Loss of coherency of the alpha/beta interface boundary in titanium alloys during deformation

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The loss of coherency of interphase boundaries in two-phase titanium alloys during deformation was analyzed. The energy of the undeformed interphase boundary was first determined by means of the van der Merwe model for stepped interfaces. The subsequent loss of coherency was ascribed to the increase of interphase energy due to absorption of lattice dislocations and was quantified by a relation similar to the Read–Shockley equation for low-angle boundaries in single-phase alloys. It was found that interphase boundaries lose their coherency by a strain of approximately 0.5 at $T = 800°C$.

1. Introduction

In two-phase titanium alloys with a colony-alpha lamellar microstructure, the crystal lattices of the α- and β-phases satisfy the Burgers orientation relationship (OR) [1]. Accordingly, the following relationship is met when the α-phase (HCP) is formed during the decomposition of the high-temperature β-phase (BCC): $\{0001\}_\alpha \| \{110\}_\beta$; $\langle 11\bar{2}0\rangle_\alpha \| \langle 111\rangle_\beta$. The presence of the OR during phase transformations involving HCP and BCC phases in general [1,2] and between the α- and β-phases of titanium in particular [3,4] has been confirmed experimentally many times. This mutual orientation of the crystal lattices of the α and β phases provides the basis for the formation of semi-coherent interphase boundaries. In fact, direct observations via high-resolution transmission electron microscopy (TEM) have indicated the semi-coherent nature of α/β boundaries in a Ti–Cr β-titanium alloy (e.g. [5]).

In the most general case, a coherent interface is defined as a boundary between two phases in which the planes of one phase are parallel to and collinear with the

planes of the other phase without any gaps. Assuming that the interatomic spacing of the two phases differs only slightly, the mismatch may be accommodated solely by means of elastic deformation along portions of the boundary. If the length of the boundary is small enough (e.g. a matrix–particle interface), such a boundary may be considered as coherent.

In the case of a larger mismatch between the lattices of the two phases or longer interphase boundaries, the accumulated mismatch cannot be accommodated by elastic deformation alone. In such cases, two other mechanisms of accommodation have been proposed: (i) by two mutually perpendicular arrays of dislocations which lie in the plane of the boundary [6,7] or (ii) by structural ledges [8–10]. The boundary remains coherent in the spaces between the misfit dislocations or ledges. Therefore, if the lattice parameters of both phases are close to each other and coherent parts of the boundary are long enough, the boundary can be considered as semi-coherent. A decrease in the length of the coherent parts due to increased mismatch between the crystal lattices of the phases obviously leads to a decrease in the level of coherency and to an increase in the boundary energy. Hence, the magnitude of the interface boundary energy can be used to quantify the degree of coherency; i.e. higher energy corresponds to lower coherency.

As has been shown in a number of investigations (e.g. [11]), a dislocation can move/glide across each of the semi-coherent α/β interfaces within a colony of alpha lamellae. In such a case, the α/β colony behaves like a grain, at least at the beginning of deformation. However, during deformation, the coherency of interphase boundaries decreases (and simultaneously the energy increases) because of the interaction between boundaries and dislocations [11]. As a result, interphase boundaries become barriers for dislocations, and deformation tends to localize within each phase, thus inducing the formation of internal boundaries within the phases and thereby breaking down the initial lamellar microstructure. Consequently, the loss of coherency between the phases may be considered as a necessary condition for the onset of the transformation of the lamellar structure into a globular one (i.e. globularization). The effect of a decrease in the level of coherency on globularization during hot working of a two-phase titanium alloy was also discussed in [12]. Here, the authors suggested that the loss of coherency increases the rate of diffusion along the interphase boundaries resulting in an acceleration of the rate of globularization of the two phases.

The evolution of an initially semi-coherent interphase boundary and its associated energy during deformation is of great interest with respect to the accommodation of deformation and the effect of interface energy on the kinetics of dynamic or static spheroidization of a lamellar microstructure. However, this subject has not been investigated sufficiently.

The aim of this study was to establish the relationship between the energy and coherency of the interphase boundary during the deformation of a two-phase titanium alloy and to evaluate the level of deformation necessary for the elimination of coherency of the interphase boundary. Attention was focused on the behavior of the widely used titanium alloy Ti–6Al–4V at elevated temperatures (~800°C) at which deformation processing is usually conducted.

2. Energy of α/β boundaries in undeformed two-phase titanium alloys

As mentioned in Section 1, the simplest way to accommodate a mismatch across interphase boundaries consists of inserting in the more closely spaced lattice extra half-planes of atoms which terminate at the boundary. According to this idea, the lattice mismatch across a planar semi-coherent interphase boundary is accommodated by two mutually perpendicular arrays of dislocations which lie in the plane of the boundary [6]. Consequently, the energy of the interface boundary can be calculated as the sum of the elastic strain energies of the individual dislocations [6,7]. An increase in the mismatch leads to a reduced spacing between the dislocations and a corresponding increase in the energy per unit area.

In a different description, first proposed by Hall et al. [8], the lattice mismatch is accommodated by so-called "structural ledges". The structural-ledge model replaces the planar interface (and the atomic habit plane) by a series of stepped planes in both phases which provide the best fit. At the edge of the terraces, at which the degree of atomic matching across the interface begins to deteriorate, the overall interface steps up to the next parallel plane where the fit is better. This model was subsequently developed in a number of other efforts [3,5,9–11,13]. Extensive investigations, including high-resolution TEM analysis [11,13], have shown that the structural-ledge model describes α/β interfaces in two-phase titanium alloys more reliably than the planar-dislocation model. The energy of the stepped (ledged) interface boundary also depends on the difference in the lattice parameters of both phases. To assess the interface energy of such boundaries in a quantitative fashion, the crystallography/geometry of α/β boundaries must be introduced.

The crystallography of the alpha and beta phases in titanium alloys is well established [3,5,11,13,14]. Based on the data in [5], the relationship between the planes and directions in the alpha and beta phases is as follows (Figure 1):

(a) According to the Burgers OR, the side face of the α-plate is formed by $(0001)_\alpha||(110)_\beta$ planes and the directions in the α- and β-lattices are related as: $[\bar{1}100]_\alpha||[\bar{1}\,1\,2]_\beta$ and $[11\bar{2}0]_\alpha||[\bar{1}\,1\,\bar{1}]_\beta$.

(b) The broad face of the α-plate has an irrational habit plane close to $(11\,\overline{15}\,4\,0)_\alpha||(11\,\overline{11}\,1\,3)_\beta$. This habit plane results from the uniform arrangement of structural ledges which step down along the $\sim[335]_\beta$ direction with $(\bar{1}100)_\alpha||(\bar{1}\,1\,2)_\beta$ terraces [5,11,13].

(c) The growth face of the α-plate is approximately $(19\,7\,\overline{26}\,0)_\alpha||(\bar{3}3\bar{5})_\beta$.

A method to quantify the energy of stepped interfaces was proposed by van der Merwe et al. [10,15–17]. This approach is briefly summarized and applied here for the specific case of α/β titanium interfaces; a more-detailed description can be found elsewhere [15].

Figure 2 shows the crystallography of the ledges on the broad face, viewed along $[1\,1\,0]_\beta//[0\,0\,0\,1]_\alpha$, in terms of the unit cells of the α and β phases in the Burgers orientation. A Cartesian coordinate system with the z-axis normal to the interface and the x- and y-axes along the rectangular interfacial axes was used. Ledges facing the x-direction are designated as x-ledges. From geometrical considerations, a

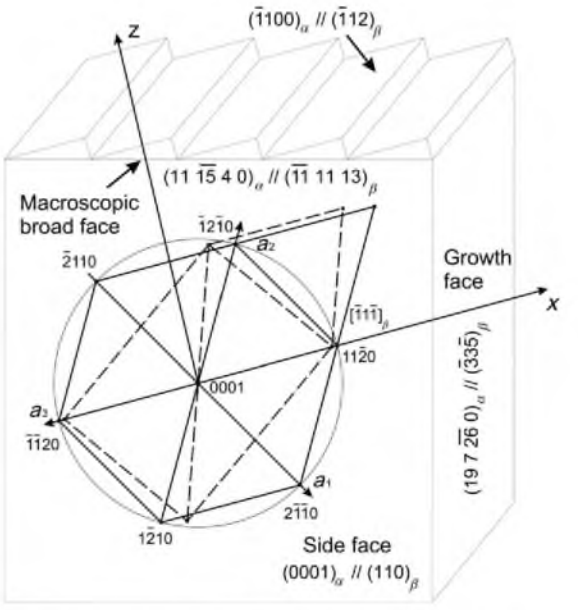

Figure 1. Crystallography of the α- and β-phases in titanium alloys.

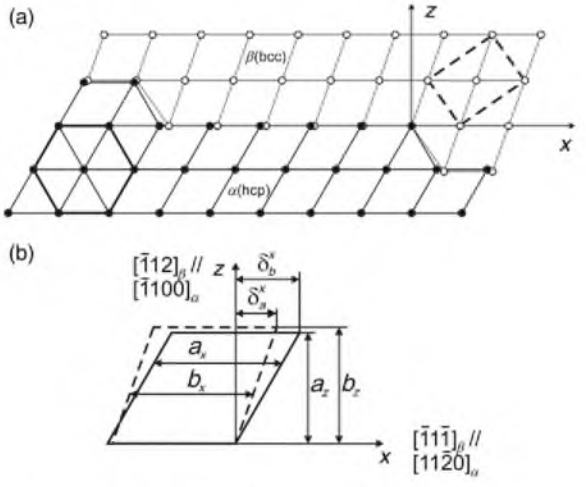

Figure 2. Schematic illustrations of: (a) Accommodation of misfit at a stepped interface between β (BCC) and α (HCP) crystals by a sequence of structural ledges (viewed along $[1\,1\,0]_\beta//[0\,0\,0\,1]_\alpha$) and (b) the β (BCC) and α (HCP) unit cells having a Burgers orientation relation: $\{0001\}_\alpha||\{110\}_\beta$; $\langle 11\bar{2}0\rangle_\alpha||\langle 111\rangle_\beta$.

number of parameters required for further calculations are introduced (Table 1, Figure 2b):

$$\text{Atomic-pattern advance in the } x\text{-direction: } \delta_X = \delta_x^a - \delta_x^b. \tag{1}$$

Table 1. Input data for calculating α/β interface energy.

x-direction	y-direction	z-direction
a_x (nm) = 0.295	a_y (nm) = 0.468	a_z (nm) = 0.256
b_x (nm) = 0.284	b_y (nm) = 0.464	b_z (nm) = 0.268
δ_x^a (nm) = 0.147		
δ_x^b (nm) = 0.095		
δ_x (nm) = 0.052		
c_x (nm) = 0.289	c_y (nm) = 0.466	c_z (nm) = 0.262
$f_x = 0.038$	$f_y = 0.0078$	$f_z = 0.048$
p_x (nm) = 7.69		
l_x (nm) = 1.39		

Reference lattice parameter in the i-direction: $$c_i = \frac{2b_i a_i}{(b_i + a_i)}, \quad (i = x, y, z). \tag{2}$$

Period of vernier in the x-direction: $$p_x = \frac{a_x}{|b_x - a_x|}. \tag{3}$$

Interfacial misfit: $$f_i = \frac{c_i}{p_i}, \quad (i = x, y, z). \tag{4}$$

Length of terrace (step periodicity): $$l_x - \frac{c_x}{f_x\left(\frac{\delta_x^a}{a_x} - \frac{\delta_x^b}{b_x}\right)}. \tag{5}$$

It is assumed that only x-ledges are present in the interface while misfit along the y-direction is compensated by misfit dislocations [3]. The overall energy of the interface E_Σ is then

$$E_\Sigma = E_x^S + E_y^P. \tag{6}$$

Here, E_x^S denotes the energy of a stepped interphase boundary and E_x^p is the energy of the planar misfit attributed to a sequence of conventional misfit dislocations in the y-direction.

According to [15], the energy of a stepped interphase boundary E_x^S is the sum of (i) the energy E_x^T of interaction at the terrace–patch interface, allowing for elastic relaxation; (ii) the energy E_x^Z of tilt misfit dislocations, compensating for the difference in "height" of two opposing steps ($b_z - a_z$, Figure 2); and (iii) the line energy Γ of the misfitted ledge-ledge interface, *viz.*,

$$E_x^S = E_x^T + E_x^Z + \Gamma. \tag{7}$$

The first term in Equation (7), the energy of interaction at the terrace–patch interface, can be calculated from

$$E_x^T = \frac{\mu U_o^2}{\pi^2 d} \sum_{n=1}^{\infty} \frac{1}{n(n + n_0)}. \tag{8}$$

In Equation (8), μ denotes the temperature-dependent (average) shear modulus at the interface, $\mu = (\mu_\alpha + \mu_\beta)/2$, in which μ_α and μ_β are the shear moduli of the α and β phases, respectively. For Ti–6Al–4V at temperature 800°C, $\mu_\alpha \approx 2.9 \times 10^{10}$ Pa and $\mu_\beta \approx 2.3 \times 10^{10}$ Pa. Thus, $\mu = 2.6 \times 10^{10}$ Pa. The symbol U_0 represents the maximum relative tangential displacement of corresponding atoms on either side of the interface, $U_0 = \frac{1}{2}\,\delta_x$; and d is the equilibrium separation of atomic planes across the interface, $d \approx c_z$. The term n_0 in Equation (8) is defined by the following relations:

$$n_0 = \frac{\mu l x}{2\pi d \lambda} \tag{9}$$

$$\lambda = \frac{1 - \nu_a}{\mu_a} + \frac{1 - \nu_b}{\mu_b} \tag{10}$$

in which ν_α and ν_β are the Poisson's ratios of the α and β phases, respectively. Here, $\nu_\alpha \sim \nu_\beta = 0.3$.

The energy of tilt misfit dislocations in the surfaces normal to the x-direction can be calculated as

$$E_x^Z = \frac{\mu c_z^z}{2\pi^2(1 - 2\nu)d} F(\bar{\beta}_x) \tag{11}$$

in which

$$F(\bar{\beta}_x) = 1 + \bar{\beta}_x - (1 + \bar{\beta}_x^2)^{\frac{1}{2}} - \bar{\beta}_x \ln\left[2\bar{\beta}_x(1 + \bar{\beta}_x^2)^{\frac{1}{2}} - 2\bar{\beta}_x^2\right] \tag{12}$$

$$\bar{\beta}_x = \frac{\pi d(1 - 2\nu)\lambda}{3\bar{p}_x \mu}, \quad d \approx c_x. \tag{13}$$

Tilt misfit dislocation spacing,

$$\bar{p}_x = l_x\left(\frac{1 - 0.5 f_z}{f_z}\right) + \delta_x^a \frac{(1 + 0.5 f_x)}{f_x}. \tag{14}$$

The line energy of the misfitted ledge–ledge interface is the following:

$$\Gamma = \frac{E_y^P(\beta_y) c_x}{l_x}. \tag{15}$$

The energy of a planar misfit in the y-direction is calculated as

$$E_y^P = \frac{\mu c_y^z}{4\pi d} F(\beta_y). \tag{16}$$

Here, $F(\bar{\beta}_y)$ and $\bar{\beta}_y$ are calculated using expressions analogous to Equations (12) and (13), i.e.

$$F(\bar{\beta}_y) = 1 + \bar{\beta}_y - \left(1 + \bar{\beta}_y^2\right)^{\frac{1}{2}} - \bar{\beta}_y \ln\left[2\bar{\beta}_y\left(1 + \bar{\beta}_y^2\right)^{\frac{1}{2}} - 2\bar{\beta}_y^2\right] \tag{17}$$

$$\bar{\beta}_y = \frac{\pi d(1 - 2\nu)\lambda}{3\bar{p}_y \mu}, \quad d \approx c_y. \tag{18}$$

Using the data in Table 1 and Equations (1)–(19), the energy of the stepped interface E_x^S was found to be $0.012\,J/m^2$; the energy of planar misfit in the y-direction $E_x^p = 0.039\,J/m^2$. The overall energy of the interface is therefore estimated to be $E_\Sigma = E_x^S + E_y^p = 0.012 + 0.039 = 0.051\,J/m^2$. It is of interest to compare this value of E_Σ with the interface energy for which the misfit in both directions (x and y) is compensated by mutually perpendicular arrays of dislocations, i.e.

$$E^P = E_x^P + E_y^P. \tag{19}$$

The value of E_x^P in this case can be calculated using expressions similar to Equations (17)–(19) with the appropriate subscripts. The planar interface energy E^P is then found to be equal to $0.07 + 0.039 = 0.11\,J/m^2$, or approximately twice that obtained for the stepped interface.

It should be noted that the energy of a planar interface evaluated in accordance with the model of Liebmann [7] (see also [18]) also yields values of interface energy of the same magnitude as the above results. In this other model, the lattice mismatch is completely accommodated by mutually perpendicular arrays of dislocations which lie in the plane of the boundary. Consequently, the energy of the interface boundary E_L^P is the sum of the elastic strain energies of the separate dislocations:

$$E_L^P = \frac{\mu}{4\pi(1-\nu)}\left\{|a_x - b_x| \ln\frac{a_x}{|a_x - b_x|} + |a_y - b_y| \ln\frac{a_y}{|a_y - b_y|}\right\} \tag{20}$$

in which μ is the shear modulus, ν is the Poisson's ratio, a_x and b_x are the interatomic distances in the two phases along the x-direction; and a_y and b_y are the respective interatomic spacings in the y-direction (Figures 1 and 2). To avoid physically implausible (negative) values of energy, the numerator of the natural-logarithm terms should be taken as the greater of a_x or b_x (first term) and the greater of a_y or b_y (second term). The value of E_L^P estimated from Equation (20) for an interface consisting of the planes $(\bar{1}100)_\alpha || (\bar{1}12)_\beta$ is $0.16\,J/m^2$. This value is approximately 70% higher than that obtained via the van der Merwe model. Nevertheless, such a difference may be considered as acceptable in view of the approximate nature of the models themselves.

The nature of the α/β interface along the three different sides of an α-plate is different from a crystallography standpoint. Application of the Liebmann model for the other faces of an α lamella in the β matrix yields a predicted energy of $0.22\,J/m^2$ for the $(0\,0\,0\,1)_\alpha \parallel (1\,1\,0)_\beta$ planes and $4.8\,J/m^2$ for the growth face. The high value of the energy for the growth face may be associated with migration of the boundary in the normal direction. Specifically, for fully and partially coherent boundaries, diffusional growth is not possible when the crystal structures of the matrix and precipitate differ to a significant degree. Such migration would require that substitutional atoms be temporarily placed in interstitial sites as the matrix plane bounding the fully coherent areas of the interface is converted atom by atom to another structure [3]. Hence, either the boundaries must be incoherent (as in the case of the growth face), or precipitate growth must occur via a ledge mechanism. As per the ledge-mechanism model, the terraces of the ledges are partially or fully coherent (e.g. $(\bar{1}100)_\alpha || (\bar{1}12)_\beta$), and the risers have a disordered structure [3].

3. Change of the interphase-boundary energy during deformation

To quantify the evolution of the α/β interface energy due to deformation, attention is focused on the broad face, namely the $(\bar{1}100)_\alpha||(\bar{1}12)_\beta$ interface. This boundary has the lowest energy and largest area and, consequently, its influence on the properties of two-phase titanium alloys is the most pronounced. In addition, because of its large area, this boundary is most often intersected by the surface of foils used in TEM investigations.

It may be assumed that changes in the nature of the α/β interface during deformation are a result of the formation of dislocation arrays in the plane of the boundary that result in the gradual loss of coherency. Each dislocation entering the boundary brings an increment of energy, thus increasing the total energy of the boundary. The increase in the energy for a small strain can be estimated in a manner analogous to that used for low-angle boundaries in single-phase materials. For such materials, the grain-boundary energy as a function of misorientation was first calculated by Read and Shockley [19] and van der Merwe [6], and can be expressed as follows [20,21]:

$$E_d = \frac{\mu b \theta}{4\pi(1-\nu)}\left(\ln\frac{\chi}{2\pi\theta} + 1\right) \tag{21}$$

in which b is the Burgers vector, θ is the misorientation of the dislocation boundary (in radians), χ is the dislocation-core parameter, i.e. $\chi = b/r_0$ where r_0 is the size of the dislocation core. The magnitude of the core parameter usually lies in the range of 1–3 [16,20,21]. In this study, this parameter was assumed to be equal to 1.5.

It has also been found that the misorientation of a dislocation boundary is a function of strain ε and can be described through the linear relationship [22]:

$$\theta = K\varepsilon \tag{22}$$

in which K denotes a constant dependent on the specific processing conditions that quantifies the dislocation boundary misorientation rate during deformation. By combining Equations (22) and (23), E_d can be expressed as

$$E_d = \frac{\mu b K \varepsilon}{4\pi(1-\nu)}\left(\ln\frac{\chi}{2\pi k\varepsilon} + 1\right). \tag{23}$$

The coefficient K can vary over a wide interval. For the cold deformation of copper [23] and stainless steel [24], the value of K has been found to be approximately 0.1. An increase in deformation temperature in the case of hot rolling of stainless steel results in an increase in K to 0.21 [24]. However, the presence of interphase boundaries in two-phase alloys considerably decreases the free path for dislocations and increases the rate of formation of dislocation walls. Thus, K is expected to be higher than the value typically found for single-phase metals. To quantify the rate of departure from the OR for the α/β titanium alloy Ti–6Al–4V in this study, therefore, a specimen measuring 8 mm diameter and 12 mm height was compressed at 800°C to a height reduction of 25%, 50%, or 75%. Thin samples were cut from the center of each specimen parallel to the compression axis for TEM investigation. To determine the angles between the normals to the (0 0 0 1) plane in the HCP lattice of the α-phase and the (1 1 0) plane in the BCC lattice of the β-phase, a single reflection

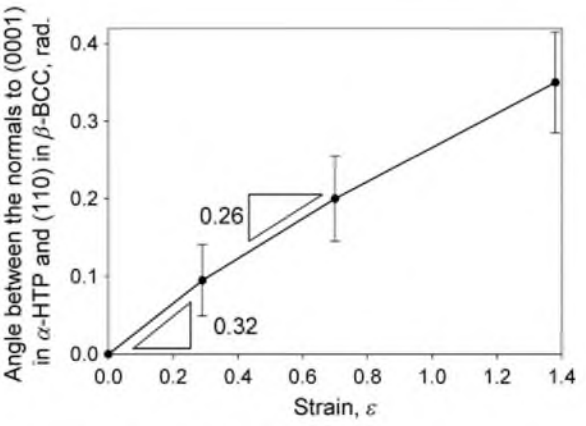

Figure 3. Angle between the normals to the (0 0 0 1) plane in the HCP lattice of the α-phase and the (1 1 0) plane in the BCC lattice of the β-phase as a function of strain.

method was used [25,26]. This method is based on the direct determination of the laboratory coordinates of the normal relative to the reflecting plane. The procedure consists of obtaining at least two (or preferably three) diffraction spots (reflections) of different planes at different goniometer angles. The best reflecting positions correspond to a maximum brightness in a dark-field image. Then, an orientation matrix which describes the orientation of the crystal can be calculated. Using the method of single reflections, the relative orientation of the phases as a function of strain was determined (Figure 3). Taking the angle θ between the (0 0 0 1) plane in the HCP lattice of the α-phase and the (1 1 0) plane in the BCC lattice of the β-phase in the initial condition to be equal to zero, the value of K was estimated from the slope of a plot of $\theta(\varepsilon)$. For the case of Ti–6Al–4V compressed at 800°C to a reduction between 25% and 50%, K was found to be ~0.3 on average, and in the range of 0.2–0.35 when the possible uncertainty associated with the fitting of the slope within the experimental scatter is taken into account.

4. Total boundary energy

The *total* interface energy as a function of strain is the sum of the Equations (6) and (23), i.e.

$$E = E_{\Sigma} + E_d. \tag{24}$$

Taking K equal to 0.3 in the expression for E_d, the dependence of overall boundary energy on strain was obtained for the $(\bar{1}100)_{\alpha}||(\bar{1}12)_{\beta}$ interface (Figure 4; the cross-hatched area corresponds to the variation of the coefficient K from 0.2 to 0.35). Figure 4 reveals that the boundary energy exhibits an asymptotic behavior, as prescribed by the Read–Shockley equation, reaching a maximum of ~0.26 J/m^2 at a strain of ~0.8, which corresponds to a height reduction of ~55%. At this strain,

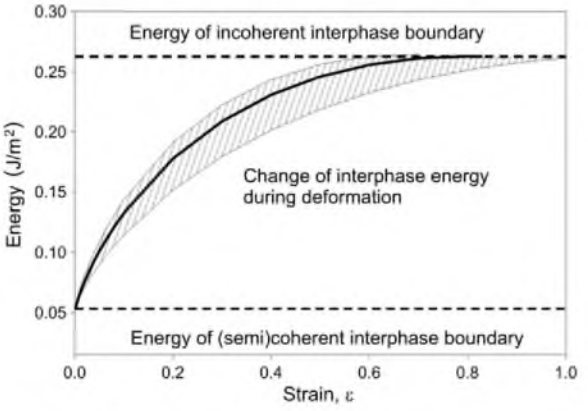

Figure 4. Boundary energy for the $(\bar{1}100)_{\alpha}||(\bar{1}12)_{\beta}$ interface as a function of strain for Ti–6Al–4V with a lamellar microstructure. The cross-hatched area corresponds to a variation of the coefficient K from 0.2 to 0.35 corresponding to the uncertainty in the determination of the slope in Figure 3.

the mutual rotation of the phases reaches approximately 0.25 radians (~15°) with respect to the initial OR (Figure 3). This corresponds to the limit of low-angle boundaries described by the Read–Shockley expression (i.e. $\theta < 15°$).

The present results are in good agreement with previous work in which the acceleration of dynamic spheroidization of Ti–6Al–4V during compression at 600°C and 800°C in the interval of 25–50% height reduction ($\varepsilon \approx 0.3$–0.7) was established by TEM and EBSD analysis [4,27]. This phenomenon was ascribed to the loss of coherency of the α/β boundaries. Indeed, as semi-coherent interfaces gradually become fully incoherent, the boundaries become essentially impenetrable obstacles for dislocations, and flow localizes within each phase, thereby intensifying the spheroidization process.

The boundary energy corresponding to an incoherent interface after rather large deformation is markedly higher than that of the semi-coherent boundary prior to deformation. Specifically, the results in Figure 4 suggest that deformation increases the boundary energy by a factor of 5. Moreover, the increment above the initial level of the energy due to the absorption of lattice dislocations is a factor of 4. Also, the present results show that dislocations increase the energy and reduce the coherency of the boundary relatively quickly with as a function of strain. The absorption of additional dislocations by the boundaries may lead to a further increase of energy, but not to any further loss of coherency, because the boundaries are already incoherent. The evolution of boundary energy at such large strains, however, cannot be described in terms of the Read–Shockley equation.

The present estimate for the interface energy (~0.26 J/m^2) is in good agreement with an interface energy of ~0.4 J/m^2 which was deduced to be appropriate in describing the kinetics of static spheroidization and static coarsening of α/β titanium alloys during thermomechanical processing at both hot and warm working temperatures [28–30].

It is worth noting that the analysis is applicable to any alloy which forms a lamellar microstructure during cooling provided appropriate input data are available for the model.

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