Molecular dynamics investigation on tilt grain boundary energies of beta-titanium and tungsten at high temperature

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Keywords: molecular dynamics simulation, grain boundary energy, beta-titanium, tungsten

Abstract
The grain boundary energies (GBEs) of symmetric tilt grain boundaries (STGBs) and asymmetric tilt grain boundaries (ATGBs) for W at 0 and 2400 K and \(\beta\)-Ti at 1300 K were calculated by means of molecular statics and dynamics simulations to investigate the effects of temperature on GBE and the relationships between GBEs and grain boundary (GB) planes. Generally, the variation trends of GBE with the tilt angle are similar for the three cases, when the tilt axis is specified. It is of course that these similarities result from their similar GB microstructures in most cases. However, the variation trends of GBE with tilt angle are somewhat different between \(\beta\)-Ti at 1300 K and W at 2400 K for STGBs with \(<100>\) and \(<110>\) tilt axes. This difference mainly stems from the following two reasons: firstly, the GB microstructures of W at 2400 K and \(\beta\)-Ti at 1300 K are different for some STGBs; secondly, the atoms at the STGB of \(\beta\)-Ti at 1300 K tend to evolve into the local \(\omega\)- or \(\alpha\)-like structures distributed at the STGB for some STGBs with \(<110>\) tilt axis, which makes the corresponding STGBs more stable, thereby decreasing the GBEs. Furthermore, a geometric parameter \(\theta\), the angle between the misorientation axis and the GB plane, was defined to explore the relationships between GBEs and GB planes. It was found that the relationships between GBEs and GB planes can be described by some simple functions of \(\sin(\theta)\) for the GBs with definite lattice misorientation, which can well explain and predict the preferred GB planes for the GBs having the same lattice misorientation. Our calculations not only extend the investigation of GBs to higher temperature, but also deepen the understanding on the temperature contributions to the microstructure evolution at GBs and on the relationships between GBEs and possible geometric parameters.

1. Introduction

The grain boundaries (GBs) play an important and even decisive role on the performance of polycrystal materials [1]. The atomic configurations of GBs essentially determine the GB stability and the other GB properties, such as grain growth, elements segregation, diffusion and so on [2–9], while the GB stability can be quantitatively evaluated using the grain boundary energy (GBE).

In recent three decades, many atomistic simulation works have been devoted to calculate GBEs and study the relationships between GBEs and geometric factors, such as the inverse density of coincidence site lattice (CSL), misorientation angle, GB plane, excess volume and so on [10–19]. It was reported that the variation trends of GBE functioned with the tilt (twist) angle are similar for metals having the same crystal structure, when the tilt (twist) axis is specified [11–14, 19], but the relationships between the GBEs and the geometric factors has not been clearly understood yet and it is still a challenge to uncover it by some simple functions. Furthermore, most of the available simulation works focused on symmetric tilt grain boundaries (STGBs) [11–13], whereas the systematic studies on the asymmetric tilt grain boundaries (ATGBs) were rare, although the ATGBs were more...
Correspondingly, the parameter feature that one of the misorientation axes between the two adjacent grains is parallel to the GB plane. otherwise, the TGB is an ATGB. The parameter the lattice sites of the two adjacent grains are mirror symmetric with respect to the GB plane, the TGB is a STGB; misorientation axis and the corresponding misorientation angle are also called as tilt axes and tilt angles. When the minimum misorientation angle among all possible misorientation axes between the two adjacent grains.

The LAMMPS code

2.2. Computational details

The construction of the TGB models was based on the method proposed by Olmsted et al [17], by which the CSL GBs including arbitrary type of GBs were built in an orthogonal box with the limited size, under the framework of periodic boundary conditions (PBCs). The limited size of the orthogonal box is \(20a_0(X) \times 10a_0(Y) \times 10a_0(Z)\), where \(a_0\) is the lattice parameter, and X, Y and Z represent the directions which are normal, parallel and parallel to the GB plane, respectively. Then all the TGBs constituted of STGBs and ATGBs were selected from the constructed GBs. Such method to construct TGBs ensures that the obtained TGB set contains as many types of tilt axes as possible, such as the tilt axes of \(<100>, <110>, <111>, <210>, <211>, <310>\).

Figure 1 shows two typical TGB models, the STGB model of \(\Sigma 3 \{211\}, 109.5^\circ/\langle 110\rangle\) and the ATGB model of \(\Sigma 3 \{111\} \{511\}, 109.5^\circ/\langle 110\rangle\). As shown in figure 1, the TGB models are characterized by the geometric feature that one of the misorientation axes between the two adjacent grains is parallel to the GB plane. Correspondingly, the parameter \(\varphi\) labeled in figures 1(a) and (b) is misorientation angle. The special misorientation axis and the corresponding misorientation angle are also called as tilt axes and tilt angles. When the lattice sites of the two adjacent grains are mirror symmetric with respect to the GB plane, the TGB is a STGB; otherwise, the TGB is an ATGB. The parameter \(\theta\) labeled in figure 1(b) represents the angle between the misorientation axis and the GB plane. Particularly, the misorientation axis here refers specially to the one with the minimum misorientation angle among all possible misorientation axes between the two adjacent grains.

2.2. Computational details

The LAMMPS code [26] was used to calculate the GBEs of W at 0 and 2400 K and \(\beta\)-Ti at 1300 K, and the MS and MD simulations were adopted to calculate the GBEs at 0 K and higher temperature, respectively. The GBE is calculated as the following expression:
\[ \gamma_{GB} = \frac{E_{GB} - NE_{bulk}}{2A}, \]  

where \( \gamma_{GB} \) labels the GBE, \( E_{GB} \) is the system potential energy of the GB, \( E_{bulk} \) is the potential energy of per-atom in a bulk system at the same temperature as the GB system, \( N \) is the number of atoms of the GB system and \( A \) is the area of the GB plane of the GB supercell. The \( 2A \) in the denominator is due to the existence of two equivalent GBs in a GB supercell, one at the middle and one at the boundary of the supercell.

### 2.2.1. Molecular static simulations

The conjugate-gradient method in LAMMPS package \[26\] was used to minimize the total energies of a serial of GB systems of W at 0 K and its bulk with the embedded-atom method (EAM) potential developed by Zhou \[27\]. The accuracy of the EAM potential of W has been validated in other works \[28\].

The length of the computational cell along X axis was extended to more than 22 \( a_0 \) for every GB model to avoid the interaction between two GBs of the supercell.

The \( \gamma \)-surface method \[17, 18, 29–31\], which has been utilized in many previous works, was adopted to calculate the GBE of each GB model by MS simulations. For every GB model obtained by joining two perfect grains, the two grains on both sides of the boundary were shifted with respect to each other on a grid with the size of \( a_0/9 \times a_0/9 \). Thus, a set of microscopic GBs was obtained by the shifts and the GBEs were calculated followed by MS simulations. Finally, the microscopic GB with the lowest GBE was believed to be the most preferable GB in ground state, and the lowest GBE was considered as the GBE of the corresponding GB model.

### 2.2.2. Molecular dynamics simulations

Higher temperature close to the melting temperature may increase the disorder arrangements of atoms at GB \[24\]. To stabilize \( \beta \)-Ti at relatively low temperature, MD simulations were performed at 1300 K (0.67 \( T_{melt} \)) for \( \beta \)-Ti with EAM/FS potential developed by Mendelev \[32\]. Besides, the GBEs of W at 2400 K (0.65 \( T_{melt} \)) were also calculated by MD simulations. Meanwhile, the calculation of GBEs of \( \Sigma 3 \) and \( \Sigma 9 \) TGBs in W at 1200 and 1800 K were also done. The minimum length of the computational cell along X directions is 50 \( a_0 \) to avoid the interaction of the two GBs in the computational cell for every GB model. Then the computational cells were relaxed in NPT ensemble for 14 \( ns \). The timestep was 2 \( fs \) and the time average of the total potential energy in the last 2 \( ns \) was used to calculate the GBEs at higher temperature.

### 3. Results and discussions

The calculated GBEs of W in this work were compared with those of W in previous works \[29, 33–35\] for STGBs with \( <100> \) and \( <110> \) tilt axes, as shown in figure 2. The variation trends of GBE curves of W calculated by Frolov et al \[33\] and by this work are similar. Besides, the GBEs calculated in this work have better agreement with the existing DFT calculations \[29, 34, 35\]. Accordingly, the good consistency between our calculations and the previous works not only validates the accuracy of our calculation methods and GB models, but also gives us confidence to extend our studies to MD simulations of GBs at high temperature for W and \( \beta \)-Ti.
3.1. The grain boundary energies of STGBs

With different tilt axes of \(<100\>, \(<110\>, \(<111\>, \(<210\>, \(<211\>, \text{and} \,<310\)>\), the variations of the STGB energy as a function of the tilt angle for W at 0 and 2400 K and \(\beta\)-Ti at 1300 K are shown in figures 3(a)–(f), respectively. It is obviously seen that the GBEs of STGBs in W at 0 and 2400 K are similar in most cases. Such similarity of GBEs between W at 0 and 2400 K is also visible for ATGBs, as shown in figure 5. Thus, it can be speculated that the temperature effects on the GBEs of W are somewhat limited. This has been further confirmed by the GBE calculations of \(\Sigma 3\) and \(\Sigma 9\) TGBs of W at 1200, 1800 and 2400 K that the GBEs of W at 1200, 1800 and 2400 K are almost the same, as shown in figures 6(a) and (d). Meanwhile, the variation trends of GBE with tilt angle are similar for W at 2400 K and \(\beta\)-Ti at 1300 K in most cases, except for the STGBs with \(<100\>\) and \(<110\>\) tilt axes.

In order to explore the reasons why the variation trends of GBE with the tilt angle are similar for W at 0 and 2400 K and \(\beta\)-Ti at 1300 K, the GB microstructures of W at 0 and 2400 K and \(\beta\)-Ti at 1300 K were analyzed with the common neighbor analysis (CNA) method implemented within OVITO package \([38]\). The CNA method is an efficient algorithm to compute a fingerprint for pairs of atoms and to characterize the local structural environment, so it facilitates the classification of atoms in crystalline systems \([39]\). In this work, the CNA method was used to identify atoms arranged in BCC, face-centered cubic (FCC), hexagonal-close packed (HCP) and other patterns. Based on the CNA analysis of GBs, it was found that the similar variation trends of STGB energy between W at 0 and 2400 K stem from the preservation of STGB microstructures as the temperature increases.
from 0 to 2400 K, as the STGBs of W shown in figure 4. It was also found that the STGB microstructures of W at 2400 K are similar to those of β-Ti at 1300 K in most cases, even for some special STGBs having different variation trends of GBE curves between W at 2400 K and β-Ti at 1300 K at the corresponding tilt angle of these special STGBs, such as the Σ11{332}, 50.5°/<110> and Σ33{554}, 59.0°/<110> shown in figure 4. Therefore, it was concluded that the similar microstructures of STGBs is the main reason why the variation trends of STGB energies with the tilt angle are similar for W at 0 and 2400 K and β-Ti at 1300 K.

However, the variation trends of GBE curves of W at 2400 K and β-Ti at 1300 K are different in several tilt angle ranges for STGBs with <100> and <110> tilt axes, as shown in figures 3(a) and (b). For example, when the tilt angle increases from 46.4° to 47.9° or from 53.1° to 59.5° regarding to <100> tilt axis, the GBE of W at 0 and 2400 K increases synchronously, but the GBE of β-Ti at 1300 K decreases correspondingly. The comparison of the corresponding STGB microstructures of W at 2400 K and β-Ti at 1300 K indicates that such deviations are closely related to the difference of the STGB microstructures between W at 2400 K and β-Ti at 1300 K, such as STGB microstructures of Σ97{940}, 47.9°/<100> and Σ65{740}, 59.5°/<100>, as shown in figure 4. Therefore, it was concluded that the similar microstructures of STGBs is the main reason why the variation trends of STGB energies with the tilt angle are similar for W at 0 and 2400 K and β-Ti at 1300 K.

Nevertheless, the analysis of microstructures of Σ11{332}, 50.5°/<110> and Σ33{554}, 59.0°/<110> STGBs by the CNA method shows that the atoms at both the STGBs are rearranged into local HCP α-like structures for both W at 2400 K and β-Ti at 1300 K. Although the GBEs of the four STGBs are all at the low GBE region of β-Ti at 1300 K, which is different from W at 2400 K, the microstructures of β-Ti at 1300 K and W at 2400 K are not always different. Thus, it was speculated that the low GBE of the four GBs in β-Ti at 1300 K is related to the special atomic rearrangements into local hexagonal ω-like or HCP α-like structures.

Figure 4. The STGB configurations viewed along the tilt axis of <100> or <110> for W at 0 and 2400 K and β-Ti at 1300 K. The blue, red, yellow and green atoms are arranged in BCC, HCP, FCC and other patterns, respectively. The red polygons in figures are drawn to facilitate the comparison of STGB microstructures.
Generally, the HCP $\alpha$ and hexagonal $\omega$ phases are two allotropic forms of Ti, which can only be stable at low temperature and are difficult to be preserved above the phase-transition temperature [25]. Therefore, it is reasonable to infer that the special atomic rearrangements into local hexagonal $\omega$-like or HCP $\alpha$-like structures at STGBs mainly result from the special STGB microstructures since there is no any $\alpha$-phase stabilized elements being added. From the perspective of crystallographic orientation relationship, the misorientations of the two STGBs, $\Sigma3\{111\}$, $70.5^\circ/\{110\}$ and $\Sigma4\{653\}$, $80.6^\circ/\{110\}$, are close to the possible misorientations between two adjacent $\beta$ grains, $70.5^\circ/\{110\}$, which is able to maintain the Martensitic orientation relationship between GB $\omega$ and the two $\beta$ grains [25]. Similarly, the misorientations of the two STGBs, $\Sigma1\{321\}$, $50.5^\circ/\{110\}$ and $\Sigma3\{554\}$, $59.0^\circ/\{110\}$, are in accordance with the possible special misorientations between two adjacent $\beta$ grains, $49.5^\circ/\{110\}$ and $60^\circ/\{110\}$, in which cases the $\alpha$-like structures formed at this two STGBs still maintain the original Burgers orientation relationship with both $\beta$ grains [40]. From the perspective of energy, the formation of local $\omega$-like or $\alpha$-like embryos distributed at STGBs of $\beta$-Ti at 1300 K makes the corresponding STGBs more stable, due to the contributions of temperature. Furthermore, these evolutions indicate that these STGBs can provide the nucleation sites for $\omega$ and $\alpha$ phases of Ti and thus can facilitate the formation of the $\omega$ and $\alpha$ phases at these STGBs, which are much different from other STGBs. Experimentally, it was indeed observed that $\alpha$ is preferentially nucleated at GB when titanium alloys are cooled at low rates from $\beta$ phase filed to ($\alpha + \beta$) phase field [25]. Thus, the formation of hexagonal $\omega$-like or HCP $\alpha$-like structures at STGBs not only indicates the promoting effects of some special STGBs on the nucleation of $\omega$ and $\alpha$ phase, but also shows the temperature effects on the microstructure evolutions at STGBs.

3.2. The grain boundary energies of ATGBs

For ATGBs with different tilt axes of $\{100\}$, $\{110\}$, $\{111\}$, $\{210\}$, $\{211\}$ and $\{310\}$, the variations of ATGB energy with the tilt angle for W at 0 and 2400 K and $\beta$-Ti at 1300 K are shown in figures 5(a)–(f), respectively. It is obvious that the variation trends of GBCE curves are similar for the three samples in most cases.

Unlike STGBs, a tilt angle may correspond to several different ATGBs and the corresponding GBEs may span a broad spectrum, when the tilt axis is specified for ATGBs. This indicates that the GB plane has a significant influence on GBCE after the misorientation between two adjacent grains is determined. However, our calculations show that there is no direct relationship between GBE and the magnitude of boundary index even for the GBs with the same tilt axis and angle. For example, the GBE of $\Sigma3\{554\}/\{811\}$, $109.5^\circ/\{110\}$ is higher than the GBE of $\Sigma3\{111\}/\{511\}$, $109.5^\circ/\{110\}$, but lower than that of $\Sigma3\{110\}/\{411\}$, $109.5^\circ/\{110\}$. To further explore the relationships between GBCEs and GB planes, the parameter $\theta$, which is the angle between the misorientation axis and the GB plane, was defined. As shown in figure 1, the $\{111\}$ axis is the misorientation axis of both the $\Sigma3\{211\}$, $109.5^\circ/\{110\}$ STGB and $\Sigma3\{111\}/\{511\}$, $109.5^\circ/\{110\}$ ATGB, and the angle between $\{111\}$ axis and the GB plane is the parameter $\theta$ for the two TGBs, which are $0^\circ$ and $19.5^\circ$, respectively. With the variation of GB plane from parallel to the misorientation axis to perpendicular to the misorientation axis, the parameter $\theta$ increases from $0^\circ$ to $90^\circ$.

Figure 6 shows the variation of GBE with $\sin(\theta)$ for six sets of TGBs with the same lattice misorientation, including $\Sigma3\{60^\circ/\{111\}\}$, $\Sigma5\{36.9^\circ/\{100\}\}$, $\Sigma7\{38.2^\circ/\{111\}\}$, $\Sigma9\{38.9^\circ/\{110\}\}$, $\Sigma21\{44.4^\circ/\{211\}\}$ and $\Sigma49\{49.2^\circ/\{322\}\}$ TGBs. There are two special types of TGBs for every set: the one with the misorientation axis parallel to the GB plane ($\theta = 0^\circ/180^\circ$) and the other with the misorientation axis perpendicular to the GB plane ($\theta = 90^\circ$). For the former, the GB planes are different, but for the latter, the TGB plane is definite and the TGB is a twist grain boundary (TWGB). Different from the GBE curves shown in figures 3 and 5, the variation of the GBE curves in figure 6 can roughly be described with some simple functions of $\sin(\theta)$. For example, the relationships between GBEs of $\Sigma3$ GBs and $\sin(\theta)$ (shown in figure 6(a)) can be fitted and described with the following linear expressions:

$$\gamma_{W/0K} = 593 + 1829 \sin(\theta),$$

(2)

$$\gamma_{W/2400K} = 558 + 1900 \sin(\theta),$$

(3)

$$\gamma_{f-Ti/1300K} = 149 + 298 \sin(\theta),$$

(4)

where $\gamma_{W/0K}$, $\gamma_{W/2400K}$ and $\gamma_{f-Ti/1300K}$ represent the GBEs of W at 0 K, W at 2400 K, and $f$-Ti at 1300 K, respectively. In these expressions, the slopes of $\gamma_{W/0K}$ and $\gamma_{W/2400K}$ are similar, with the values of 1892 and 1900, respectively, while the slopes of $\gamma_{f-Ti/1300K}$ are much different. The approximate linear relationships between GBE and $\sin(\theta)$ can also be noted in $\Sigma3$, $\Sigma7$, $\Sigma21$ and $\Sigma49$ TGBs, as shown in figures 6(a), (c), (e) and (f), respectively. However, for $\Sigma9\{38.9^\circ/\{110\}\}$ TGBs, it is more appropriate to describe the relationships between GBE and $\sin(\theta)$ by parabolic functions, as shown in figure 6(d). The corresponding fitting parabolic functions are as follows:

$$\gamma_{W/0K} = 2655 - 1518(\sin(\theta) - 0.123)^2$$

(5)

$$\gamma_{W/2400K} = 2646 - 1337(\sin(\theta) - 0.1253)^2$$

(6)
According to the analysis above, the function types describing the relationships between TGB energies and $\sin(\theta)$ may be different for TGBs with different lattice misorientations. If the lattice misorientation is specified, the relationships between TGB energies and $\sin(\theta)$ can be described by functions of the same type for $W$ at 0 and 2400 K and $\beta$-Ti at 1300 K, but the coefficients in the three functions are different. For $W$ at 0 and 2400 K, the coefficients are close, but for $W$ at 2400 K and $\beta$-Ti at 1300 K, the coefficients are obviously different. Therefore, it is possible to roughly describe the relationships between GBE and TGB plane from viewpoint of geometric factor $\sin(\theta)$, but such description is only applicable for TGBs with the same lattice misorientation. Generally, the TGB energy increases as $\sin(\theta)$ increases from 0 to 1 when the lattice misorientation is specified. The TGB set with $\sin(\theta)$ of 0 is a special subset of TGBs with the same lattice misorientation, which generally has lower GBE. These special TGBs consist of STGBs, TWGBs and other ATGBs. Specifically, the STGBs have lower GBE in most cases, while the TWGBs generally have higher GBE. For the $\Sigma 3$ TGBs with $\sin(\theta)$ of 0, the STGB of $\Sigma 3\{211\}\{211\}$, $60^\circ/\langle 111 \rangle$ has the lowest GBE of 582, 560 and 190 mJ m$^{-2}$ for $W$ at 0 K, $W$ at 2400 K and $\beta$-Ti at 1300 K, respectively, while the TWGB of $\Sigma 3\{110\}\{110\}$, $60^\circ/\langle 111 \rangle$ has the highest GBE of 2071, 2134 and 361 mJ m$^{-2}$ for $W$ at 0 K, $W$ at 2400 K and $\beta$-Ti at 1300 K, respectively. Our investigation on the relationships between GBE and $\sin(\theta)$ is important to study the preferred GB planes for TGBs with the same lattice misorientation. For example, Wang et al [41] found that the $\Sigma 5$ GBs in pure iron has a strong preference for $\{310\}$ $\{310\}$ plane in experiments. Our calculations can give an explanation for such preference that the $\Sigma 5\{310\}\{310\}$ is a STGB with $\sin(\theta)$ of 0 and has the lowest GBE for all $\Sigma 5$ TGBs.

$\gamma_{\text{\beta-Ti/1300K}} = 701 - 537(\sin(\theta) - 0.1844)^2$ (7)

Figure 5. The ATGB energies of $W$ at 0 and 2400 K and $\beta$-Ti at 1300 K functioned with different tilt angles and different tilt axes of (a) $<100>$, (b) $<110>$, (c) $<111>$, (d) $<210>$, (e) $<211>$ and (f) $<310>$.
Accordingly, the proposition of the parameter $\theta$ is a significant attempt we made to reduce the five geometric parameters of the GB to a simple parameter that the relationships between GBE and $\sin(\theta)$ can be described by simple functions. The defined $\theta$, which is the angle between the misorientation axis and the GB plane, is actually closely related to the five geometric parameters (two parameters describing the GB plane and three parameters describing the lattice misorientation) of the GB. Thus, it can be regarded as the special parameter representing of the complex coupling effects of the five geometric parameters. In this work, the simple empirical functions of $\sin(\theta)$ are obtained from the numerical fitting method, which shows that the GBE can be estimated from the expressions of $\sin(\theta)$. However, the underlying mechanism of these empirical functions are still unknown and the exploration of the underlying mechanism still requires a lot of ongoing works.

### 4. Conclusions

In this study, the MS and MD methods were utilized to investigate the GBEs and microstructures of TGBs of W at 0 and 2400 K and $\beta$-Ti at 1300 K, as well as the relationships between TGB energies and geometric factors. In most cases, the variations of TGB energy with the tilt angle are similar for W at 0 and 2400 K and $\beta$-Ti at 1300 K, when the tilt axis is specified. The similarities result from the similar GB microstructures among the

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**Figure 6.** The TGB energies of W at 0 and 2400 K and $\beta$-Ti at 1300 K as a function of $\sin(\theta)$, where $\theta$ is the angle between the misorientation axis and the GB plane. Figures 6(a)–(f) correspond to the $\Sigma^3$, $\Sigma^5$, $\Sigma^7$, $\Sigma^9$, $\Sigma^{21}$ and $\Sigma^{49}$ TGBs, respectively. Figures 6(a) and (d) show the additional TGB energies of W at 1200 and 1800 K for $\Sigma^3$ and $\Sigma^9$ TGBs.
three cases. However, some deviations occur for the STGBs with \(<100>\) and \(<110>\) tilt axes. For the STGBs with \(<100>\) tilt axis, the GBE variation trends of \(\alpha\)-Ti at 1300K are opposite to that of W at 2400 K when the tilt angle increases from 46.4° to 47.9° or from 53.1° to 59.5°. The deviations are caused by the difference of the corresponding STGB microstructures between W at 2400K and \(\alpha\)-Ti at 1300K. For the STGBs with \(<110>\) tilt axis, the deviation of the GBE variation trends of \(\alpha\)-Ti at 1300K from that of W at 2400 K can also be observed, when the tilt angle ranges from 50° to 60°. This deviation stems from the special atomic rearrangements, which induces the formation of local HCP \(\alpha\)-like or hexagonal \(\omega\)-like structures at the STGB and the decreasing of GBE for \(\beta\)-Ti at 1300K. The special atomic rearrangements at the STGBs of \(\beta\)-Ti at 1300K result from the special lattice misorientations that the Burgers or Martensitic orientation relationship between GB \(\alpha\) and the two adjacent \(\beta\) grains or between GB \(\omega\) and the two adjacent \(\beta\) grains is able to maintain. The special properties of TGBs of \(\beta\)-Ti at the high temperature above \(T_{\text{trans}}\) provide a new perspective to study GB properties of other crystalline materials with various allotropes.

Furthermore, the geometric parameter \(\theta\), the angle between the misorientation axis and the GB plane, was defined to describe the relationships between TGB energies and GB planes. For the TGBs with the specified lattice misorientation, the correlation between GBE and \(\sin(\theta)\) can be described by some simple functions, such as linear and parabolic functions. Such correlations can well explain and predict the preferred GB plane for the TGBs with the same lattice misorientation. The geometric parameter \(\theta\) defined in this paper provides a new viewpoint to study the relationships between GBEs and geometric factors.

Acknowledgments

This research was funded by the SYNL Basic Frontier & Technological Innovation Research Project (No. L2019R10), the National Key R&D Program of China (No. 2016YFB0701302) and the CAS Frontier Science Research Project (No. QYZDJ-SSW-JSC015). We acknowledge the Special Program for Applied Research on Super Computation of the NSFC-Guangdong Joint Fund (the second phase). Some of the calculations in this study were done on Tianhe-II high performance computer system in the National Super-computer Centre in Guangzhou, China.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Author contributions

MD simulation, H H; writing—original draft preparation, H H; writing—review and editing, S M and S W; supervision, S W; project administration, S W; funding acquisition, S W All authors have read and agreed to the published version of the manuscript.

Declaration of competing interests

The authors declare no competing interests.

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