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Thermodynamics approach to the hydrogen diffusion and phase transformation in titanium particles

Weimin Gao[a,*], Weiqi Li[a,b], Jin Zhou[b], Peter D. Hodgson[a]

[a] *Centre for Material and Fibre Innovation, Deakin University, Geelong, VIC 3217, Australia*
[b] *College of Mechanical & Electrical Engineering, Nanjing University of Aeronautics & Astronautics, Nanjing 210016, China*

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ABSTRACT

The hydrogen diffusion and phase transformation in a titanium particle were studied based on thermodynamic calculation. The mechanisms of hydrogen diffusion in different phases (α-Ti, β-Ti and TiH_x) were analyzed. A mobility database was developed for titanium–hydrogen system based on the experimental works on hydrogen diffusion coefficient reported in literature and the fundamental of diffusion. To implement the calculation, a commercial software package for the simulation of diffusion-controlled phase transformation was used. The hydrogen diffusion process, hydrogen distribution, phase transformation and phase growth rate during hydrogenization of a titanium particle at temperatures of 560 K, 800 K and 1000 K were discussed. The thermodynamics and kinetics analysis provided quantitative insight into the diffusion process and improved the understanding of diffusion mechanism and phase transformation.

1. Introduction

Titanium and its alloys are attractive materials for structure application in many industrial fields because of their high ratio of strength to weight, high heat resistance, outstanding resistance to corrosion and high toughness in a wide variety of environments. Their application is, however, hampered by high gap sensitivity, low machinability and poor deformation characteristics [1]. It is known that the mechanical properties of the materials can be improved by doping or charging alloy elements, resulting in phase transformation and microstructure change. It has been demonstrated that hydrogen is one of the most important elements that can significantly affect the mechanical properties of titanium and its alloys [2]. The machinability of titanium alloys can be remarkably improved by charging with a certain level of hydrogen, whereas a higher hydrogen content in titanium alloys can deteriorate the mechanical properties of titanium products due to hydrogen embrittlement [3]. The characteristics of titanium having different hydrogen concentrations and the structures and properties of different titanium hydrogen phases have been investigated [2,4]. However, the dynamic process of hydrogen diffusion and phase transformation during hydrogenation or dehydrogenation has rarely been reported due to the experimental difficulties.

With the advent of modern computational tools regarding alloy thermodynamics and kinetics, it is possible to simulate the progress of diffusion-controlled phase transformations in multi-component alloys [5–7] and, thus, to predict mechanical properties. In this paper, the dynamic process of hydrogen diffusion and phase transformation were analyzed based on thermodynamic and kinetic calculations and by coupling with both dispersed phase model and moving boundary model. A kinetic database was also developed for titanium hydrogen system.

2. Diffusion mechanism and diffusivity of H in Ti

A finite-difference code developed for the simulation of one-dimensional diffusion controlled phase transformation in multicomponent alloy systems (DICTRA) [8] was used to model the hydrogen diffusion in titanium particles, which combines an explicit description of the diffusion equation with thermodynamic calculations assuming local thermodynamic equilibrium at moving interface. As DICTRA uses the CALPHAD approach, the diffusion flux of a species is related to the chemical potential gradient rather than the concentration gradient. When the chemical potential gradient is regarded as the driving force, mobilities are used instead of diffusivities to calculate the flux so that the thermodynamic driving forces and the diffusion coupling between elements are taken into account.

A thermodynamic database, TTTI3, published by Thermo-calc [8] was used in the present work to describe the Gibbs free energy

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[*] Corresponding author. +61 3 52272334; fax: +61 3 52271103.
E-mail address: weimin.gao@deakin.edu.au (W. Gao).

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of phases as a function of temperature, composition and pressure. Due to, so far, there has been no a kinetic database for Ti–H system available, a database is developed based on the experimental results on hydrogen diffusivity from literature to describe the diffusion coefficients of hydrogen in different phases and self diffusions of hydrogen and Ti.

There are three phases in Ti–H system [4]. Pure titanium has two kinds of allotropes. α-Ti phase (h.c.p.) is stable at temperatures below 1155 K, while at temperatures above 1155 K the dominating phase is β-Ti (b.c.c.). With the permeation of hydrogen, α-Ti can transfer to β-Ti above 576 K, while it transfers to hydrides (TiH_x) at lower temperatures than 576 K [9]. The hydrides can also be created from β-Ti as the concentration of hydrogen in titanium further increases. The hydrogen shows different mechanisms and diffusivities in different phases.

2.1. *Hydrogen diffusion in α-phase*

The diffusion mechanism of hydrogen atoms in α-Ti is interstitial diffusion. In h.c.p. α-Ti, there are two possible positions available for interstitial atoms: tetrahedral (radius = 0.34 Å), and octahedral (radius = 0.62 Å). It is widely believed that hydrogen atoms occupy the octahedron sites [9]. For a multicomponent system, as there is a relation between concentration gradients and usually the concentration of one of the component is chosen as a dependent variable in the calculations [10]. For the chosen components, the interstitial sites are not occupied and, for simplicity, it is assumed that only substitutional components contribute to the volume and all substitutional components have the same partial molar volumes [11,12]. This work is only about Ti–H system, this and the following descriptions of diffusion mechanism, however, allow the interstitial elements of hydrogen to be treated in future mobility assessments.

A few expressions have been reported to describe the temperature dependence of hydrogen diffusion coefficient in α-Ti, as presented in Fig. 1.

Wasilewski and Kehl [13] measured the H diffusion coefficient in α-Ti at temperatures from 773 K to 1097 K with volumetric measurement method and obtained the following fitted expression for hydrogen diffusivity in α-Ti, D_α.

$$D_\alpha = 1.8 \times 10^{-6} \exp\left[\frac{-12380 \pm 680}{RT}\right] \quad (\mathrm{m}^2/\mathrm{s}) \tag{1}$$

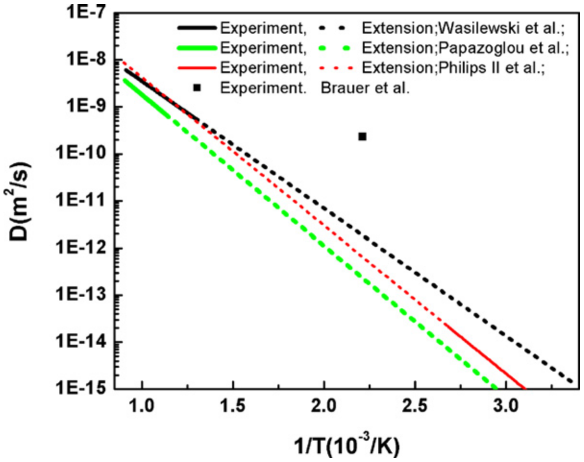

Fig. 1. Hydrogen diffusion coefficients in α-Ti (the solid lines denote the experimental results reported by Wasilewski and Kehl [13], Papazoglou and Hepworth [14] and Philips et al. [17], respectively, the dashed lines are the extrapolation of their experimental results and the filled square is the experimental result of Brauer et al. [18]).

With the same measurement method, Papazoglou and Hepworth [14] studied the hydrogen diffusion coefficient from 884 K to 1102 K and reported:

$$D_\alpha = 3 \times 10^{-6} \exp\left[\frac{-14700 \pm 650}{RT}\right] \quad (\mathrm{m}^2/\mathrm{s}) \tag{2}$$

The principle of the volumetric measurement method has been described in detail in [15,16]. The method involved placing a pretreated pure α-Ti sample in a prescribed vessel, infusing hydrogen, measuring the hydrogen pressure in the vessel, educing the relative saturation of hydrogen in titanium from the variation of hydrogen pressure and, finally, calculating the hydrogen diffusion coefficient based on its relationship with the relative saturation. Since it is easy to produce β-Ti during the creation of α-Ti samples, the control of β-Ti formation is important when using the method. Wasilewski and Kehl [13] produced α-Ti by exposing long cylindrical titanium specimens to hydrogen at a sufficiently high pressure. The sample preparation is likely to form a surface layer of β-Ti for the duration of the isothermal experiment. To determine the hydrogen concentration profile in α-Ti, the β-Ti layer was removed by Wasilewski and Kehl before testing. To avoid the formation of β-Ti on sample surface, Papazoglou and Hepworth [14] controlled the hydrogen pressure in vessels to be lower than the equilibrium value of the formation of β-Ti.

The effect of temperature on the kinetics of hydrogen in α-Ti was studied by Philips et al. [17] with the cathode charging method. They measured the hydrogen contents and the thicknesses of hydride layers formed during galvanostatic cathodic polarization in 0.05 M H_2SO_4 at a current density of 1 $\mathrm{mA/cm^2}$ at temperatures of 25, 40, 60, 80 and 100 °C. The hydrogen diffusion coefficient in α-Ti was calculated from the thickness of hydride layer and described as

$$D_\alpha = 6 \times 10^{-6} \exp\left[\frac{-14400 \pm 800}{RT}\right] \quad (\mathrm{m}^2/\mathrm{s}) \tag{3}$$

Brauer et al. [18] studied the diffusion phenomenon of hydrogen in titanium and Ti alloys with a nuclear physics method based on the reaction of $^{15}\mathrm{N} + {}^{1}\mathrm{H} \rightarrow {}^{12}\mathrm{C} + {}^{4}\mathrm{He} + \gamma$ (4.43 MeV). The concentration of hydrogen was calculated from the number of γ rays and the diffusion coefficient was extracted from the hydrogen depth profile based on the principle of diffusion. It was reported that the diffusion coefficient of hydrogen in α-Ti at 452 K, D_α(452 K), is 2.3×10^{-10} $\mathrm{m^2/s}$. Comparing with the extrapolation of the diffusion coefficients measured with the volumetric measurement method (Eqs. (1) and (2)) yields D_α(452 K) = 1.5×10^{-12} $\mathrm{m^2/s}$.

In comparing the measurement methods, one finds that the formation of β-Ti and titanium hydrides was avoided in the experiments of Papazoglou and Hepworth [14]. This is unlikely to in the experiments of Wasilewski and Kehl [13] and Philips et al. [17]. Although the method used by Brauer et al. [18] is unlikely to form those phases, the measured value of hydrogen diffusion coefficient is several orders of magnitude higher than those obtained from the volumetric measurement method and the nuclear physics method. Therefore, the experimental results of Papazoglou and Hepworth [14] have revealed the diffusion characteristics of a pure α-Ti system and Eq. (2) was used in this modeling work.

2.2. *Hydrogen diffusion in β-Ti*

The crystal lattice of β-Ti also has two kinds of sites, tetrahedral and octahedral. There are some debates about the site of hydrogen atom.

Considering the binding energy, Han [9] reported that the position of hydrogen atoms is not fixed in β-Ti (H) crystal. It was proposed that hydrogen atoms occupy octahedral sites in relatively low hydrogen content titanium, while they are apt to occupy tetrahedral sites in titanium with high hydrogen content. In 2Ti + 1H β-Ti (H), the binding energy of hydrogen in tetrahedral sites is 0.005 eV higher than that in octahedral sites; in 4Ti + 1H β-Ti (H), the binding energy of hydrogen in tetrahedral sites is 0.018 eV lower than that in octahedral sites. Huang et al. [4], however, reported that, as interstitial atoms, hydrogen atoms should occupy tetrahedral sites due to the tetrahedral interstitial radius is bigger than the octahedral one in a bcc structure. Han [9] pointed out that although the interstitial radius of tetrahedral sites is larger than that of octahedral sites in the b.c.c. structure (the interstitial radius of β-Ti octahedral sites, r_x, is 0.2778 Å and r_x is 0.4278 Å for tetrahedral sites), the octahedral interstitial sites are not persymmetric. The interstitial atoms can only lead to two atoms departing their equilibrium position markedly, while the others have no distinct departure. Then, the lattice distortion is not severe. Therefore, in some kinds of b.c.c. structure metals, interstitial atoms occupy tetrahedral interstitial sites, such as carbon atoms in molybdenum, but in other b.c.c. metals, interstitial atoms occupy octahedral ones, such as carbon atoms in α-Fe.

Through the same method as for α-Ti, Wasilewski and Kehl [13] investigated the hydrogen diffusion coefficient in β-Ti at temperatures of from 923 K to 1273 K and reported that the variation of hydrogen diffusion coefficient with hydrogen concentration is not remarkable in β-Ti except at very low hydrogen concentration. The hydrogen diffusion coefficient as a function of temperature can be expressed by

$$D_\beta = 1.95 \times 10^{-7} \exp\left[\frac{-6640 \pm 500}{RT}\right] \quad (\mathrm{m^2/s}) \tag{4}$$

Papazoglou and Hepworth [14] measured the diffusivities in b.c.c. structure at 1122 K, 1162 K and 1173 K. Sevilla et al. [19] studied the hydrogen diffusion with pulsed field gradient-nuclear magnetic resonance at the temperature of 620–830 K and obtained:

$$D_\beta = 6.3 \times 10^{-8} \exp\left[\frac{-14184 \pm 966}{RT}\right] \quad (\mathrm{m^2/s}) \tag{5}$$

The diffusion coefficient of hydrogen in β-phase is a few orders of magnitude higher than that in α-phase. The coefficient as a function of temperature is illustrated in Fig. 2. It can be seen that the results reported by different coefficient are almost the same at high temperatures. The difference between the results of Wasilewski and Kehl [13] and Papazoglou and Hepworth [14] may be attributed to the samples used by Papazoglou and Hepworth [14] having a lower hydrogen concentration. At very low hydrogen concentration (<10% saturation), the diffusivity depends on the hydrogen concentration [13,14]. However, this was not taken into account in the mobility database developed in this work due to the lack of experimental data. The experimental results of Wasilewski and Kehl [13] and Sevilla et al. [19] were extended to compare their predictions to the diffusion coefficient at low temperatures, as shown in Fig. 2. A large difference can be found between the predictions from Eq. (4) and the experimental results of Sevilla et al. [19]. Eq. (5) derived from the experimental data at 620–830 K by Sevilla et al. [19] also shows a good prediction for the coefficients at high temperatures and a good agreement with the measurement of Papazoglou and Hepworth [14]. Thus, Eq. (5) was used to determine the hydrogen diffusion coefficient in β-Ti at the present work.

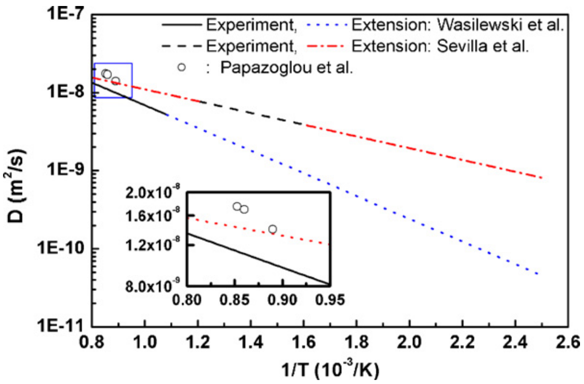

Fig. 2. H diffusion coefficient in β-Ti (the solid line and dashed line denote the experimental results reported by Wasilewski and Kehl [13] and Sevilla et al. [19], respectively; the dotted line and dot-dashed line are the extrapolation of their experimental results, respectively, and the opened circles are the experimental result of Papazoglou and Hepworth [14]).

2.3. Hydrogen diffusion in titanium hydrides

There are three kinds of titanium hydrides [20]. δ-Phase with f.c.c. structure has an atom ratio of hydrogen to titanium between 1.5 and 1.99, which is the eutectoid product of β-phase. δ-Phase can also form when excessive hydrogen permeates into α-Ti. TiH_2 is called ε-phase and has a f.c.t. structure. γ-Phase with a metastable f.c.o. structure separates out from α-phase. Hydrogen atoms in δ-phase occupy tetrahedron sites. This kind of hydride has lattice parameters a = 0.4454 nm. After δ-phase becomes ε-hydride, all the tetrahedral sites are occupied. γ-Phase has lattice parameters of a = 0.4168 nm, b = 0.4234 nm and c = 0.4577 nm. The sizes of these hydrides are all much larger than α-Ti (a = 0.295 nm) [21].

Many researchers have studied the diffusivity of hydrogen in titanium hydrides with different methods, such as pulsed field gradient-nuclear magnetic resonance (PFG-NMR) [22], inelastic neutron-scattering measurements [23,24], nuclear magnetic resonance measurements [25], diffraction-enhanced X-ray imaging (DEI) method [26] and mechanical spectroscopy [27]. The results on hydrogen diffusion coefficient reported by different authors [22,23,27–29] are nearly the same. The data reported by Kaess et al. [22] were used and Eq. (6) was derived to calculate the diffusion coefficient of hydrogen in TiH_x in the present work. The variation of the hydrogen diffusion coefficient with the atom ratio of H to Ti, x, and the temperature is also illustrated in Fig. 3:

$$D_{TiH_x} = (2 - x)3.17 \times 10^{-7} \exp\left[\frac{-11700}{RT}\right]$$
$$(1.5 \le x \le 1.95) \quad (\mathrm{m^2/s}) \tag{6}$$

2.4. Diffusion data for modeling

In a multicomponent system, there are a number of concentration-dependent and interrelated diffusion coefficients. In

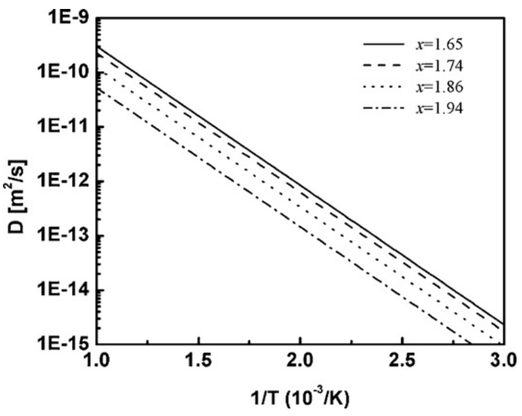

Fig. 3. H diffusion coefficient in titanium hydrides.

order to perform the simulation of phase transformation and diffusion in the multicomponent system, atomic mobilities are generally used, rather than diffusion coefficients, to reduce the number of parameters stored in the database and make the parameters are independent, as only one unique mobility is required for a component in the multicomponent system [8]. Although, theoretically, the diffusive reactions of the present work can be modeled with the diffusion coefficients, which were evaluated from experimental measurements in the above sections, a mobility database was created by considering the extension of the kinetic database for more complex Ti-H alloy systems. The composition-independence mobilities in α and β phases were extracted from Eqs. (2) and (5), respectively, by defining $\phi_i = -Q_i + RT\ln D_i$ for element i, where Q_i is the activation energy of the element. For TiH_x phase, the composition dependency was described with a linear combination of the values at each endpoint of the composition space and a Redlich–Kister expression [11,30]. In the calculations the interdiffusion coefficients in α-phase and β-phase were then obtained by means of the Einstein relation, while the composition dependent interdiffusion coefficients in TiH_x were related to the mobilities and mole fraction of components and thermodynamic factors by the use of the Darken relation [11]. This method has been discussed elsewhere [11,31–33]. The mobility database, in conjunction with a Ti-based alloy thermodynamics database (TTTI3) and the CALPHAD technique, was also used to calculate the local equilibrium conditions at phase interfaces in order to determine the moving boundary migration rate, phase fractions, phase compositions and chemical potentials.

3. Diffusion and phase transformation

The isothermal hydrogen diffusion process and phase transformation in a titanium particle of 0.5 mm in radius were simulated in this paper. According to phase diagram [4], there are four characteristic temperature ranges. At each range, there is a specific phase transformation process during hydrogen diffusion. They are of less than 573 K, 573–956 K, 956–1155 K and above 1155 K. Because only β phase exists in the system and no phase transformation occurs above 1155 K, the simulation was only performed for the hydrogen diffusion and phase transformation processes at the first three temperature ranges. The titanium particles have an initial hydrogen content of 0.003 wt%.

One-dimensional spherical model was used and 100 cells were applied for the region from the center to the surface of the spherical particle. The grid points in the modeling region were distributed geometrically with a geometrical factor of 0.8, so that a higher number of grid points in the surface region of the titanium particle were yielded to result in more accurate value for the region of interest. This is an optimized gridding scheme, which can reach a fast computation and make the final results independent of the grid distribution. A closed boundary was applied for the center of the particle. The fluxes of hydrogen and titanium are then zero at the center. The third boundary condition was employed to model the hydrogen diffusion at titanium surface exposed to the hydrogen-content atmosphere and was expressed by

$$\left.\frac{\partial C}{\partial x}\right|_{x=r} = -\beta(C_{x=r} - C_s) \qquad (7)$$

where β is hydrogen transfer coefficient at the surface of titanium particles. $C_{x=r}$ and C_s denote the hydrogen concentration at the titanium surface and the hydrogen potential in atmosphere, respectively.

As, up to now, there is no literature relating to the hydrogen transfer coefficient at titanium surface, experiments of hydrogenization of pure titanium slabs at 650 °C and 950 °C were performed to determine the mass-transfer coefficient that may depend on both temperature and environment composition. The depth-profiles of hydrogen in the hydrogenized sample surfaces were measured with a glow discharge optical emission spectroscopy (GD-OES) and the results were used to extract the hydrogen transfer coefficient with a method proposed by Gao et al. [34]. The uncertainty analysis of this method has also been discussed in detail in our previous work [34]. It was found that the hydrogen transfer coefficient weakly depends on the temperature and an average value of 1×10^{-7} mol/s with a uncertainty of $\pm 0.08 \times 10^{-7}$ mol/s was then used in this work no matter what phase existed in the titanium surface.

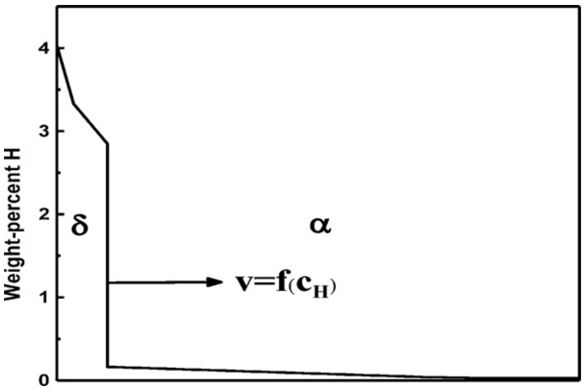

Fig. 4. Phase transformation at 560 K.

4. Results and discussion

4.1. Diffusion and phase transformation under 573 K

With the calculation, the phase transformation rate, the hydrogen concentration at the particle surface, the start and end times of phase transformation, the volume friction of phases and the average hydrogen concentration in the titanium particle at any time can be obtained.

At a temperature less than 573 K, α phase is presented in a titanium particle with 0.003 wt% hydrogen. With the diffusion of hydrogen into the particle, α phase transfers to titanium hydride (δ-Ti) until the amount of atomic hydrogen in TiH_x becomes saturated (Fig. 4). The hydrogen diffusion and the phase transformation from α-Ti to δ-Ti at 560 K were calculated with moving boundary model. The hydrogen concentration in the atmosphere, C_s, is 1%.

The phase transformation rate is a function of hydrogen concentration. Fig. 5 shows that the velocity of the phase boundary increases sharply with an increase on hydrogen in the system and achieves a maximum value of approximate 5.8×10^{-3} μm/s at

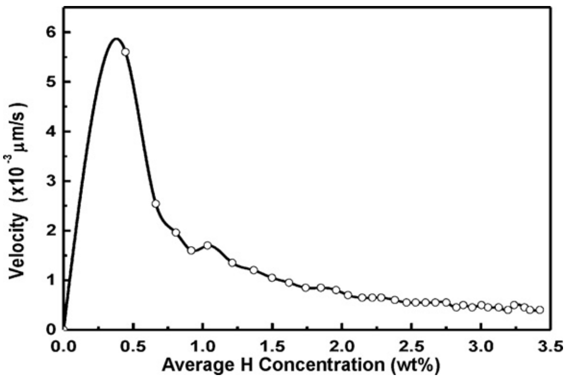

Fig. 5. Variation of moving velocity of δ-Ti boundary with average H concentration.

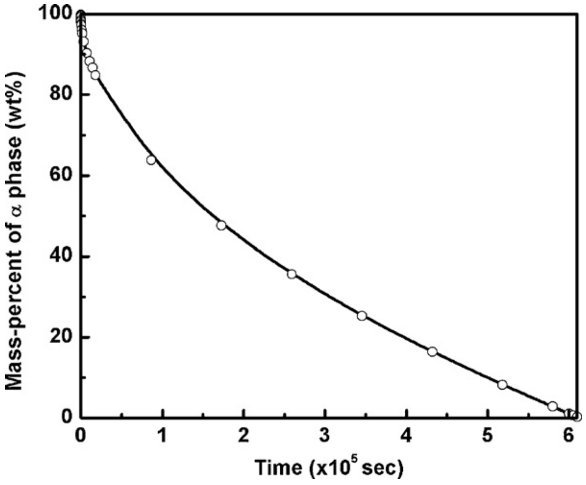

Fig. 6. The reduction of α phase at 560 K.

a hydrogen concentration of 0.38 wt%. The velocity then rapidly drops to about 1.5×10^{-3} μm/s and descends more slowly with a further increase in hydrogen. This can be attributed to the formation of the hydride phase, which has a low hydrogen diffusion coefficient. The barrier hydride layer blocks the penetration of hydrogen and, in turn, leads to a slower phase growth rate [35]. This results in a slow volume-average rate of phase transformation and the larger the titanium particle size the slower the average phase transformation and hydrogen diffusion velocities. The simulation results show that it takes more than 160 h to transfer all of the α phases to TiH$_x$ for a particle with a diameter of 1 mm at the temperature of 560 K (Fig. 6).

4.2. Diffusion and phase transformation at 573–956 K

To investigate the hydrogen diffusion and phase transformation characteristics at 573–956 K, the hydrogen diffusion process at 800 K was calculated. At this temperature, with the diffusion of hydrogen into the titanium particle, β-Ti firstly forms from α-Ti and then transforms to TiH$_x$, which becomes the only composition in the final system. It was found that β-Ti forms at the grain boundaries, while the formation of δ-Ti is mainly intergranular within the β-Ti, as shown in Fig. 7. This can be confirmed from experiments [36,37].

A constant phase growth rate was found for δ-Ti (Fig. 7b). However, the transformation velocity of α-Ti to β-Ti interface increases during the hydrogen diffusion and reaches a maximum of 0.42 μm/s (Fig. 8), which is more than 70 times faster than that for the formation of δ-Ti from α-Ti at 560 K (Fig. 5). It was also found that the fastest phase transformation rate occurs when the β phase reaches to about 30 wt%.

Due to the high hydrogen diffusion coefficient in β-Ti and the fast phase growth rate, the phase transformation from α-Ti to β-Ti and, then, to TiH$_x$ in a 1 mm titanium particle can finish in about 2.2 h at 800 K. The transformation process from α-Ti to β-Ti takes about 24 min, starting at 5 min and finishing at about 29 min (Fig. 9a). The formation of TiH$_x$ starts after 1 h 27 min of hydrogen diffusion and finishes within 52 min (Fig. 9b). A constant transformation rate of 0.033 wt% per second was found. As the titanium hydride formation is mainly intergranular, the effect of the hydride layer on the penetration of H can be ignored and the velocity is stable.

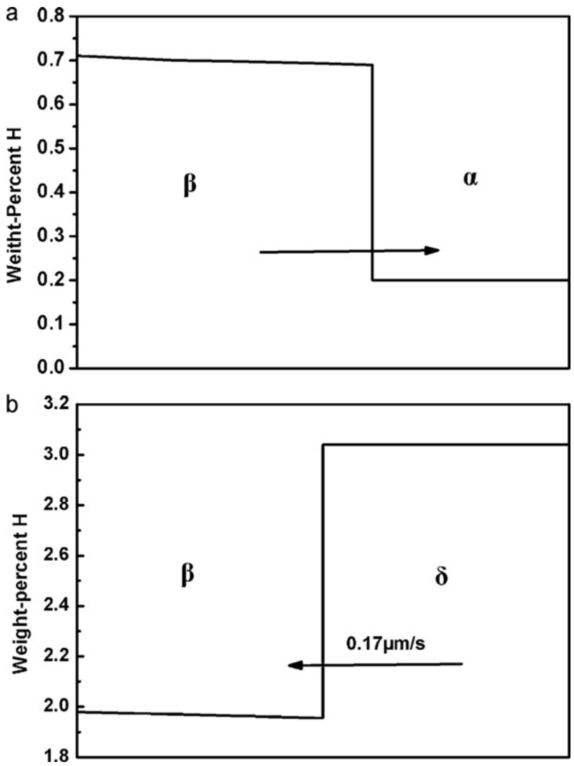

Fig. 7. Phase transformation at 800 K.

4.3. Diffusion and phase transformation at 956–1155 K

The characteristics of hydrogen diffusion at 956–1155 K were studied by modeling the diffusion process at 1000 K. As hydrogen diffuses into the titanium particle from the atmosphere, β-Ti forms from the initial α-Ti. Because the hydrogen diffusion coefficient in β-Ti is much higher than that in α-Ti, the hydrogen can quickly transfer to the phase boundaries between β-Ti and α-Ti from the particle surface and, as a result, the diffusion controlled phase transformation is very fast (Fig. 10). As observed for the variation of the β-Ti growth rate with hydrogen concentration at 800 K, the phase growth rate at 1000 K also increases at first and, then, reaches a maximum value when the content of β-Ti in the system is about 30 wt%. This implies that the β-Ti formation mechanisms at both 800 K and 1000 K are the same. However, the phase transformation rate is faster at 1000 K then at 800 K, due to higher hydrogen diffusion coefficient at 1000 K. The fastest boundary velocity is

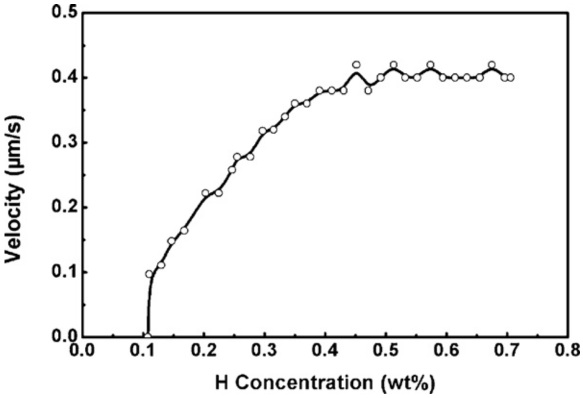

Fig. 8. Variation of β-Ti boundary moving velocity with H concentration.

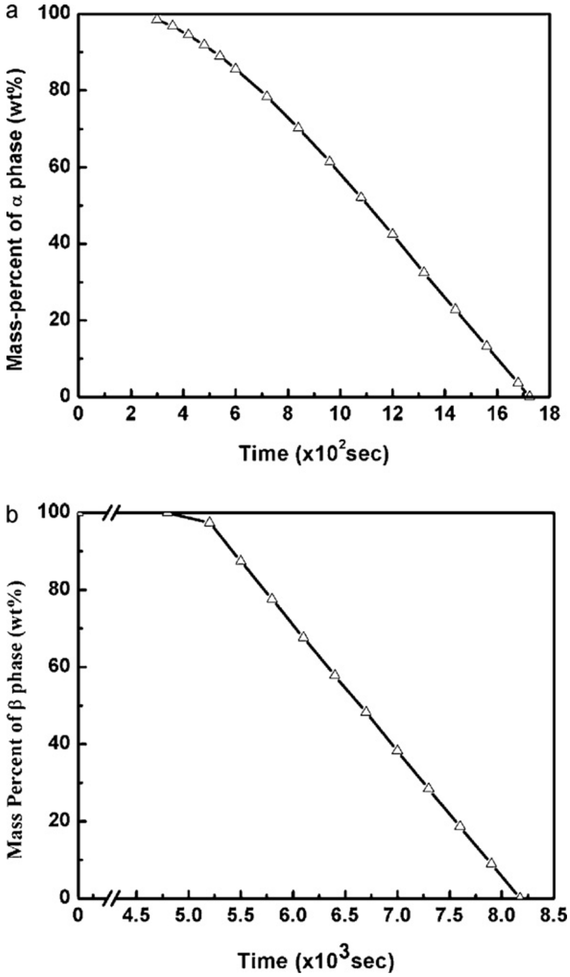

Fig. 9. The reduction of α phase (a) and β phase (b) at 800 K.

1.28 μm/s and the phase transformation in the particle can be finished within 6.5 min.

4.4. Variation of hydrogen concentration

Fig. 11 shows the variation of volume-average hydrogen concentration during the hydrogenization of titanium particles at different temperatures. At 560 K, the average hydrogen concentration in the titanium particle increases very slow because of the formation of the δ-Ti barrier layer. At 800 K, as the transformation rate from α-Ti to β-Ti is faster than that from β-Ti to TiH_x and because of the high hydrogen diffusion coefficient in β-Ti, the hydrogen concentration in the system increases sharply when β-Ti exists in the system. It can be seen that, in the first 3 h, the hydrogen concentration increases up to 3.3 wt% from the initial concentration of 0.003 wt%. However, when TiH_x is the only phase in the system, the hydrogen diffusion rate becomes very slow. Fig. 11 also shows that the hydrogen increases to 1.77 wt% within 2 h at 1000 K. It should be noticed that the hydrogen diffusion process depends on the hydrogen transfer coefficient at the titanium surface and the hydrogen potential of the atmosphere. The hydrogen transfer coefficient may changes with the formation of new phases at the surface of titanium particles. However, in this study, a constant surface transfer coefficient was employed for all phases.

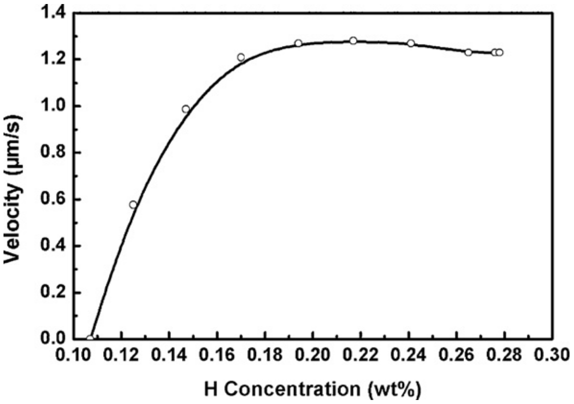

Fig. 10. β-Ti boundary moving velocity as a function of average H concentration.

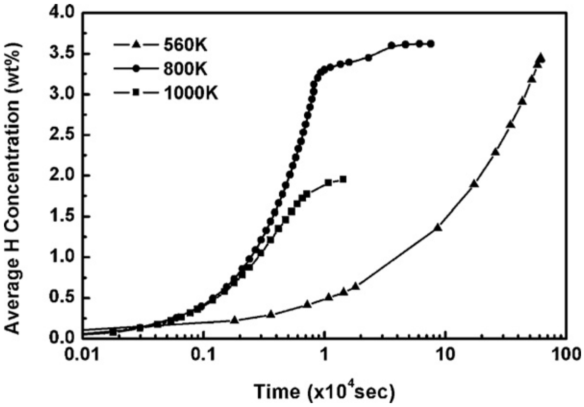

Fig. 11. Variety of average H concentration during hydrogenization.

5. Conclusions

A mathematic model was developed based on thermodynamics and kinetics to calculate the hydrogen diffusion and phase transformation during the hydrogenization and dehyrogenization of titanium and its alloys. In this paper, the model was successfully used to predict the hydrogen diffusion process, hydrogen distribution, phase transformation and phase growth rate during charging of hydrogen into a titanium particle at temperatures of 560 K, 800 K and 1000 K. The calculation results show that, at a temperature of below 573 K the formation of a TiH_x layer results in a slow hydrogenization rate of titanium. The phase transformation rate of β-Ti from α-Ti above 573 K increases with an increase in hydrogen content and reaches a maximum value. The formation of δ-Ti at temperatures of 573–956 K is intergranular, which leads to a constant rate of δ-Ti formation. The boundary moving velocity of δ-Ti is 0.17 μm/s at 800 K.

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