# Tailoring hydrogenation, thermodynamic properties and oxidation resistance of TiFe alloy by only regulating stoichiometric ratio of Ti and Fe elements

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## 1. The picture of the home-made Sieverts-type apparatus

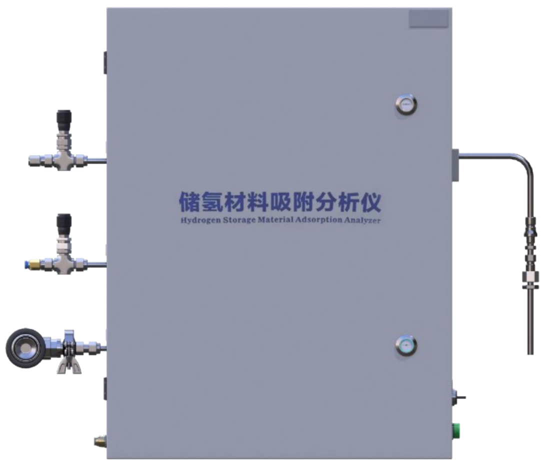


Fig.S1- The picture of the home-made Sieverts-type apparatus

## 2. Apparent Activation energy of hydrogen absorption

This is an example process for calculating the apparent activation energy using the Arrhenius equation.

$$\ln k = \frac{-E_a}{RT_p} + \ln A\#(1)$$

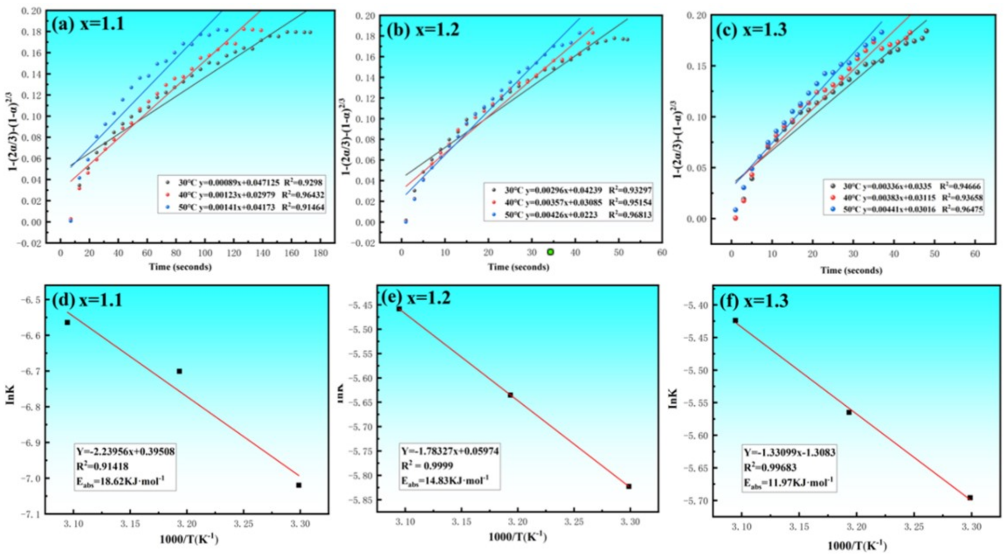


Fig.S2- GB3D-fitted hydrogen absorption curves of $Ti_xFe_{2-x}$ (x = 1.1, 1.2, 1.3) alloys at different temperatures (a–c). Arrhenius fitting of $Ti_xFe_{2-x}$ (x = 1.1, 1.2, 1.3) alloys (d-f).

Taking the alloy with x=1.1 as an example, the activation energy (Ea) was calculated based on the Arrhenius equation. The natural logarithm of the rate constant K(lnK) obtained from the linear fitting in Fig. 11a (values:0.00089, 0.00123, 0.00141) was plotted against 1000/T. According to $\ln k = -E_a/RT + \ln A$, the slope of the fittedline is $-E_a/R$. With a slope of −2.23956 and the gas constant $R = 8.314\ J\cdot mol\cdot K^{-1}$, the apparent activation energy of the hydrogen absorption was calculated to be 18.62 kJ/mol.

### 3. Activation energy of hydride decomposition

This is an example process for calculating the activation energy of hydride decomposition using the Kissinger equation.

$$\ln\frac{\beta}{T_p^2} = C - \frac{E_a}{RT_p}\#(2)$$

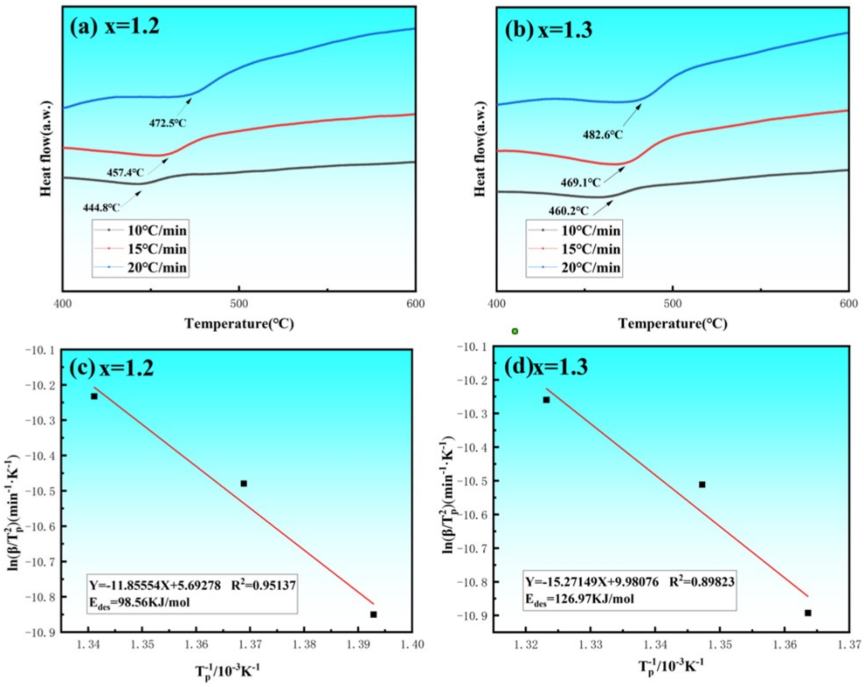


Fig.S3 – DSC curves of x=1.2 and x=1.3 alloys at different heating rates (a-b). Fitted curves by using Kissinger equation of x=1.2 and 1.3 alloys (c-d).

Taking the alloy with x=1.2 as an example, the decomposition activation energy ($E_a$) of the hydride was calculated using the Kissinger method. Three heating rates ($\beta$ = 10, 15, 20 °C/min) were adopted, and the corresponding peak temperatures ($T_p$) of hydride decomposition were determined as 472.5 °C, 457.4 °C and 444.8 °C, respectively. A linear fitting was performed by plotting $\ln(\beta/T_p^2)$ versus $1/T_p$. According to the Kissinger equation $\ln(\beta/T_p^2)= C-E_a/(RT_p)$, the slope of the fitted line is $-E_a/R$. With a slope of -11.85554 and the gas constant $R=8.314\ J\cdot mol^{-1}\cdot K^{-1}$, the decomposition activation energy was calculated to be 98.5 kJ/mol**.**

**4. Thermodynamic parameter calculation**

This is an example process for calculating the thermodynamic parameters (enthalpy change ΔH and entropy change ΔS) of hydride decomposition using the Van't Hoff equation.

$$\ln\left(\frac{P_{ep}}{P_0}\right) = \frac{\Delta H}{RT} - \frac{\Delta S}{R}\#(3)$$

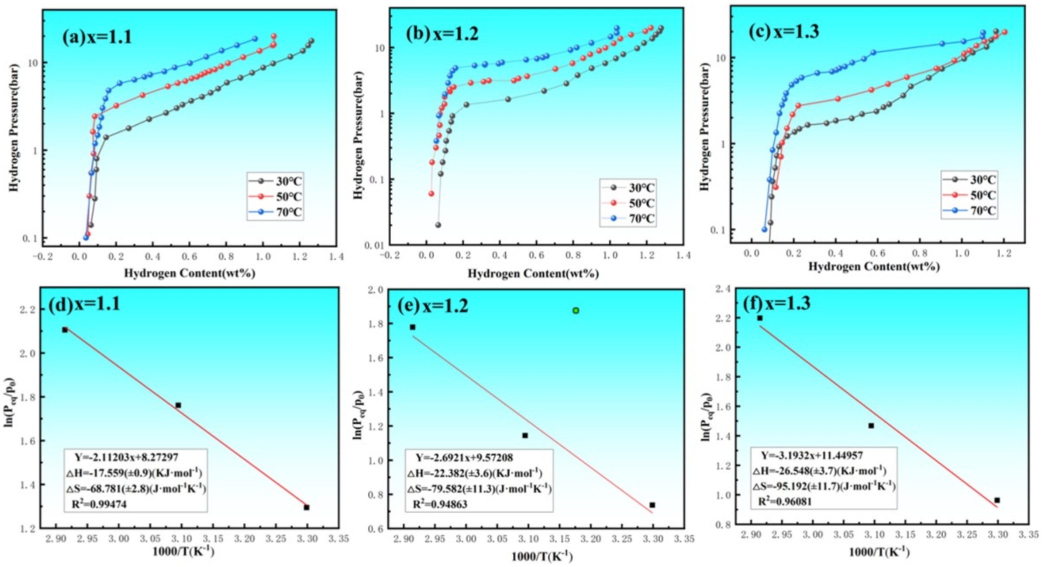


Fig.S4 – PCT curves at different temperatures (a–c) and Van't Hoff fitting plots for $Ti_xFe_{2-x}$ (x=1.1, 1.2, 1.3) alloys (e–f).

Taking the alloy with x=1.1 as an example, the thermodynamic parameters (enthalpy change ΔH and entropy change ΔS) were calculated using the Van't Hoff equation. The equilibrium plateau pressures ($P_{eq}$) at 30, 40 and 50 °C were measured, and $\ln(P_{eq}/P_0)$ ($P_0$: standard atmospheric pressure) was plotted against 1000/T. According to $\ln(P_{eq}/P_0)=\Delta H/RT-\Delta S/R$, the slope and intercept of the fitted line correspond to $-\Delta H/R$ and $\Delta S/R$, respectively. With a slope of −2.11203 and an intercept of 8.27297, the enthalpy and entropy changes were calculated as $\Delta H=-17.56\ kJ\cdot mol^{-1}$ and $\Delta S=-68.78\ J\cdot mol^{-1}\cdot K^{-1}$ ($R=8.314\ J\cdot mol^{-1}\cdot K^{-1}$).