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Изучение упрочнения и охрупчивания ω -фазы β -титановых сплавов в рамках первопринципного подхода

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Выделение ω -фазы в β -титановых сплавах приводит к увеличению их прочности при значительном ухудшении пластичности. В работе исследован механизм упрочнения и охрупчивания ω -фазы в рамках первопринципного метода на основе теории функционала плотности. Рассчитаны обобщенные энергии дефектов упаковки для различных систем скольжения в β - и ω -фазах. Эффекты упрочнения и охрупчивания ω -фазы описываются путем сравнения энергетических барьеров скольжения систем в β - и ω -фазах с использованием различных ориентационных соотношений. Показано, что упрочнение и охрупчивание ω -фазы связано с гораздо более высокими значениями энергетических барьеров скольжения в ω -фазе, за исключением $(\bar{2}020)[0001]_{\omega}$, чем в β -фазе. При снижении содержания Мо и увеличении степени разрушения структуры энергетический барьер скольжения наиболее активной системы $(\bar{2}020)[0001]_{\omega}$ в ω -фазе увеличивается. Это свидетельствует об усилении эффектов упрочнения и охрупчивания ω -фазы в процессе старения.

Ключевые слова: титановые сплавы, фаза, охрупчивание, обобщенная энергия дефекта упаковки, расчеты из первых принципов

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Origin of the ω -strengthening and embrittlement in β -titanium alloys: Insight from first principles

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The ω -phase precipitates in β -Ti alloys increase the strength but significantly degrade the ductility of the alloys. In the present work, the mechanism of ω -strengthening and embrittlement is investigated by using a first principles method based on density functional theory. The generalized stacking fault energies of various slip systems in both the β and ω phases are calculated. The strengthening and embrittlement effects of the ω phase are discussed by comparing the slip energy barriers of slip systems in the β and ω phases with different orientation relationships. It is found that the slip energy barriers of slip systems in the ω phase, except for $(\bar{2}020)[0001]_{\omega}$, are much higher than those of slip systems in the β phase, which explains the ω -strengthening and embrittlement effects. The slip energy barrier of the most active slip system in the ω phase, $(\bar{2}020)[0001]_{\omega}$, increases with the depletion of Mo and increasing extent of structure collapse, suggesting that aging treatment enhances the ω -strengthening and embrittlement effects.

Keywords: titanium alloys; ω phase; embrittlement; generalized stacking fault energy; first-principles calculations

1. Introduction

Beta-titanium alloys (β -Ti), with body centered cubic (bcc) crystal lattice, are widely used in aerospace, ocean development and biomedical area due to their high specific strength, corrosion resistance and

biocompatibility [1]. In general, β -Ti alloys contain transition metal elements such as Mo, Cr, V, Nb (β stabilizers) [2]. In these alloys, ω phase precipitates with nonclose-packed hexagonal lattice are commonly observed [3–6]. The ω particles may form du-

ring quenching from high temperature without atomic diffusion, termed as athermal ω phase. Alternatively, the ω phase may precipitate during the isothermal aging, termed as isothermal ω phase [7–9], where element partitioning occurs between the ω and β phases. Many efforts have been made to investigate the β – ω transition pathway. A generally accepted mechanism is that the ω phase forms through the collapse of two adjacent $(111)_\beta$ atomic planes of the β matrix toward the plane in between them [9, 10]. This results in the $[110]_\beta \parallel [1120]_\omega$ orientation relationship between the ω and β phases. Because bcc structure has four equivalent $\langle 111 \rangle_\beta$ directions, the ω phase has four variants in the β matrix, i.e., ω_1 with $(111)_\beta \parallel (0001)_\omega$, ω_2 with $(\bar{1}11)_\beta \parallel (0001)_\omega$, ω_3 with $(1\bar{1}1)_\beta \parallel (0001)_\omega$, and ω_4 with $(\bar{1}\bar{1}1)_\beta \parallel (0001)_\omega$ [11]. Banerjee et al. [12] found that the extent of dislocation collapse depends on the stability of the ω phase. In alloys enriched with β stabilizing element, e.g. Ti-Mo, the crystal structure of the athermal ω phase is only partially collapsed. During the following isothermal annealing, the rejection of Mo from ω precipitates stabilizes the ω phase, leading to a developed ω lattice with full collapse of atomic planes, i.e., two $(111)_\beta$ planes merge into one.

The presence of ω phase has a crucial influence on the mechanical properties of β -Ti alloys. Experiments demonstrated that the ω particles strengthen significantly the β -Ti alloys but have a remarkable embrittlement effect. Extensive researches have shed some light on such influences. Generally, the strengthening effect of ω phase is ascribed to the higher stiffness of the ω phase than that of the β matrix. This was confirmed by the Young's modulus of the ω phase (220 GPa) relative to that of the β phase (70 GPa) [13]. For Ti-Mo, Ti-Mn, and Ti-V alloys, the strength increases with the volume fraction of the ω particles while the ductility decreases with increasing ω size during the aging process [6]. Chen et al. [14] reported a ductile-to-brittle transition in Ti-Mo with increasing aging time. It was suggested that this transition is attributed to the evolution of the composition and crystal structure of the ω phase during the annealing. Several mechanisms were proposed to describe the behavior of ω particles in deformation, such as shearing, bypassing, disordering and reorientation [15–17]. In Ti-Mo alloy, some ω variant was observed to keep the original hexagonal lattice after a $\{112\}\langle 111 \rangle_\beta$ dislocation slip through. On the other hand, the crystal lattice of the others is heavily dis-

torted, indicating these ω particles block the slip of the dislocations. In spite of the aforementioned research efforts, the mechanism of ω -strengthening and embrittlement at atomistic level is still to be explored.

In this work, the influence of ω phase on the mechanical properties of β -Ti alloys is investigated by using a first principles method based on density functional theory (DFT). We calculated the generalized stacking fault energies (GSFEs) of the various planes of both ω and β phases. The comparison between the GSFEs of the two phases is used to measure the compatibility of dislocation movement in them, and, to predict the strengthening and embrittlement effects of the ω phase. The effects of the partition of Mo atoms between the ω and β phases and the degree of lattice collapse on GSFE and the dislocation slip are studied as well, which shed light on the influence of aging on the ω -strengthening and embrittlement effects.

2. Methodology and calculations details

2.1. Generalized stacking fault energy

The generalized stacking fault energy (γ surface) is expressed as

$$\gamma = \frac{E_{xy} - E_0}{S}, \quad (1)$$

where E_{xy} is the total energy of a crystal with the top half atomic planes shifted relative to the bottom half by displacement of (x, y) along the slip plane, E_0 is the energy of the unshifted system, S is the area of the stacking fault.

The GSFE may be calculated readily by using first principles methods with supercell model with vacuum (Fig. 1). The slip plane is set as the xy plane of the supercell. The total number of atomic layers is $2N$. The GSFE may be obtained by shifting the top N layers against the bottom N layers step by step along the slip plane and calculating the corresponding energy [18]. The number of atomic layers N and vacuum thickness are carefully tested to make the calculated GSFE converge with an error no more than 0.01 J/m^2 . It is noted that N varies with the orientation of the slip plane and the phases. The shape and volume of the supercell are fixed while the atoms are allowed to relax in the direction perpendicular to the slip plane.

For the Ti- x Mo alloys ($x = 0$ –25 at %), the random distribution of the alloying atoms Mo in the system is described within the framework of special quasi-random structure (SQS) scheme [19] implemented in the Alloy Theoretic Automated Toolkit (ATAT) [20–22]. The supercells model for Ti- x Mo is schemati-

Fig. 1. The supercell models of pure Ti (a), Ti-xMo alloy (b) for the calculations of generalized stacking fault energy (color online)

cally shown in Fig. 1, b. The random distribution of Mo atoms destroys the symmetry of crystal lattice such that the atomic layers for the same slip planes are no longer equivalent. Therefore, in this work, we calculate the GSFEs of each individual atomic layers. The overall GSFE is taken as the average of all the individual GSFEs.

2.2. Calculation details

The total energies of β and ω supercells are calculated by using plane-wave pseudopotential method [23], implemented in Vienna Ab initio Simulation Package (VASP) [24–26]. The generalized gradient approximation (GGA) parameterized by Perdew, Burke, and Ernzerhof (PBE) [27] is adopted to describe the electronic exchange and correlation. We adopt the plane-wave cut-off energy (E_{cut}) of 500 eV and the k -point mesh density of about 0.3 nm^{-1} in our calculations. The convergence criterions are set as 10^{-5} eV for the total energy and 10^{-1} eV/nm for the interatomic forces. To limit the interaction between defects (stacking faults), we adopt supercells which have more than 18 atomic layers and a vacuum layer with thickness of 1.5 nm.

3. Results

3.1. GSFEs of β and ω phases of pure Ti

There are three main slip planes in β -Ti, i.e., $(110)_{\beta}$, $(112)_{\beta}$ and $(123)_{\beta}$ planes [1]. The calculated

GSFE surfaces for these slip planes are shown in Figs. 2, a, c, and e. The easiest slip direction (i.e., with lowest energy barrier) is $[1\bar{1}1]_{\beta}$ for $(110)_{\beta}$ -plane, $[11\bar{1}]_{\beta}$ for $(112)_{\beta}$ and $(123)_{\beta}$ plane. Figures 2, b, d, and f display the GSFEs along the slip systems. The displacement refers to the ratio of moving distance of atoms to the length of Burgers vector. The maximum GSFE (i.e., the unstable stacking fault energy, γ_{us}) along the slip systems are 0.20, 0.25 and 0.24 J/m^2 for $\{110\}\langle 111 \rangle_{\beta}$, $\{112\}\langle 111 \rangle_{\beta}$ and $\{123\}\langle 111 \rangle_{\beta}$, respectively.

It is noted that, for the $\{112\}\langle 111 \rangle_{\beta}$ and $\{123\}\langle 111 \rangle_{\beta}$ slip systems, some of the stacking fault energies are found to be negative, indicating that the structures with face defects are more stable than the perfect β lattice. It is known that β -Ti is a high temperature phase and is not stable at low temperature. Therefore, it is not surprising that 0 K DFT calculations yield some negative stacking fault energy due to the instability of the β phase.

For the ω phase, we calculate the GSFE surfaces for the slipping planes, considering the possible orientation between the slip systems of β and ω phases which will be detailed in Sect. 4 and listed in Table 1.

The GSFE surfaces of $(11\bar{2}0)_{\omega}$ and $(10\bar{1}\bar{1})_{\omega}$ slip planes of ω phase which are parallel to $\{110\}_{\beta}$ are shown in Figs. 3, a and c. From the GSFE surface, the GSFE curves along the minimum energy barrier slip paths are extracted. These slip paths are $(11\bar{2}0)[0001]_{\omega}$ (Fig. 3, b), $(11\bar{2}0)[1\bar{1}01]_{\omega}$ (Fig. 3, b), and $(10\bar{1}\bar{1})[\bar{1}10\bar{1}]_{\omega}$ (Fig. 3, d). The unstable stacking fault energy γ_{us} are 0.71, 0.80, and 1.07 J/m^2 , respectively.

Figures 4, a, c, and e display the GSFE surfaces of $(\bar{1}012)_{\omega}$, $(12\bar{3}1)_{\omega}$, $(\bar{2}020)_{\omega}$. The GSFE curves for the slip systems $(\bar{1}012)[1\bar{1}01]_{\omega}$, $(12\bar{3}1)[\bar{1}10\bar{1}]_{\omega}$, and $(\bar{2}020)[0001]_{\omega}$, which are connected to $\{112\}\langle 111 \rangle_{\beta}$ are shown in Figs. 4, b, d and f. The unstable stacking fault energy γ_{us} are 4.38, 1.08 and 0.42 J/m^2 . For the plane $(\bar{1}012)_{\omega}$, the GSFEs are extremely high direct along the path $(\bar{1}012)[1\bar{1}01]_{\omega}$. We adopt the GSFEs along the easiest path denoted with the red dashed line in Fig. 4, a. In addition, as shown in Fig. 4, f, there exists a local minimum of the GSFE curve at the displacement of 0.5 for $(\bar{2}020)[0001]_{\omega}$, indicating that the full $(\bar{2}020)[0001]_{\omega}$ dislocation tends to dissociate into two partial dislocations with Burgers vector of $1/2[0001]_{\omega}$, which has been experimentally observed [14].

Fig. 2. GSFE surfaces for $(110)_\beta$ (a), $(112)_\beta$ (c), and $(123)_\beta$ planes (e) and the GSFEs for the corresponding minimum slip energy barrier path $[1\bar{1}1]_\beta$ (b), $[11\bar{1}]_\beta$ (d) and $[11\bar{1}]_\beta$ (f) (color online)

The GSFE surfaces and curves of $(\bar{1}540)[0001]_\omega$, $(53\bar{2}1)[01\bar{1}1]_\omega$, $(134\bar{2})[1\bar{1}0\bar{1}]_\omega$ and $(\bar{1}2\bar{1}3)[10\bar{1}1]_\omega$ parallel to $\{123\}\langle 111 \rangle_\beta$ slip systems are shown in Fig. 5. The γ_{us} are 0.83, 1.07, 3.64, and 4.45 J/m², respectively.

3.2. GSFEs of ω with various compositions and extents of collapse

During the aging process, the composition and extent of collapse of ω phase change with increasing aging time. Therefore, in order to understand the ef-

fect of aging on the ω strengthening and embrittlement effect, it is crucial to know how the Mo content and extent of collapse influence the mobility of the slip system in the ω phase. As presented in Sect. 3.1, the energy barrier for the $(\bar{2}020)[0001]_\omega$ is the lowest among all slip systems of the ω phase considered in this work. Namely, the mobility of $(\bar{2}020)[0001]_\omega$ slip system is the highest among them. Therefore, we take $(\bar{2}020)[0001]_\omega$ slip system to investigate the influences of Mo content and collapse extent.

Table 1. The 10 orientations between ω phase and the three main beta slip systems, the calculated γ_{us} and the ratio $\gamma_{us}^{\omega} / \gamma_{us}^{\beta}$ are also given below

β slip systems	ω variants	ω slip system	$\gamma_{us}, \text{J/m}^2$	$\gamma_{us}^{\omega} / \gamma_{us}^{\beta}$
$\{110\}\langle 111 \rangle_{\beta}$			0.20	
	ω_1	$(11\bar{2}0)[0001]$	0.71	3.55
	$\omega_{2,3}$	$(11\bar{2}0)[1\bar{1}01]$	0.80	4.00
	ω_4	$(10\bar{1}\bar{1})[1\bar{1}01]$	1.07	5.35
$\{112\}\langle 111 \rangle_{\beta}$			0.25	
	ω_1	$(\bar{1}012)[10\bar{1}\bar{1}]$	4.38	16.22
	$\omega_{2,3}$	$(12\bar{3}1)[\bar{1}01\bar{1}]$	1.08	4.00
	ω_4	$(\bar{2}020)[0001]$	0.42	1.68
$\{123\}\langle 111 \rangle_{\beta}$			0.23	
	ω_1	$(\bar{1}540)[0001]$	0.83	3.61
	ω_2	$(53\bar{2}1)[01\bar{1}\bar{1}]$	1.07	4.65
	ω_3	$(1342)[1\bar{1}0\bar{1}\bar{1}]$	3.64	15.83
	ω_4	$(\bar{1}2\bar{1}3)[10\bar{1}\bar{1}]$	4.45	19.35

Figure 6 presents the unstable stacking fault energy γ_{us} of $(\bar{2}020)[0001]_{\omega}$ against the Mo content x ($0 < x < 25$ at %). The ω phase is assumed to be fully collapsed. The solid circles represent the γ_{us} of each individual slip layers for the same slip plane but with different atomic environment, and the empty circles represent the average γ_{us} of the slip planes. It is seen

that the individual γ_{us} are scattered, indicating that local atomic environment influences notably the unstable stacking fault energy. However, the average γ_{us} decreases with increasing Mo content.

Figure 7 schematically shows the structures of the β , partially collapsed ω , and fully collapsed ω phase and the GSFE curves of ω -Ti against the col-

Fig. 3. GSFE surfaces for $(11\bar{2}0)_{\omega}$ (a) and $(10\bar{1}\bar{1})_{\omega}$ (c) planes and the corresponding minimum slip energy barrier paths (b) red line for $(11\bar{2}0)[0001]_{\omega}$, black line for $(11\bar{2}0)[1\bar{1}01]_{\omega}$ and (d) for $(10\bar{1}\bar{1})[\bar{1}10\bar{1}]_{\omega}$ (color online)

Fig. 4. GSFE surfaces for $(\bar{1}012)_\omega$ (a), $(12\bar{3}1)_\omega$ (c) and $(\bar{2}020)_\omega$ (e) planes and the corresponding minimum slip energy barrier paths $(\bar{1}012)[1\bar{1}01]_\omega$ (b), $(12\bar{3}1)[\bar{1}10\bar{1}]_\omega$ (d) and $(\bar{2}020)[0001]_\omega$ (f)

lapse extent. The collapse extent varies from $Z_\omega = 0$ for the uncollapsed β phase to $Z_\omega = 1/6[0001]_\omega$ for the fully collapsed ω phase with a step of $1/48[0001]_\omega$. As seen in the figure, for $Z_\omega = 0-3/48[0001]_\omega$, the values of γ_{us} are 0.2–0.3 J/m², at the same level as that of the $\{112\}\langle 111 \rangle_\beta$ slip system of the β phase. For $Z_\omega = 4-5/48[0001]_\omega$, γ_{us} increases significantly with Z_ω . γ_{us} of ω phases with $Z_\omega = 6-8/48[0001]_\omega$ are 0.42–0.43 J/m² at the same level as that of the $(\bar{2}020)[0001]_\omega$ slip system of the fully collapsed ω phase. The shape of the GSFE curve also changes with Z_ω . At high collapse extent, there are two peaks

on the GSFE curves. The local minimum in between the two peaks indicates that there exists a stable stacking fault in the structure of ω with high collapse extent. The two peaks of the GSFE curve merge gradually into one with decreasing Z_ω , indicating that the stable stacking fault disappears.

4. Discussion

4.1. Strengthening and embrittlement of ω phase

In $\omega + \beta$ dual phase alloys, the strengthening effect depends on how easily the dislocation in β ma-

Fig. 5. GSFE surfaces for $(\bar{1}540)_\omega$ (a), $(5\bar{3}21)_\omega$ (c), $(1342)_\omega$ (e), and $(\bar{1}2\bar{1}3)_\omega$ (g) planes and the corresponding minimum slip energy barrier paths $(\bar{1}540)[0001]_\omega$ (b), $(5\bar{3}21)[01\bar{1}1]_\omega$ (d) and $(1342)[\bar{1}\bar{1}0\bar{1}]_\omega$ (f) and $(\bar{1}2\bar{1}3)[10\bar{1}1]_\omega$ (h) (color online)

trix can cut through the hard ω phase, of which the feasibility can be roughly measured with the ratio of the slip energy barriers (unstable stacking fault energy) of ω phase to that of β phase, i.e. $\gamma_{us}^\omega / \gamma_{us}^\beta$. A $\gamma_{us}^\omega / \gamma_{us}^\beta$ ratio closer to 1 indicates a weaker strengthening effect. Because the unstable stacking fault energies γ_{us} depend on the slip systems of both phases, $\gamma_{us}^\omega / \gamma_{us}^\beta$ varies with the orientation relationship between the slip systems of ω and β phases. Here, for

simplicity, we consider that the dislocation in the β -matrix cuts directly through the ω phase without changing gliding direction, i.e., only the dislocation of the ω slip system (both slip plane and direction) parallel to that of the β phase can be activated. Thus, the strengthening effect is determined by the ratio $\gamma_{us}^\omega / \gamma_{us}^\beta$ corresponding to the slip systems of the β and ω phases that are parallel to each other. For example, the β slip system $\{110\}\langle 111 \rangle_\beta$ is parallel to

Fig. 6. Unstable stacking fault energy of $(\bar{2}020)[0001]_{\omega}$ ω -Ti-Mo as a function of Mo content from 0 to 25%, averaged over the individual unstable stacking fault energies (scattered symbols) calculated for the atomic layers with different atomic environment (color online)

the $(11\bar{2}0)[0001]_{\omega}$ slip system of ω_1 variant, $(11\bar{2}0)[1\bar{1}01]_{\omega}$ of ω_2 and ω_3 , and $(10\bar{1}\bar{1})[1\bar{1}01]_{\omega}$ of dislocations may be easily activated by the $\{112\}\langle 111\rangle_{\beta}$ dislocations in the β matrix. For the other orientation relationship between the slip systems of the β and ω phases, the ω phase acts as strong obstacle for the movement of the dislocation in β phase. This explains why the ω phase strengthens the β -Ti alloy. The $\{112\}\langle 111\rangle_{\beta}$ dislocations blocked by the ω phase pile up ahead of the ω particles. This may induce heavy stress concentration at the β/ω interface, making microcracks nucleate along the interface or in the weak atomic plane $(\bar{2}020)$ of the ω phase such that decreases the ductility of the alloy. First-principles calculations of β/ω interface indicated that the cracks tend to initiate at interface area instead of in ω and β bulk phases [28].

$(11\bar{2}0)[0001]_{\omega}$, $(10\bar{1}\bar{1})[1\bar{1}01]_{\omega}$, and $(10\bar{1}\bar{1})[1\bar{1}01]_{\omega}$ to determine the ratio $\gamma_{us}^{\omega}/\gamma_{us}^{\beta}$ and the strengthening effect.

The possible orientation relationships between the slip systems of β and ω phases and the corresponding $\gamma_{us}^{\omega}/\gamma_{us}^{\beta}$ ratios are listed in Table 1. Among the 10 slip systems of ω phase, only the $(\bar{2}020)[0001]_{\omega}$ dislocations may be easily activated by the $\{112\}\langle 111\rangle_{\beta}$ dislocations in the β matrix. For the other orientation relationship between the slip systems of the β and ω phases, the ω phase acts as strong obstacle for the movement of the dislocation in β phase. This explains why the ω phase strengthens the β -Ti alloy. The $\{112\}\langle 111\rangle_{\beta}$ dislocations blocked by the ω phase pile up ahead of the ω particles. This may induce heavy stress concentration at the β/ω interface, making microcracks nucleate along the interface or in the weak atomic plane $(\bar{2}020)$ of the ω phase such that decreases the ductility of the alloy. First-principles calculations of β/ω interface indicated that the cracks tend to initiate at interface area instead of in ω and β bulk phases [28].

Our calculations are in agreement with the experimental observations of Chen et al. [29]. The microcompression test on the single crystalline Ti-10V-2Fe-3Al (Ti1023) alloy micropillars demonstrated that the deformation is mainly accommodated by the $\{112\}\langle 111\rangle_{\beta}$ dislocations. In the area of the slip band, the lattice of ω_1 variant with $(\bar{1}012)[1\bar{1}01]_{\omega}$ parallel to $\{112\}\langle 111\rangle_{\beta}$ is heavily distorted. On the other hand, the original hexagonal lattice of ω_4 variant with $(\bar{2}020)[0001]_{\omega}$ parallel to $\{112\}\langle 111\rangle_{\beta}$ is fully maintained. As mentioned above, the $\gamma_{us}^{\omega}/\gamma_{us}^{\beta}$ ratio for ω_1 variant with $(\bar{1}012)[1\bar{1}01]_{\omega}$ parallel to $\{112\}\langle 111\rangle_{\beta}$ is very high (16.22). Therefore, the $\{112\}\langle 111\rangle_{\beta}$ dislocations in β phase is blocked and pile up at the β/ω interface, leading to a heavy stress concentration ahead the ω phase, making the crystal lattice of the ω_1 variant distorted. The $\gamma_{us}^{\omega}/\gamma_{us}^{\beta}$ for the $(\bar{2}020)[0001]_{\omega} \parallel \{112\}\langle 111\rangle_{\beta}$ relationship for the ω_4 variant is 1.68, indicating that the ω_4 particle may be cut through by the $\{112\}\langle 111\rangle_{\beta}$ dislocations such that its original lattice remains.

4.2. Aging strengthening and embrittlement of ω phase

In the aging process, the Mo atoms are rejected from the ω to β phase, leading to a more stable ω phase with lower Mo concentration and higher extent of collapse. Our calculations demonstrated that the

Fig. 7. Schematic of lattice of β , partially collapsed ω and fully collapsed ω phase (a), and GSFE curves of $(\bar{2}020)[0001]_{\omega}$ with various collapse extents (Z_{ω}) (b) (color online)

GSFE of the ω phase increases with decreasing Mo concentration and increasing collapse extent (Figs. 6 and 7), indicating that the annealing process improves the blocking effect of the ω phase to the dislocations in the β matrix. Therefore, it is expected that the strength of alloy increase whereas the ductility decreases with aging time. This prediction is in agreement with experimental finding. The experiment of Chen et al. demonstrated [14], the elongation of the Ti-Mo (20 wt %) alloy decreases from 25 to 22% after 1 hour aging. After annealed for 7 days, the brittle fracture even took place at the very early stage of the test. The compressive fracture strength and hardness increase with the aging time. The surface morphologies of the fracture samples showed that there is no observed plastic behaviour observed in 7 days annealed sample. It is clear that, besides the volume fraction and size of the ω particles, the Mo element partition and structure evolution during the aging process contribute to the stronger ω -strengthening and embrittlement effects with longer aging time.

5. Conclusion

The mechanism of ω -strengthening and embrittlement of β alloys are systematically investigated by using a first principles method. The main results are summarized as follows.

The slip energy barriers of most of the slip systems of the ω phase are much higher than those of the β phase. Therefore, the ω particles in β -Ti alloy act as obstacles for the movement of the dislocations, which strengthens the alloy but degrades the ductility.

The slip energy barrier of the most active slip system of ω phase, $(\bar{2}020)[0001]_{\omega}$, increases with the depletion of the Mo content in and increasing collapse extent of ω phase, contributing to the enhancement of the ω -strengthening and embrittlement effects.

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