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Received: 10 November 2019; Accepted: 26 November 2019; Published: 30 November 2019

Abstract: Based on the density functional theory, the geometric structure, adsorption energy and density of states of H$_2$/α-Fe$_2$O$_3$ (001) system and (H$_2$+Ni)/α-Fe$_2$O$_3$ (001) system were determined. The results showed that the absolute value of adsorption energy between H$_2$ molecule and α-Fe$_2$O$_3$ (001) surface and the bond length of H$_2$ molecule were increased by the presence of Ni atom. The presence of Ni atom promotes the adsorption of H$_2$ molecule on α-Fe$_2$O$_3$ (001) surface. Reduction behavior of iron and nickel oxides in H$_2$ atmosphere was determined by thermogravimetric analysis. The samples included Fe$_2$O$_3$, Fe$_2$O$_3$-NiO and Fe$_2$O$_3$-Ni systems. The effect of Ni and NiO on the reduction behavior of Fe$_2$O$_3$ was investigated. The ease of reduction within the following three systems decreases sequentially: Fe$_2$O$_3$-Ni > Fe$_2$O$_3$-NiO > Fe$_2$O$_3$. The activation energy of Fe$_2$O$_3$-Ni, Fe$_2$O$_3$-NiO and Fe$_2$O$_3$ systems at two temperature stages (viz. < 400 °C and > 400 °C) were 172 kJ·mol$^{-1}$, 197 kJ·mol$^{-1}$ and 263 kJ·mol$^{-1}$ respectively.

Keywords: α-Fe$_2$O$_3$ (001) surface; adsorption; reduction kinetics; Fe-Ni-O-H system; Fe-Ni alloy

1. Introduction

Nickel is a silver-white metal with good mechanical strength, plasticity and high chemical stability. Nickel is mainly used in stainless steel, electroplating and catalyst industries [1,2]. About 2/3 of the world’s nickel resources are used to produce stainless steel. About 70% of the production cost of austenitic stainless steel is the consumption of nickel [3–5]. Nickel catalysts are widely used in the hydrogenation of various unsaturated hydrocarbons due to their good catalytic activity, high mechanical strength and good thermal conductivity. They are also good catalysts for dehydrogenation, oxidative dehalogenation and desulfurization [6].

To provide a theoretical insight into the reaction mechanism of substances by investigating the electronic structure of multi-electron systems, density functional theory (DFT), which expresses the electronic energy as a functional of the electron density, was also included in this work. It has become an important means to study the properties and reaction mechanism of substances by simulation based on density functional theory and combining with macroscopic experimental phenomena [7–9]. In the present study, based on the first principle of density functional theory, the geometric structure, adsorption energy and density of states of H$_2$/α-Fe$_2$O$_3$ (001) system and (H$_2$+Ni)/α-Fe$_2$O$_3$ (001) system were investigated.
Cores et al. [10] studied the reduction process of Fe$_3$O$_4$-NiO by pulverized coal and H$_2$. It was found that there are two steps in the reduction reaction: The first step was the reduction of NiO and NiFe$_2$O$_4$, and the second step was the reduction of iron oxides. Zhou et al. [11] studied the reaction process of Fe$_2$O$_3$-NiO by methane. It was found that the first stage of the reduction process of Fe$_2$O$_3$ was Fe$_2$O$_3$ reduced to FeO, and the second stage was FeO reduced to Fe. The addition of NiO promotes the initial stage of reduction process of Fe$_2$O$_3$. Abdel-Halim et al. [12] studied the preparation of ferronickel alloy by reduction of Fe$_2$O$_3$/NiO compound with carbon. The results showed that the reaction was carried out step by step. At low temperatures, Boudouard reaction was the controlling step. Feng et al. [13] studied the effect of chloride on sulfide adsorption on cerussite surface through DFT calculations and XPS measurements. In the presence of chloride species, it had a significant effect on the surface structures and electronic properties of cerussite.

In this paper, based on the density functional theory, the effect of Ni atom on the adsorption behavior of H$_2$ molecule on α-Fe$_2$O$_3$ (001) surface was investigated. The reduction of the Fe-Ni-O-H system was determined by a thermogravimetric analyzer. According to the weight loss curve of the sample, the kinetic mechanism was studied.

2. Computational and Experimental Methods

2.1. Computational Details

The structure of the hexagonal hematite (α-Fe$_2$O$_3$) is an R-3c space group with lattice constants of $a = b = 5.04$ Å, $c = 13.75$ Å, $\alpha = \beta = 90^\circ$, and $\gamma = 120^\circ$. α-Fe$_2$O$_3$ (001) surface is one of the dominant crystal facets of nature α-Fe$_2$O$_3$. In this paper, the nine atomic layer slab models ($P = 2 \times 2$) of the α-Fe$_2$O$_3$ (001) surface were studied [14]. A vacuum region of 15 Å was added. This region was optimized by relaxing the outmost six layers and fixing the bottom three layers [15–17]. The clean surface of α-Fe$_2$O$_3$ (001) is shown in Figure 1.

![Figure 1. Diagram of α-Fe$_2$O$_3$ (001) clean surface.](image1.png)

Calculations were processed using the Cambridge Sequential Total Energy Package (CASTEP) module. The Perdew–Burke–Ernzerhof (PBE) exchange correlation function form in the generalized gradient approximation (GGA) was selected, it is suitable for the study of iron-oxygen system [15,18]. Pseudopotential chooses the ultra-soft pseudopotentials in reciprocal space representation. The plane-wave has the cutoff energy of 350 eV in all calculations, and the value of k-points is $4 \times 4 \times 1$ [15,16,19,20]. The values of convergence criterial for energy is $2.0 \times 10^{-5}$ eV/atom, maximum force is 0.005 Ha/Å, maximum stress is 0.1 GPa, displacement in Self Consistent Field (SCF) is 0.002 Å. The spin-polarized runs through the all calculation. The optimized cell parameters ($a = b = 5.01$ Å, $c = 13.91$ Å) are in good agreement with the experimental values.
The optimized H2 molecule was placed vertically at the Fe-top adsorption site on the α-Fe2O3 (001) surface, and Ni atoms were placed at the O-top adsorption site on the α-Fe2O3 (001) surface as shown in Figure 2. The adsorption energy, E_{ads}, was calculated using following Equation [21]:

\[
E_{ads}(H2/α-Fe2O3 (001)) = EH2/α − Fe2O3 (001) − Eα − Fe2O3 (001) − EH2
\]  \( (1) \)

\[
E_{ads}(H2+Ni/α-Fe2O3 (001)) = E(H2 + Ni)/α − Fe2O3 (001) − Eα − Fe2O3 (001) − EH2 − ENi
\]  \( (2) \)

where \( E_{H2/α-Fe2O3 (001)} \), \( E(\text{H}_2 + \text{Ni})/α-Fe2O3 (001) \), \( E_{α-Fe2O3 (001)} \), \( E_{H2} \) and \( E_{Ni} \) represent the total energies of \( \text{H}_2/α-\text{Fe}_2\text{O}_3 \) (001) system, \( (\text{H}_2 + \text{Ni})/α-\text{Fe}_2\text{O}_3 \) (001) system, \( α-\text{Fe}_2\text{O}_3 \) (001) system, the adsorbate \( \text{H}_2 \) molecule and the adsorbate Ni atom, respectively.

![Figure 2](image_url)  
Figure 2. Initial adsorption location of H2 molecule and Ni atom.

2.2. Experimental Details

The Fe2O3-Ni and Fe2O3-NiO samples were mixed homogeneously by a ball mill. The three samples were studied in the experiment: Fe2O3 (200 mg), Fe2O3 + Ni (200 mg + 20 mg), Fe2O3 + NiO (200 mg + 25 mg). The mass of Ni component in Fe2O3 + NiO and Fe2O3 + Ni samples was the same. A thermogravimetric analyzer (HENGJIU Inc., Beijing, China) was used to study the reduction experiment of Fe-Ni-O system in H2 atmosphere. The three samples were reduced by H2 (99.95%) with gas flow rate of 30 mL/min and a heating rate of 10 °C/min from 20 to 1000 °C. The phase composition of the samples was determined by X-ray diffraction (JEOL Inc., Tokyo, Japan). The diffraction spectra in the range 10° to 90° at a rate of 10°/min were measured.

2.3. Kinetic Approach

Study on kinetics of reduction process by thermal analysis [22–24], the kinetic equation under non-isothermal conditions is obtained.

\[
\frac{d\alpha}{dT} = \frac{A}{\beta} \exp\left(-\frac{E}{RT}\right)f(\alpha)
\]  \( (3) \)

where \( \alpha \) is the degree of conversion, \( \beta \) is the heating rate, \( E \) is the activation energy of the reaction, \( R \) is 8.314 J·mol\(^{-1}\)·K\(^{-1}\), \( f(\alpha) \) is the differential mechanism function.

The kinetic equation of reduction process is obtained by Coats–Redfern approximation equation.

\[
\ln\left[\frac{G(\alpha)}{T^2}\right] = \ln\left[\frac{AR}{\beta E}\left(1 - \frac{2RT}{E}\right)\right] - \frac{E}{RT}
\]  \( (4) \)
For most reactions, the activation energy $E >> RT$, and Equation (4) can be simplified:

$$\ln \left( \frac{G(\alpha)}{T^2} \right) = \ln \left( \frac{AR}{\beta E} \right) - \frac{E}{RT}$$  \hspace{1cm} (5)

For a constant heating rate, the linear relationship between $\ln(G(\alpha)/T^2)$ and $1/T$ can be obtained, and $E$ can be determined from the slope.

3. Results and Discussion

3.1. Computational Results of H$_2$ Molecule on the $\alpha$-Fe$_2$O$_3$ (001) Surface in the Presence of Ni Atom

The structure parameters and adsorption energy of H$_2$/α-Fe$_2$O$_3$ (001) system and (H$_2$ + Ni)/α-Fe$_2$O$_3$ (001) system are shown in Table 1. Negative value of $E_{ads}$ represents a stable adsorption configuration. The greater the absolute value of adsorption energy represents stronger interaction and the stronger interaction between adsorbate and substrate. As shown in Table 1, the absolute value of adsorption energy of (H$_2$ + Ni)/α-Fe$_2$O$_3$ (001) system is 0.93 eV higher than that of H$_2$/α-Fe$_2$O$_3$ (001) system. It is shown that the presence of Ni atom strengthens the interaction between the H$_2$ molecule and the α-Fe$_2$O$_3$ (001) surface. When Ni atom was added to H$_2$/α-Fe$_2$O$_3$ (001) system, the bond length of H$_2$ molecule increased from 0.758 to 0.889 Å and a 63.36° tilt occurred between the H$_2$ molecule and the α-Fe$_2$O$_3$ (001) surface. The variation of structure parameters of H$_2$ molecule indicates that the existence of Ni atom can affect the structure of H$_2$ molecule itself. When Ni atom was added to H$_2$/α-Fe$_2$O$_3$ (001) system, which causes the inclination angle between H$_2$ molecule and the α-Fe$_2$O$_3$ (001) surface, thus leading to the change of surface charge distribution of α-Fe$_2$O$_3$ (001) [21,25]. Compared with H$_2$/α-Fe$_2$O$_3$ (001) system, the average bond length of Fe–O in (H$_2$ + Ni)/α-Fe$_2$O$_3$ (001) system increased from 2.0253 to 2.0258 Å, indicating that α-Fe$_2$O$_3$ (001) in (H$_2$ + Ni)/α-Fe$_2$O$_3$ (001) system has been activated, which will be more conducive to the adsorption of H$_2$ molecules on α-Fe$_2$O$_3$ (001) surface [26].

<table>
<thead>
<tr>
<th>System</th>
<th>$E_{ads}$/eV</th>
<th>$d_{H-H}$/Å</th>
<th>$d_{O-Fe}$/Å</th>
<th>$\triangle \alpha_{H_2-surface}$/°</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$/α-Fe$_2$O$_3$ (001)</td>
<td>1.88</td>
<td>0.758</td>
<td>2.0253</td>
<td>0</td>
</tr>
<tr>
<td>(H$_2$ + Ni)/α-Fe$_2$O$_3$ (001)</td>
<td>2.81</td>
<td>0.889</td>
<td>2.0258</td>
<td>63.36</td>
</tr>
</tbody>
</table>

Figure 3 shows the density of states (DOS) of α-Fe$_2$O$_3$ (001) surface and H$_2$ molecules of H$_2$/α-Fe$_2$O$_3$ (001) system in the presence or absence of Ni atom. The green dotted line in the two figures represent Fermi level. When the energy is greater than Fermi level, it is unoccupied state, and when energy is less than Fermi level, it is occupied state. As shown in Figure 3a, when the Ni atom is added to the H$_2$/α-Fe$_2$O$_3$ (001) system, within the range of $-2.0$ to $1.50$ eV, the electrons tend to move to higher energy levels, resulting in the increase in density of the electrons with higher energies. Meanwhile, within the range of $-7.50$ to $1.50$ eV, the peaks also show a slight displacement to the more positive side. It is found that the presence of Ni atom in the H$_2$/α-Fe$_2$O$_3$ (001) system leads to the transition to higher energy levels of electron of H$_2$ molecule, and thus an obvious displacement of the peaks to more positive side is shown Figure 3b. Moreover, a new peak was found in the unoccupied states. These results indicate that the stability of the H$_2$ molecule decreases and the tendency of cracking occurs with the addition of Ni atom [27].
When the ordinate value of Figure 4 is 1.0, it means the reduction degree is 100%. Comparing the three samples, Fe$_2$O$_3$ is easier to reduce. When NiO was added to Fe$_2$O$_3$, within the Fe$_2$O$_3$ system, the morphological structure of samples changed significantly and the porosity of the compacts increased and promoted the reduction of Fe$_2$O$_3$ in H$_2$ atmosphere, and we will validate this conclusion through experiments.

### 3.2. Reduction Behavior in the Fe-Ni-O-H System

The reduction curves of Fe$_2$O$_3$, Fe$_2$O$_3$-Ni and Fe$_2$O$_3$-NiO exposed to H$_2$ are shown in Figure 4. When the ordinate value of Figure 4 is 1.0, it means the reduction degree is 100%. Comparing the reduction degree curves of three samples, reduction reaction of Fe$_2$O$_3$-Ni was firstly completed, followed by Fe$_2$O$_3$-NiO, and Fe$_2$O$_3$ was finally completed. It can be considered that Ni components were determined as accelerator in Fe$_2$O$_3$ system, and final reaction temperature of Fe$_2$O$_3$ was reduced. There are two reasons for the promotion behavior of Ni components. Firstly, Ni has large specific surface area, many surface active sites and strong adsorption capacity for H$_2$ [28]. When Ni is present within the Fe$_2$O$_3$ system, Ni adsorbs more hydrogen atoms and transfers them to Fe$_2$O$_3$ system, which promotes the reduction reaction of Fe$_2$O$_3$ system. Secondly, NiO reacts with Fe$_2$O$_3$ to produce NiFe$_2$O$_4$, which is easier to reduce. When NiO was added to Fe$_2$O$_3$ system, the morphological structure of samples changed significantly and the porosity of the compacts increased and promoted the reduction of Fe$_2$O$_3$ [12,29]. Compared with Ni, the promotion effect of NiO is not as obvious. The reaction rate curves of Fe$_2$O$_3$, Fe$_2$O$_3$-Ni and Fe$_2$O$_3$-NiO are shown in Figure 5. The temperature corresponding to the maximum reaction rate of the three samples ranged from low to high: Fe$_2$O$_3$-Ni < Fe$_2$O$_3$-NiO < Fe$_2$O$_3$. As shown in Figure 5, the reaction rate curves of three samples are mainly composed of two peaks, and the boundary point of the two peaks is about 400 °C. According to the result, we analyzed the reduction products of three samples at different temperatures by XRD and explored the reduction process of three samples in H$_2$ atmosphere.
were characterized by XRD. Figure 6a shows that the phases of reduction products of Fe₂O₃ at different temperatures. The phases present are Fe₂O₃ and Fe₃O₄ at 380 °C. At 550 °C, the phases present are Fe₃O₄ and Fe. At 590 °C, FeO diffraction peaks appear, and the phases present are Fe₃O₄, FeO and Fe. At 1000 °C, Fe₂O₃ and H₂ react completely, and the phase present is Fe. From the results of XRD, the reduction of Fe₂O₃ by H₂ is a multi-stage process [30,31]. When the temperature is less than 400 °C, Fe₂O₃ is reduced to Fe₃O₄. In the temperature range of 400–570 °C, the following reaction occurred: Fe₂O₃→Fe. When the temperature is higher than 570 °C, the following reactions occurred: Fe₃O₄→FeO→Fe. Figure 6b shows that the constituent phases of Fe₂O₃-NiO after reduction at different temperatures. Fe₂O₃, Fe₃O₄ and Ni are the phases present at 380 °C. At 570 °C, awaruite [FeNi₃] diffraction peaks appear. At this temperature, the phases present are Fe₃O₄, Fe and FeNi₃. When the temperature is increased to 590 °C, the phases present are Fe₃O₄, FeO, Fe and FeNi₃. At 1000 °C, Fe₂O₃ and NiO are completely reduced and the phases present are Fe and FeNi₃. From the results of XRD, the reduction process of Fe₂O₃-NiO is divided into two steps. The first step is mainly the reduction of NiO and the transformation of Fe₂O₃ to low-valent iron oxides. At the same time, a small amount of Fe-Ni alloy is formed. The second step is the reduction of low-valent iron oxides and the formation of Fe-Ni alloys [32]. Comparing Figure 6b,c, we can see that the reduction products of Fe₂O₃-Ni and...
Fe₂O₃-NiO at different temperatures have the same constituent phases, and the reduction process is basically the same. The first step is the reduction of Fe₂O₃ to Fe₃O₄, and the second step is the reduction of Fe₃O₄ and the formation of Fe-Ni alloys.

### 3.3. Reduction Kinetics of Fe-Ni-O-H System

Because the reaction rate curves of three samples are mainly composed of two peaks, and the boundary point of the two peaks is about 400 °C. The kinetic calculation was divided into two sections (above 400 °C and below 400 °C). Table 2 lists the fifteen commonly used mechanism functions in gas-solid reactions, by analyzing the curve of \( \ln(G(\alpha))/T^2 \) versus \( 1/T \) of fifteen mechanism functions and finding out the best mechanism function with the maximum correlation coefficient. For reduction of Fe₂O₃ by hydrogen at temperatures less than 400 °C, the best mechanism function was the Anti-Jander 3D function. This indicated that the reduction was dominated by a 3D diffusion model. For temperatures >400 °C, Jander 2D (\( n = 2 \)) function was determined to be the mechanism function of the Fe₂O₃-Ni-H₂ systems, and the reduction reaction follows a 2D diffusion model. The reduction process for the Fe₂O₃-Ni and Fe₂O₃-NiO systems was divided into two stages, <400 °C and >400 °C, and the kinetic mechanisms investigated. For temperatures <400 °C, Anti-Jander 3D function was the best mechanism function for the Fe₂O₃-Ni-H₂ systems, and the reduction reaction follows a 3D diffusion model. For temperatures > 400 °C, Mampel Power (\( n = 2 \)) function was determined to be the mechanism function of the Fe₂O₃-Ni-H₂ systems, and the reduction reaction follows the Mampel Power law. For the Fe₂O₃-NiO-H₂ system, at temperatures <400 °C, the Anti-Jander 3D function was the best mechanism.
At temperatures above 400 °C, Jander 2D (n = 2) function was the best mechanism function, and the reduction reaction follows a 2D diffusion model. The apparent activation energies for the reduction reactions are shown in Table 3.

Table 2. Some mechanism functions for gas-solid reactions.

<table>
<thead>
<tr>
<th>No.</th>
<th>Equation</th>
<th>G(α)</th>
<th>f(α)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Mampel Power (n = 1)</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>Mampel Power (n = 3/2)</td>
<td></td>
<td>2/3α⁻¹/²</td>
</tr>
<tr>
<td>3</td>
<td>Mampel Power (n = 2)</td>
<td></td>
<td>1/2α⁻¹</td>
</tr>
<tr>
<td>4</td>
<td>Jander 2D (n = 2)</td>
<td></td>
<td>(1 - α)²/³[1 - (1 - α)²/³]⁻¹</td>
</tr>
<tr>
<td>5</td>
<td>Jander 3D (n = 2)</td>
<td></td>
<td>3/2(1 - α)²[1 - (1 - α)²/³]⁻¹</td>
</tr>
<tr>
<td>6</td>
<td>G-B</td>
<td></td>
<td>3/2[(1 - α)⁻¹/³ - 1]⁻¹</td>
</tr>
<tr>
<td>7</td>
<td>Anti Jander 3D</td>
<td></td>
<td>3/2(1 + α)²/³[1 + α]¹/³ - 1]⁻¹</td>
</tr>
<tr>
<td>8</td>
<td>Avrami-Erofeev (n = 3/2)</td>
<td></td>
<td>2/3(1 - α)[−ln(1 - α)]⁻¹/²</td>
</tr>
<tr>
<td>9</td>
<td>Avrami-Erofeev (n = 2)</td>
<td></td>
<td>1/2(1 - α)[−ln(1 - α)]⁻¹</td>
</tr>
<tr>
<td>10</td>
<td>Avrami-Erofeev (n = 3)</td>
<td></td>
<td>1/3(1 - α)[−ln(1 - α)]⁻²</td>
</tr>
<tr>
<td>11</td>
<td>Avrami-Erofeev (n = 4)</td>
<td></td>
<td>1/4(1 - α)[−ln(1 - α)]⁻³</td>
</tr>
<tr>
<td>12</td>
<td>Interface Reaction R3 (n = 1/3)</td>
<td></td>
<td>3(1 - α)²/³</td>
</tr>
<tr>
<td>13</td>
<td>Reaction Order (n = 1/4)</td>
<td></td>
<td>4(1 - α)³/⁴</td>
</tr>
<tr>
<td>14</td>
<td>Interface Reaction R3 (n = 3)</td>
<td></td>
<td>1 - (α)²/³</td>
</tr>
<tr>
<td>15</td>
<td>Reaction Order (n = 3)</td>
<td></td>
<td>(1 - α)²/³</td>
</tr>
</tbody>
</table>

Table 3. Apparent activation energies and mechanism functions for the reduction of Fe₂O₃, Fe₂O₃-Ni and Fe₂O₃-NiO compacts.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Temperature Range (°C)</th>
<th>Activation Energy (kJ·mol⁻¹)</th>
<th>Mechanism</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe₂O₃</td>
<td>&lt;400</td>
<td>180</td>
<td>Anti-Jander 3D</td>
</tr>
<tr>
<td></td>
<td>&gt;400</td>
<td>83</td>
<td>Jander 2D (n = 2)</td>
</tr>
<tr>
<td>Fe₂O₃-Ni</td>
<td>&lt;400</td>
<td>106</td>
<td>Anti-Jander 3D</td>
</tr>
<tr>
<td></td>
<td>&gt;400</td>
<td>66</td>
<td>Mampel Power (n = 2)</td>
</tr>
<tr>
<td>Fe₂O₃-NiO</td>
<td>&lt;400</td>
<td>127</td>
<td>Anti-Jander 3D</td>
</tr>
<tr>
<td></td>
<td>&gt;400</td>
<td>70</td>
<td>Jander 2D (n = 2)</td>
</tr>
</tbody>
</table>

According to the data in Table 3, the activation energy of Fe₂O₃ system doped with Ni components is lower than that of Fe₂O₃ system at two temperature ranges, whether the reaction temperature is lower than 400 °C or higher than 400 °C. The high activation energy is not conducive to the reaction, indicating that doping Ni components in Fe₂O₃ system is conducive to the reduction reaction. The activation energies of reduction process of Fe₂O₃-Ni, Fe₂O₃-NiO and Fe₂O₃ are 172 kJ·mol⁻¹, 197 kJ·mol⁻¹ and 263 kJ·mol⁻¹, respectively. The difficulty of reduction reaction in three systems is represented from low to high: Fe₂O₃-Ni < Fe₂O₃-NiO < Fe₂O₃; it is consistent with the conclusion in Figure 4.

4. Conclusions

Based on DFT calculation, it can be seen that H₂ molecule is more easily adsorbed on the α-Fe₂O₃ (001) surface when Ni atoms exist. It can be concluded that Ni components can promote the reduction of Fe₂O₃ in H₂ atmosphere. This conclusion is verified by reduction degree curve and reduction kinetics. The absolute value of adsorption energy of (H₂ + Ni)/α-Fe₂O₃ (001) system is 0.93 eV higher than that of H₂/α-Fe₂O₃ (001) system. It is shown that the presence of Ni atom promotes the adsorption of H₂ on α-Fe₂O₃ (001) surface. The existence of Ni atom has a great influence on the structure of H₂ molecule and α-Fe₂O₃ (001) surface. The reduction of Fe₂O₃ by H₂ is a multi-stage process, when the temperature is below 400 °C and the reduction reaction follows a 3D diffusion model. At temperatures above 400 °C the reduction reaction follows a 2D diffusion model. The activation energies of two temperature stages are 180 kJ·mol⁻¹ and 83 kJ·mol⁻¹, respectively. Ni components
are determined as accelerators in Fe\textsubscript{2}O\textsubscript{3} system, and the reaction termination temperatures of Fe\textsubscript{2}O\textsubscript{3} were reduced. When Ni components were added, the activation energies of reduction process of Fe\textsubscript{2}O\textsubscript{3} system decreased.

**Author Contributions:** Funding acquisition, H.W.; investigation, H.Z. and B.L.; methodology, H.Z., B.L., Y.W. and H.W.; project administration, B.L. and Y.W.; resources, B.L., Y.W. and H.W.; software, H.Z.; supervision, H.W.; writing—original draft, H.Z. and B.L.; writing—review and editing, B.L., Y.W. and H.W.

**Acknowledgments:** This research was funded by the Key R&D Program of Yunnan Province (2018IA055), National Natural Science Foundation of China (No. U1602272 and 51664039) and the Analysis and Testing Foundation of Kunming University of Science and Technology (2018M20172102040).

**Conflicts of Interest:** The authors declare no conflict of interest.

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