and the δ-phase into the β-phase under para-equilibrium condition.

Growth Velocities



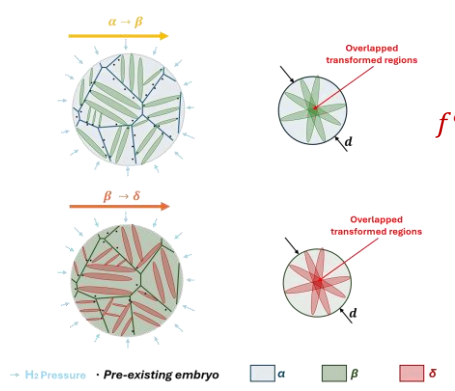
$$v^{\beta} = \frac{(c_H^{\alpha} - c_H^{\alpha\beta})}{(c_H^{\beta\alpha} - c_H^{\alpha\beta})} \cdot \frac{D^{\alpha}}{r^{\beta}} = \mathbf{924\ \mu m\ s^{-1}}$$



$$v^{\delta} = \frac{(c_H^{\beta} - c_H^{\beta\delta})}{(c_H^{\delta\beta} - c_H^{\beta\delta})} \cdot \frac{D^{\beta}}{r^{\delta}} = \mathbf{81\ \mu m\ s^{-1}}$$

Figure 4: Hydrogen concentration profile ahead the tip of the **(a)** β- and **(b)** δ- phase growing with lenticular shape into the α- and β- matrixes, respectively.

Jhonson-Mehl-Avrami-Kolmogorov



$$f^{\beta}(t) = 1 - \exp\left(-I^{\beta} \cdot \frac{\pi}{6} \cdot e \cdot d^3 \cdot t\right), for\ t \le t_{0,99}^{\beta}$$

$$f^{\delta}(t) = 1 - \exp\left(-I^{\delta} \cdot \frac{\pi}{6} \cdot e \cdot d^3 \cdot \left(t - t_{0,99}^{\beta}\right)\right), for\ t > t_{0,99}^{\beta}$$

Figure 5: Schematic representation of β- and δ- phase grains simplified as spherical grains with grain size d, The representation also highlights the overlapped transformed regions that are taken into account in the extended transformed volume of the β- and δ- phases.

Nucleation Rate

$$I^{\beta} = I_0^{\beta} \cdot exp\left(\frac{-Q_a^{\beta}}{\Delta\mu_H^{\alpha\to\beta}}\right) \qquad I^{\delta} = I_0^{\delta} \cdot exp\left(\frac{-Q_a^{\delta}}{\Delta\mu_H^{\beta\to\delta}}\right)$$

Experimental Results

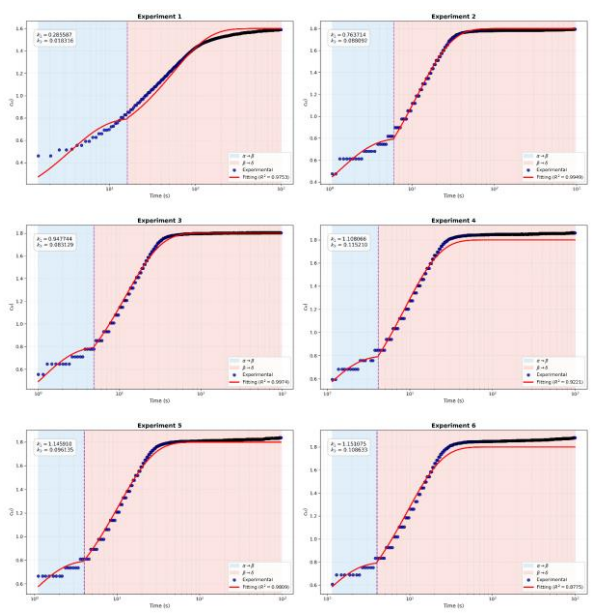


Figure 6: Experimental and Fitted Kinetics curves for the TiVNbCr alloy.

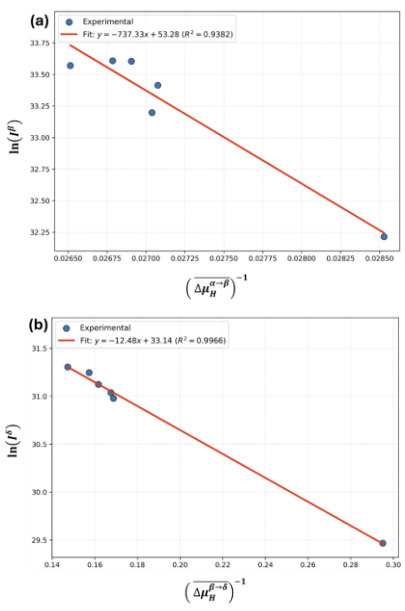


Figure 7: Plot of $\ln(I)$ versus $1/\Delta\mu_H$ for **(a)** β- and **(b)** δ- phase for the TiVNbCr alloy.

Table 1: Pre-exponential constants and activation energy for nucleation of β- and δ-phase for the TiVNbCr alloy.

I_0^{β} $(m^{-3} \cdot s^{-1})$	Q_a^{β} (kJ/mol H)	I_0^{δ} $(m^{-3} \cdot s^{-1})$	Q_a^{δ} (kJ/mol H)
1.38x10^{23}	737.33	2.48x10^{14}	12.48

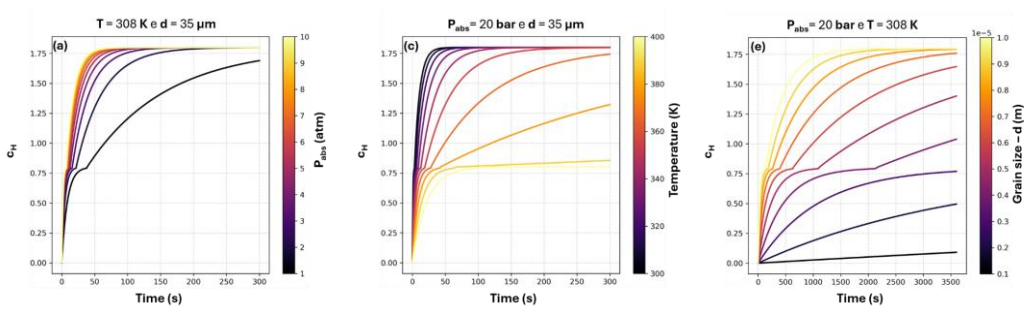


Figure 8: Calculation of the kinetics curves of the TiVNbCr BCC alloy for: **(a)** T = 308 K and d = 35 um; **(b)** P_{abs} = 20 bar and d = 35 um; **(c)** P_{abs} = 40 bar and d = 35 um;

Conclusions

Estimation of the growth velocities suggests that, for smaller particle sizes (< 100 µm), the kinetics of the β- and δ-phase formation are controlled by nucleation rate. A nucleation model that considers the nucleation rate proportional to the H chemical overpotential was proposed. The JMAK equation for the proposed mechanism was derived and validated using experimental data from different absorption kinetics curves for the TiVNbCr multicomponent alloy.

Agradecimentos

FAPESP CNPq CAPES