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A MODEL FOR EXPERIMENTALLY-OBSERVED HIGH-STRAIN-RATE DYNAMIC STRAIN AGING IN TITANIUM

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Abstract—Recent high-strain-rate experimental results have shown an anomalous response by commercially pure titanium at relatively high temperatures: for a fixed high strain rate and a suitable strain, the flow stress which is a monotonically decreasing function of the temperature, suddenly begins to increase with increasing temperature, and then begins to decrease, displaying a dynamic strain-aging behavior. This phenomenon may be caused by the interaction between moving dislocations and mobile point defects in the dislocation core area. Based on this supposition, a model is developed which, both qualitatively and quantitatively, describes the experimentally observed results. This model assumes that the anomalous response is, in fact, dynamic strain aging caused by the drag of the core atmosphere, the evolution of the dislocation structure, and the associated interaction processes. The model combines the concepts of athermal long-range and thermally activated, short-range barriers, with the model of a “trough” for the thermally activated breakaway of dislocations from the core atmosphere. The evolution of the core atmosphere concentration is included in the model, based on the strong interaction force between dislocations and point defects in the core area. The final product is a unified model which seems to accurately predict the response of commercially pure titanium, over a broad range of strain rates and temperatures. © 2000 Acta Metallurgica Inc. Published by Elsevier Science Ltd. All rights reserved.

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1. INTRODUCTION

The phenomena related to the interaction between moving dislocations and mobile point defects include dynamic strain aging [3], abnormal strain-amplitude-dependent internal friction [4] and high-temperature creep [5]. There are two types of interaction between dislocations and point defects, depending on their relative positions. One is when the point defects are distributed outside the dislocation core area, in which case the solute distribution is called a Cottrell, Snoek or Suzuki atmosphere, and the other is when the point defects are distributed in the dislocation core area, forming a *core atmosphere*. Both types of point defect distributions lead to interaction between dislocations and point defects, but each through a different mechanism.

When the point defects are distributed outside the core area, their mobility is limited by volume diffusion in the crystal lattice. For the core atmosphere (i.e. when point defects are within the dislocation core), the mobility of the point defects is limited by the pipe diffusion along the dislocation core, or the directional diffusion under the strong interaction force between the dislocation and point defects when the dislocation is in motion. In the field of internal friction study, both of the above microscopic processes are manifested macroscopically through the abnormal strain-amplitude-dependent internal friction peaks.

The dynamic strain-aging effect due to the drag of the point defect atmosphere by volume diffusion, has been (and continues to be) studied extensively in the literature [3]. Except for a few cases [6–8], the dynamic strain-aging effect caused by core atmosphere drag has not been fully explored. Recently, the plastic deformation properties of commercially pure titanium have been investigated experimentally [1] over the temperature range of 77–1000 K and strain rate range of 10^{-3} – 10^4 /s. The experimental results [1] show that:

1. at a fixed strain rate and a suitable strain, and

[†] I report with sadness the sudden death of my coauthor, Professor Jingyi Cheng at the young age of 37, on 14 February 2000, Hefei, China. Sia Nemat-Nasser.

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with a monotonically increasing temperature, the monotonically decreasing flow stress may suddenly begin to increase at a critical temperature and, after attaining a peak value, may begin to decrease;

2. the critical temperature for the start of the sudden increase in the flow stress, shifts to higher values as the strain rate is increased; and
3. a critical strain level is needed for the occurrence of this phenomenon. Hence, depending on the temperature and strain rate, the flow stress may display three stages of deformation regimes, generally observed at low strain rates, but now at high strain rates and high temperatures [1].

The experimental results strongly suggest a relation to the dynamic strain-aging effect, caused by the interaction between moving dislocations and mobile point defects, the solute atoms. The analysis of solute atoms diffusing to and with dislocations leads to the suggestion that the effects may be caused by the drag due to the dislocation core atmosphere, because the estimated activation energy for the solute diffusion rules out the possibility of drag due to the solute atmosphere outside the dislocation core area [1].

In this paper, a detailed explanation of the mechanisms responsible for the observed anomalous behavior of commercially pure titanium is presented, using a new physically based model of interaction between moving dislocations and mobile point defects. The mechanism of dynamic strain aging at high strain rates is examined in detail. It is concluded that the drag on the dislocations due to the point defect atmosphere within the core of dislocations, the evolution of dislocation structure and the corresponding interactions are the underlying key mechanisms. It is therefore surmised in this paper that the experimentally observed phenomenon is indeed the dynamic strain aging, produced by the drag force acting on mobile dislocations due to the point defects residing within their core area, i.e. the core atmosphere.

To establish an appropriate constitutive model for dynamic strain aging caused by the drag due to the dislocation core atmosphere, the idea of a "trough model" [2] for the thermally activated breakaway of dislocations from the core atmosphere is integrated with concepts of short- and long-range barriers to the motion of dislocations, arriving at a unified model which seems to have good predictive capabilities over a broad range of strain rates and temperatures.

While the proposed model is based on the physics of the processes which occur at the atomic and dislocation scale, lending physical meaning to the involved constitutive parameters, the formulation is macroscopic and phenomenological, minimizing the

required number of independent parameters. In view of the many remaining uncertainties in the involved microscopic events, this appears to be an effective and useful approach.

2. CONSTITUTIVE MODEL FOR MECHANICAL BEHAVIOR

2.1. Rate equation for plastic deformation

Plastic deformation of most crystalline materials is due to the motion and multiplication of dislocations. The effective plastic strain rate, $\dot{\gamma}$, is usually approximated by Orowan's equation,

$$\dot{\gamma} = \beta b \rho_m \bar{v}, \quad (1)$$

where β is the orientation factor, b is the magnitude of the Burgers vector, ρ_m is the density of the mobile dislocations, and \bar{v} is the average velocity of the mobile dislocations.

For thermally activated dislocation motion, the average velocity of moving dislocations is modeled by an Arrhenius type of equation [9],

$$\bar{v} = l \nu_0 \exp\left(-\frac{\Delta G}{kT}\right), \quad (2)$$

where l is the average distance the dislocations travel after a successful activation event, ν_0 is the attempt frequency of the dislocation segment, ΔG is the activation energy, k is the Boltzmann constant, and T is the absolute temperature.

Therefore, the rate of plastic deformation can be written as

$$\dot{\gamma} = \dot{\gamma}_0 \exp\left(-\frac{\Delta G}{kT}\right), \quad (3)$$

where the pre-exponential factor $\dot{\gamma}_0 = \beta b \rho_m l \nu_0$ is generally considered a constant, the physical reason for this being that a decrease in the dislocation free path is partially compensated by an increase in the mobile dislocation density. In addition, the mathematical structure of (3) is such that, the variation of the pre-exponential factor does not affect the function ΔG in a substantial way.

To evaluate the activation energy, a detailed model for the interaction between dislocations and local obstacles opposing the motion of dislocations is needed. For solution-hardened materials, the main local thermal barriers to the dislocation motion are forest dislocations and solute atoms. It is usually assumed that both the forest dislocations and the solutes act as fixed discrete obstacles. Mobile dislocations overcome them individually under the assistance of thermal activation. This fixed-discrete-obstacle model has dominated the interpretation of solution hardening over the past years. As pointed out by Kocks [2], the fixed-discrete-obstacle model is untenable for many crucial experimental reasons. Instead, Kocks favors a

trough model in which the effect of the solutes is postulated to be equivalent to a continuous locking of the dislocations along their entire lengths, during every waiting time. The trough model was invented to describe the unlocking of dislocations from segregated solute atmospheres (in particular, in Fe-C) [10], and has been used in a description of internal friction [11, 12]. Investigating the properties of this model, Kocks [2] concludes that the model appears to satisfy all the requirements of a viable theory. He further points out that the model continues to apply, as the solute mobility is increased with increasing temperature.

2.1.1. Trough model. During the time a dislocation is held up at forest dislocations, it interacts with solute atoms to temporarily form a low energy configuration. The dislocation breaks away from this low energy valley through a thermally activated nucleation of a “bulge”. Figure 1 shows the pertinent configuration for thermally activated nucleation of a “bulge” from a “trough”. While the solutes are shown individually, they are treated as if they were smeared out along the dislocation, giving it a lower line energy: one may say that the solutes make a trough for the dislocation. To move on, the dislocation has to leave the bound state and reacquire its high “free” line energy. It does so by nucleating a bulge. In this paper, the length of the “bulge” is assumed to equal the length of the dislocation segment. The shape of the bulge is determined by the applied stress and the equilibrium between the two end line tensions.

According to Kocks *et al.* [9], the activation energy, ΔG , for a “bulge” to nucleate can be generally expressed as

$$\Delta G = F_0 \left[1 - \left(\frac{\tau^*}{\hat{\tau}} \right)^p \right]^q, \tag{4}$$

where F_0 is the *total* free energy necessary to overcome the obstacle without the aid of external work, the effective stress $\tau^* = \tau - \tau_a$ is the thermal part of the resistance to the dislocation motion, τ is the applied stress, τ_a is the athermal part of the resistance to the dislocation motion, $\hat{\tau}$ is the maximum glide resistance to the dislocation motion at 0 K, usually being called the mechanical threshold stress, and $0 < p \leq 1$ and $1 \leq q \leq 2$ are parameters representing the profile of the obstacle.

The physical parameters F_0 and $\hat{\tau}$ are assumed to relate to the properties of dislocations and obstacles as follows

$$F_0 \propto \sqrt{F_D F_B} w \tag{5}$$

and

$$\hat{\tau} \propto \frac{F_0}{b l_d w}, \tag{6}$$

where F_D is the free energy per unit length of the dislocation without the effect of solutes, F_B is the binding free energy per unit length, w is the effective width of the trough, and $l_d \approx l$ is the length of the dislocation segment. The binding free energy, F_B , is proportional to the interaction strength of each solute atom, F_{B0} , times the concentration of solutes along the dislocation line, C ,

$$F_B \propto F_{B0} C. \tag{7}$$

Therefore, the solute-concentration dependence of the thermal activation energy and the mechanical threshold stress can be expressed as follows

$$F_0 = F_0' \sqrt{\frac{C}{C_0}} \tag{8}$$

and

- : Solute Atoms
- : Forest Dislocations
- : Initial Position of the Dislocation Line
- : Activated Position of the Dislocation Line

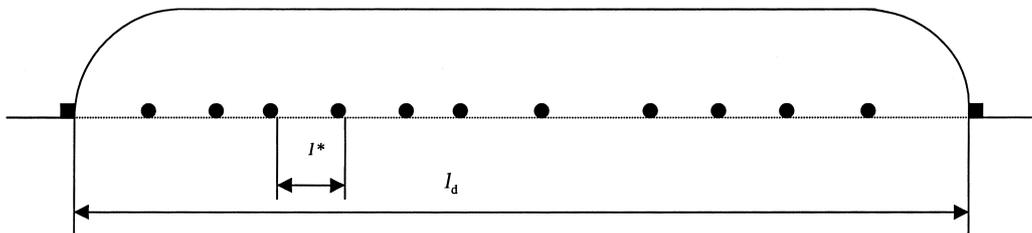


Fig. 1. Thermally activated nucleation of a “bulge” from a “trough”.

$$\hat{\tau} = \tau_0 \sqrt{\frac{C}{C_0}} \left(\frac{l_0}{l_d} \right), \quad (9)$$

respectively. Here F'_0 is the activation energy at a solute concentration of C_0 , and $\tau_0 = (F'_0/bl_0w)$, is a constant, with l_0 and l_d being the initial and current average dislocation spacings, i.e. $(l_d/l_0) = (\rho_0/\rho)^{1/2}$, where ρ_0 and ρ are the initial and current dislocation densities.

The essence of bulge nucleation is that the length of the dislocation "bulge" is not related to the spacing of individual solute atoms: the bulge is a breakaway from a trough. The solutes behave as if they were smeared out along the dislocation, and only their interaction energy per unit length matters. This energy is proportional to the interaction strength of each solute atom times the concentration along the dislocation line.

To complete the description of the plastic behavior of the material, the evolution of the structural parameters, such as the dislocation segment length l_d , the athermal resistance to the dislocation motion, τ_a , and the concentration of solutes along the dislocation line, C , must be quantified.

2.2. Variation of microstructure

The variation of the dislocation microstructure and its relation to the mobile point defects play key roles in the mechanical behavior of this commercially pure titanium. With continued plastic deformation, a large number of dislocations are produced, resulting in an increase in the strength of the interaction between dislocations. Therefore, the required force to move a dislocation also increases, leading to a workhardening effect.

Most materials eventually lose their ability to further workharden, as they reach a saturated steady-state deformation because of dynamic recovery. The microstructure of the saturated state depends on the temperature and strain rate. Experimental evidence shows that the dislocation density is higher, or the average dislocation spacing is smaller, for samples of the same material that have been deformed at lower temperatures or at higher strain rates. The macroscopic behavior of a material is the representation of the evolution of the microstructure towards its saturated state. When the evolution of the microstructure towards saturation is rapid, then the workhardening rate is high. Usually the saturated state is difficult to approach at low temperatures. In fact, the saturated states are seldom reached at low temperatures, and the material workhardens continuously till failure.

† Note that, while $l_d/l_0 = (\rho_0/\rho)^{1/2}$ can be a state variable, the plastic strain, γ , cannot; here, ρ_0 and ρ are the initial and current dislocation densities. Hence, (12) is an empirical relation without a thermodynamic basis.

At high temperatures, the saturated state is relatively easy to approach. During the high-temperature deformation process, the flow stress essentially reaches its saturation value after a small plastic strain.

The presence of mobile solute atoms affects the deformation response of the material. To develop a general model, the variation of the microstructure must be quantified. In the present case, the essential microstructural parameters to be considered are the average length of the dislocation segments, the athermal resistance to the dislocation motion, and the average concentration of solutes along the dislocation core.

2.2.1. Variation of the average length of dislocation segments. The variation of the average length of dislocation segments relates to the workhardening of the material. Nemat-Nasser and Li [13] have proposed a simple empirical model to estimate this average length. Assuming that the average dislocation spacing is a decreasing function of the accumulated plastic strain and an increasing function of the temperature, the variation of the average length of the dislocation segments is expressed as

$$l_d = \frac{l_0}{f(\gamma, T)}, \quad (10)$$

with the following constraining conditions for the dimensionless function f

$$\begin{aligned} f(\gamma, T) &> 0, \quad f(0, T_0) = 1 \\ \frac{\partial f(\gamma, T)}{\partial \gamma} &\geq 0, \quad \frac{\partial f(\gamma, T)}{\partial T} \leq 0, \end{aligned} \quad (11)$$

where l_0 is the initial average dislocation spacing, γ is the plastic strain, and T_0 is the initial temperature.† As an example, the following relations are used in [13] for application to OFHC copper

$$\begin{aligned} l_d &= \frac{l_0}{1 + a(T)\gamma^{n_0}} \\ a(T) &= a_0 \left[1 - \left(\frac{T}{T_m} \right)^2 \right]. \end{aligned} \quad (12)$$

Here, a_0 and n_0 are viewed as adjustable constitutive parameters, with n_0 between 0 and 1, and T_m is the melting temperature.

In this paper, equation (12) is used to describe the evolution of the average length of the dislocation segments.

2.2.2. Athermal resistance. The athermal resistance to the dislocation motion represents the long-range effect of all other dislocations, grain boundaries and defects. It is expressed by the following empirical relation

$$\tau_a = g(\gamma, d_G, \dots)\tau_a^0, \quad (13)$$

where γ is the plastic strain, d_G is the average grain size, τ_a^0 is a constant with the dimension of stress, and g is a dimensionless function of the indicated arguments. In this paper, it is assumed that,

$$\tau_a = \tau_a^0 \gamma^{n_1}, \quad (14)$$

where n_1 is a constant. Note again that, the use of the plastic strain γ here does not have any thermodynamic basis, and it is more appropriate (but less convenient) to use dislocation density.

2.2.3. Solute concentration on dislocation line. Point defects, such as vacancies, interstitials, and substitutional solute atoms, have substantial influence on the mechanical behavior of materials. They act as local obstacles to the dislocation motion and are overcome by thermal activation. At low temperatures, they are essentially immobile, but attain mobility when the temperature is high enough. Mobile point defects move to and with the dislocations under the corresponding interaction forces. Hence, the concentration of the solutes along the dislocation line changes, resulting in phenomena such as dynamic strain aging and abnormal strain-amplitude-dependent internal friction.

The most important point defects in commercially pure titanium are interstitial solute atoms such as oxygen, nitrogen, carbon, and hydrogen [14]. Due to the interaction of point defects with the elastic strain field of dislocations, the point defects segregate to dislocations to form point defect atmospheres around dislocations, outside their core area. Additionally, point defects can be present in the dislocation core. In fact, the dislocation core may attract point defects more strongly than other sites within the elastic field.

For the point defect atmosphere outside the dislocation core area, the analysis of the diffusion process is relatively simple, because the interaction force between point defects and dislocations is known through an elastic calculation. This interaction force depends only on the type of dislocations and point defects. Even so, a full analytical treatment of the drag due to the point defect atmosphere acting on moving dislocations, is difficult [15].

The analysis becomes more complicated when dealing with the diffusion of solute atoms within the dislocation core area, especially when the dislocations are in motion. The dislocation core offers a short-cut circuit for atoms to diffuse. For other than interstitial atoms, the activation energy for pipe diffusion along the dislocation core is much lower than that for volume diffusion, usually equaling about one third to one half of that of the volume diffusion [16]. Some experimental evidence shows that the diffusion of interstitial atoms along the dislocation pipe is even more difficult than in the bulk, due to the strong binding force between

the dislocations and interstitial atoms in the dislocation core area. For an interstitial atom to diffuse in the dislocation core area, the binding force must be overcome first. Therefore, the interstitial atoms are more stable in the dislocation core than in the bulk.

When a dislocation is in motion, or under the action of applied stresses, it exerts a driving force on each of its core solutes, causing their directional diffusion. Assuming that the average spacing between solute atoms along the dislocation core is $l^* = 1/C$, under the applied stress τ , the dislocation exerts a force $F = \tau b l^* = \tau b / C$ on each of the solute atoms. We assume that the width of the potential for a solute atom diffusion is a^* , the total interaction energy between a dislocation and a solute atom is Q_i , and the total potential energy, or the activation energy, for diffusion, is Q . If the mechanical work done by the applied stress is less than the interaction energy of the dislocation and the solute atom, $\tau b l^* a^* < Q_i$, then the forward jump frequency, ν , to overcome the potential barrier for the solute atom is,

$$\nu = \nu'_0 \exp\left(-\frac{Q - \tau b l^* a^*}{kT}\right), \quad (15)$$

because part of the energy needed is provided by the work done by the applied force on the solute atom. Here ν'_0 is the attempt frequency of the solute atom. When $\tau b l^* a^* > Q_i$, the forward jump frequency becomes,

$$\nu = \nu'_0 \exp\left(-\frac{Q - Q_i}{kT}\right). \quad (16)$$

Taking into account the backward jumps when the applied stress is low, the diffusion velocity of the interstitial atoms is,

$$\begin{aligned} v_D &= a_0 \nu'_0 \left[\exp\left(-\frac{Q - \tau b l^* a^*}{kT}\right) \right. \\ &\quad \left. - \exp\left(-\frac{Q + \tau b l^* a^*}{kT}\right) \right] \\ &= \frac{D}{a^*} \sinh\left(\frac{F a^*}{kT}\right), \end{aligned} \quad (17)$$

where a_0 is the jump distance, and

$$D = a_0 a^* \nu'_0 \exp\left(-\frac{Q}{kT}\right) = D_0 \exp\left(-\frac{Q}{kT}\right) \quad (18)$$

is the diffusion coefficient, with $D_0 = a_0 a^* \nu'_0$ being the pre-exponential factor for diffusion. When the force exerted on the solute atoms is small, i.e. when $(F a^* / kT) \ll 1$, equation (17) reduces to the Einstein mobility relation,

$$v_D = \frac{D}{kT} F. \quad (19)$$

When the diffusion velocity of the interstitial atoms is high enough so that they can move along with the dislocations over a distance, during this movement, dislocations encounter and capture more interstitial atoms. The resistant force to the dislocation motion is increased due to the increase of the concentration of the core atoms. Dynamic strain aging can result from this increase of the resistant force to the dislocation motion. Because of the increase in the number of interstitial atoms along the dislocation core, the average spacing between interstitial atoms, l^* , decreases. If the applied stress is not increased, then, the driving force for interstitial atoms to diffuse, F , is decreased, resulting in a decreased mobility of the interstitial atoms. Therefore, the number of solutes captured by the moving dislocation has an upper limit at a given applied stress level. On the other hand, as suggested by Louat [17], the probability of the solute atom coming to a core site is proportional to the fraction of available core sites. Here also, a saturated value for the solute concentration must exist. A simple empirical expression for the variation of the solute concentration with the characteristic saturation property, is

$$C - C_0 = (C_s - C_0) \left\{ 1 - \exp \left[- \left(\frac{t_w}{t_D} \right)^\alpha \right] \right\}. \quad (20)$$

The local concentration C varies between the nominal value, C_0 , and the saturation concentration, C_s , with the characteristic diffusion time t_D . t_w in equation (20) is the average waiting time of dislocations at the obstacles, and $\alpha = 1/3$ or $2/3$ according to the diffusion mechanisms of the solute atoms, the former corresponding to pipe diffusion along the dislocation line, and the latter corresponding to volume diffusion in the crystal lattice [18]. The process of a dislocation bowing out and capturing solutes is similar to the process of a dislocation meeting forest dislocations, with the solutes diffusing to its core through pipe diffusion along the forest dislocation lines, while the dislocation is waiting at the obstacles. Therefore, α is equal to $1/3$.

The saturation concentration of the core atmosphere depends on the area the dislocation sweeps, under the equilibrium bowing-out of the dislocation segment. The greater the resolved shear stress acting on the dislocation, the greater the sweeping area. Consequently, there are more solute atoms being captured by the dislocation segment, as the stress level increases. Therefore, the saturation concentration is an increasing function of the effective stress. On the other hand, due to the pinning effect of the solute atoms on the dislocations, the higher the concentration of the solute atoms along the dislocation core, the more difficult it is for the dislocation segment to bow out, i.e. the saturation

concentration is inversely proportional to the core atmosphere concentration. Also, because of the increase in the dislocation density, the length of the dislocation segment reduces with increasing strain. Under the same applied stress, the bowing-out area is therefore reduced. Hence, the saturation concentration should be a decreasing function of the effective strain, at large strains. At small strains, the bowing-out area of the dislocation segment should be an increasing function of the strain, because the increasing strain requires greater stress, while the variation of the average length of the dislocation segments is still small. A simple description of this behavior is proposed here as follows

$$\frac{C_s}{C_0} - 1 = \left(\frac{\tau - \tau_a}{\tau_1 C_0} \frac{\gamma}{\gamma_1} \exp \left(1 - \frac{\gamma}{\gamma_1} \right) \right)^{n_2}, \quad (21)$$

where τ_1 , γ_1 and n_2 are constants.

When the plastic strain rate is constant, the average waiting time has its steady state value. According to Orowan's equation, neglecting the running time of the dislocation between obstacles, the average waiting time is related to the plastic strain rate by,

$$t_w = \frac{\dot{\gamma}_0}{v_0 \dot{\gamma}}. \quad (22)$$

The characteristic diffusion time, t_D , is obtained in terms of the applied stress and temperature from (17),

$$t_D = \frac{a_0}{v_D} = \frac{a_0 a^*}{D \sinh \left(\frac{\tau b l^* a^*}{kT} \right)}, \quad \text{when} \quad (23)$$

$$\tau b l^* a^* < Q_i,$$

and

$$t_D = \frac{a_0}{v_D} = \frac{a_0 a^*}{D \exp(Q_i/kT)}, \quad \text{when} \quad (24)$$

$$\tau b l^* a^* > Q_i.$$

In the case of this commercially pure titanium, the solute concentration is very low, so that $\tau b l^* a^* > Q_i$ can be assumed (and used through out this paper). Therefore, equation (24) is used to determine the characteristic diffusion time.

2.3. Final constitutive relation

From the above analysis, the final constitutive relation is obtained as follows

$$\dot{\gamma} = \dot{\gamma}_0 \exp \left\{ - \frac{F'_0 \sqrt{C/C_0}}{kT} \left[1 - \left(\frac{\tau - \tau_a}{\tau'_0 \sqrt{C/C_0} f(\gamma, T)} \right)^p \right]^q \right\}, \quad (25)$$

with

$$f(\gamma, T) = 1 + a_0 \left[1 - \left(\frac{T}{T_m} \right)^2 \right] \gamma^{n_0}, \quad (26)$$

$$\tau_a = \tau_a^0 \gamma^{n_1}, \quad (27)$$

$$\frac{C}{C_0} - 1 = \left(\frac{C_s}{C_0} - 1 \right) \left\{ 1 - \exp \left[- \left(\frac{\Omega}{\gamma} \exp \left(- \frac{Q - Q_i}{kT} \right) \right)^z \right] \right\}, \quad (28)$$

and

$$\frac{C_s}{C_0} - 1 = \left(\frac{\tau - \tau_a}{\tau_1 C/C_0} \frac{\gamma}{\gamma_1} \exp \left(1 - \frac{\gamma}{\gamma_1} \right) \right)^{n_2}, \quad (29)$$

where $\Omega = \beta b \rho_m h'_0 = \dot{\gamma}_0 (v'_0/v_0)$ is a constant.

When the solute concentration along the dislocation line does not vary with time (in the case when the solute atoms are immobile, or are saturated at high temperatures), the above equation reduces to the model of Nemat-Nasser and Li [13], with only a minor difference, i.e. in the present paper, the pre-exponent factor $\dot{\gamma}_0$ is considered to be a constant.

3. EVALUATION OF MODEL CONSTANTS AND COMPARISON WITH EXPERIMENTAL RESULTS

To evaluate the model constants, we may express the model as follows

$$\tau = \tau'_0 \sqrt{\frac{C}{C_0}} \left\{ 1 - \left[- \frac{kT}{F'_0 \sqrt{C/C_0}} \left(\ln \frac{\dot{\gamma}}{\dot{\gamma}_0} \right) \right]^{1/q} \right\}^{1/p} \times \left\{ 1 + a_0 \left[1 - \left(\frac{T}{T_m} \right)^2 \right] \gamma^{n_0} \right\} + \tau_a^0 \gamma^{n_1} \quad (30)$$

and

$$\frac{C}{C_0} = 1 + \left(\frac{\tau - \tau_a^0 \gamma^{n_1}}{\tau_1 C/C_0} \frac{\gamma}{\gamma_1} \exp \left(1 - \frac{\gamma}{\gamma_1} \right) \right)^{n_2} \times \left\{ 1 - \exp \left[- \left(\frac{\Omega}{\gamma} \exp \left(- \frac{Q - Q_i}{kT} \right) \right)^z \right] \right\}. \quad (31)$$

Among the parameters in the above constitutive relations, the Boltzmann constant k equals $1.38 \times 10^{-23} \text{ JK}^{-1}$, which is a universal constant, the melting temperature of titanium is 1935 K, and the activation energy for the volume diffusion of oxygen in titanium is 200 KJ/Mole [19]. The exponents, p and q , are chosen to be the same as those used by Nemat-Nasser and Isaacs [20] and Nemat-Nasser and Li [13] for tantalum and copper, i.e. 2/3 and 2, respectively. It has been suggested by Ono [21] and Kocks *et al.* [9] that these values of p and q provide a sufficiently accurate description of the profile of the energy barrier in most cases.

In the absence of dynamic strain ageing, expression (30) reduces to the model used by Nemat-Nasser *et al.* [1]. Indeed, setting $C = C_0$, (30) becomes

$$\tau = \tau'_0 \left\{ 1 - \left[- \frac{kT}{F'_0} \left(\ln \frac{\dot{\gamma}}{\dot{\gamma}_0} \right) \right]^{1/q} \right\}^{1/p} \times \left\{ 1 + a_0 \left[1 - \left(\frac{T}{T_m} \right)^2 \right] \gamma^{n_0} \right\} + \tau_a^0 \gamma^{n_1}. \quad (32)$$

For all constitutive parameters in (32), we have used the values obtained in [1]. The model parameters are $\dot{\gamma}_0$, τ'_0 , F'_0 , a_0 , τ_a^0 and n_1 . Their values (see Table 1) have been obtained in [1] following a systematic procedure outlined by Nemat-Nasser and Isaacs [20]. In this approach, first the athermal part of the flow stress is established using the high-temperature data, since at high temperatures, this part of the flow stress is not significantly affected by the short-range barriers to the dislocation motion. Indeed, high-strain-rate experimental data at a 998 K initial temperature show good correlation with the model prediction, as can be seen from Figs 4(d) and 7(c). Once the expression for the athermal part of the flow stress is fixed, the experimental results for temperatures and strain rates outside the

Table 1. Summary of material constants

Constants	Values	Constants	Values
τ'_0	140 MPa	F'_0	173 KJ/Mole
$\dot{\gamma}_0$	$4 \times 10^8/s$	a_0	19
n_0	0.55	τ_a^0	110 MPa
n_1	0.15	Ω	$1 \times 10^{12}/s$
Q_i	100 KJ/Mole	τ_1	300 MPa
n_2	2.5	γ_1	0.18

dynamic strain-aging range are used directly to evaluate $\dot{\gamma}_0$, τ'_0 , F'_0 and a_0 . As has been shown in [1], the model is in good accord with the experimental data outside the range of dynamic strain-aging effects, for both very low (e.g. 77 K) and very high (e.g. 900 K and higher) temperatures, at high strain rates, where the solute mobility effects are not significant.

The resistance to the motion of dislocation can change due to the variation in the density of the dislocation core atmosphere, leading to the dynamic strain-aging phenomenon. This effect is included in the model by simply modifying the activation energy and mechanical threshold stress to account for the added resistance to dislocation motion due to the presence of the solute atoms. In the model, this effect is introduced by the term C/C_0 . The parameters defining the dependence of this quantity on temperature, stress, strain rate and the density of dislocations (empirically represented by the strain γ), are then obtained by fitting of the experimental data, while the structure of the expression (31) is established based on the physics of the process. The activation energy corresponding to the dynamic strain aging is estimated to be $Q-Q_i=100$ eV, as discussed in [1]. The other parameters in (31) are then obtained in order to best fit the observed results. The model parameters are given in Table 1.

The experimental procedure and results have been reported in [1]. Here, our focus is on the high-strain-rate dynamic strain-aging phenomenon. Therefore, only high-strain-rate data are examined. Figure 2 shows by the dotted curves the experimentally obtained variation of the flow stress with tem-

perature, for a strain rate 2200 s^{-1} and indicated strains. The solid curves are the corresponding theoretical predictions. As is seen, good correlation between the experimental and model results is obtained. Figures 3 and 4 show the stress-strain relation for a 2200 s^{-1} strain rate and eight different initial temperatures. Figure 5 shows the flow stress as a function of the temperature for an 8000 s^{-1} strain rate, and indicated strains. The individual stress-strain relations are shown in Figs 6 and 7. All these results suggest that the model adequately captures the essence of the response of this material.

Detailed explanations of the experimental results according to the model proposed here are given in the next section.

4. DISCUSSION

4.1. Mechanisms of dynamic strain aging

A key feature of thermally activated dislocation motion is that the dislocations spend most of their time in interacting with local obstacles, such as forests of dislocations, vacancies and solute atoms. This period of time is usually called the waiting time in the literature. After the dislocation overcomes a set of obstacles, it runs very fast until it is stopped at the next group of obstacles. The average velocity of the dislocation is determined by the spacing between the obstacles and the waiting time spent during the thermal activation process. The dislocation moves in a jerky way. Actually, the average velocity of dislocations is small during the

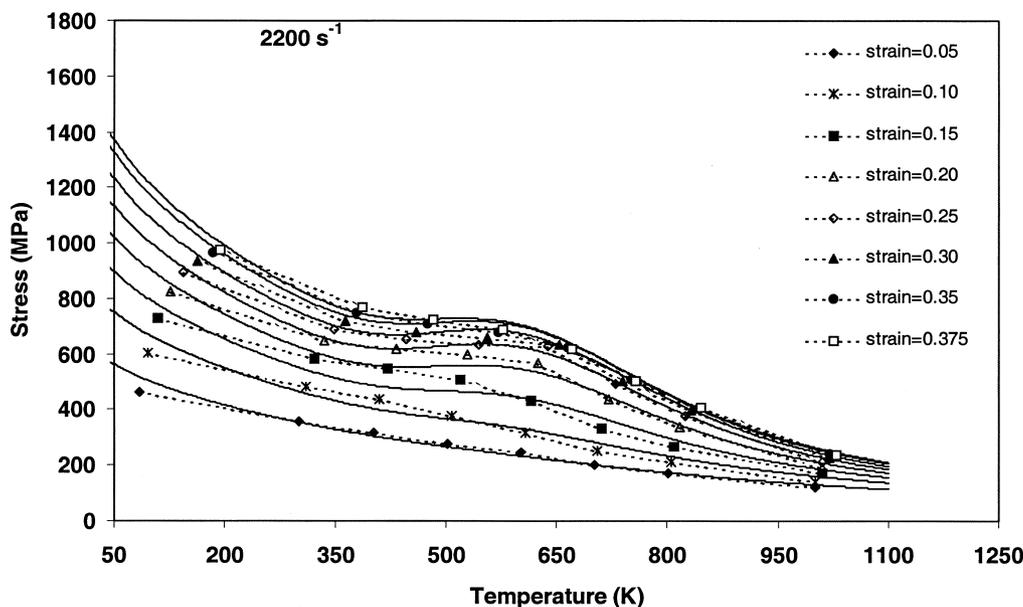


Fig. 2. Flow stress vs temperature curves of CP-Ti at indicated plastic strains (dotted lines: experimental; solid lines: theoretical).

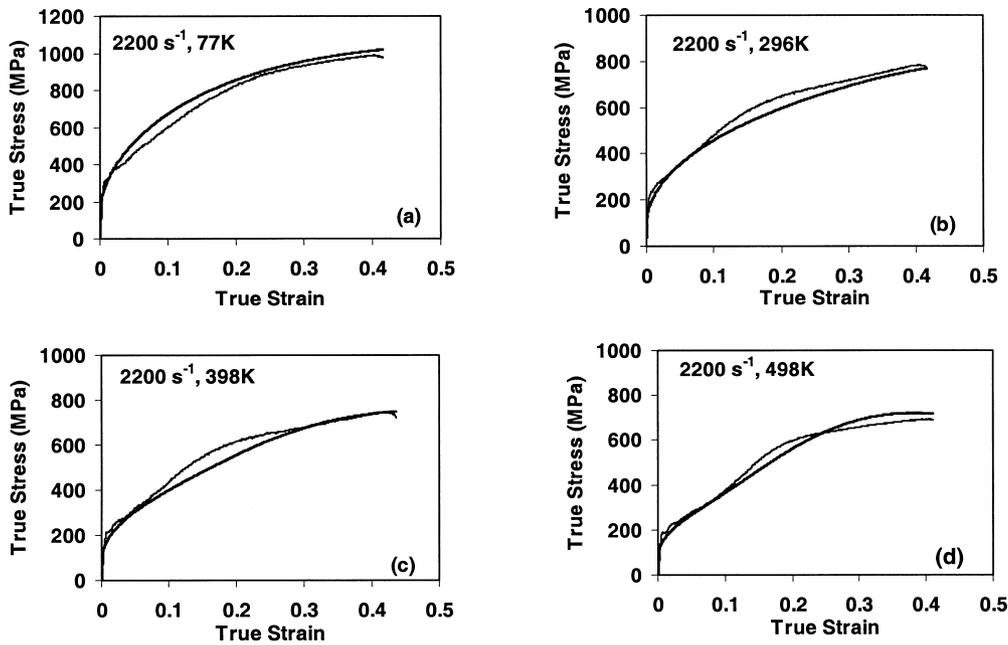


Fig. 3. Experimental (thin solid) and model (thick solid) stress-strain curves.

process of thermal activation. The effect of the drag by point defects becomes evident when the time for the point defects to diffuse to and with the dislocations is comparable to the waiting time of the dislocations. That is, the dynamic strain-aging effect is observed at suitable combinations of strain rates and temperatures.

At present, all models proposed for explaining the dynamic strain-aging phenomenon are based on

the idea of solute atoms diffusing to dislocations. That is, the dislocations are waiting passively for the solutes to diffuse to them and to form an atmosphere around them. The model developed in the present paper is based on a different mechanism. In the present model, the dislocations are not waiting passively for the solutes to diffuse to them, but rather they capture the solutes during their bowing-out process, under the applied stress, while

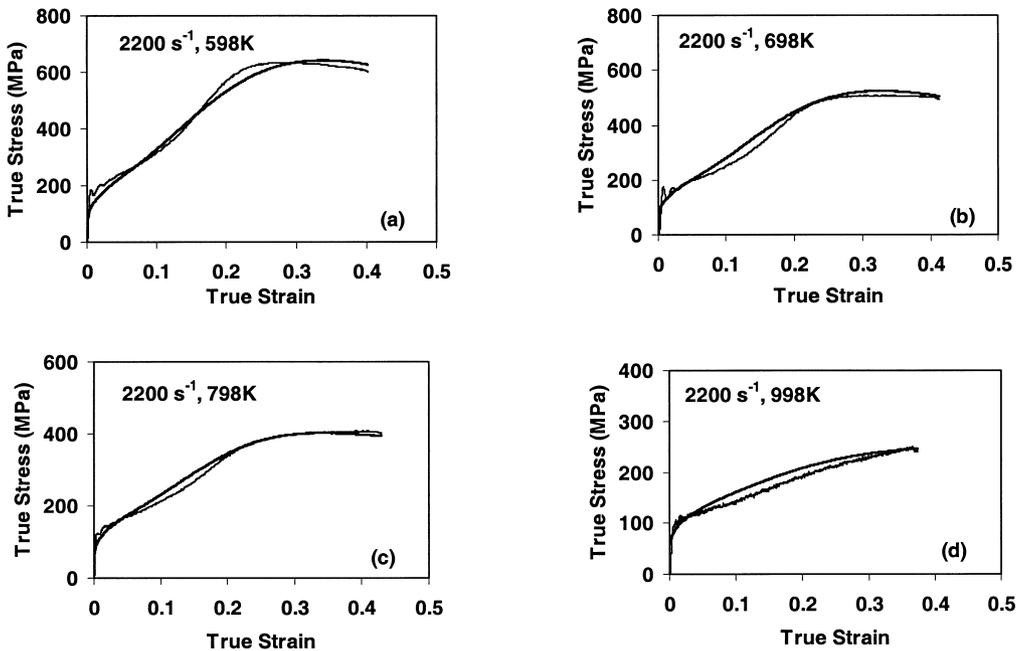


Fig. 4. Experimental (thin solid) and model (thick solid) stress-strain curves.

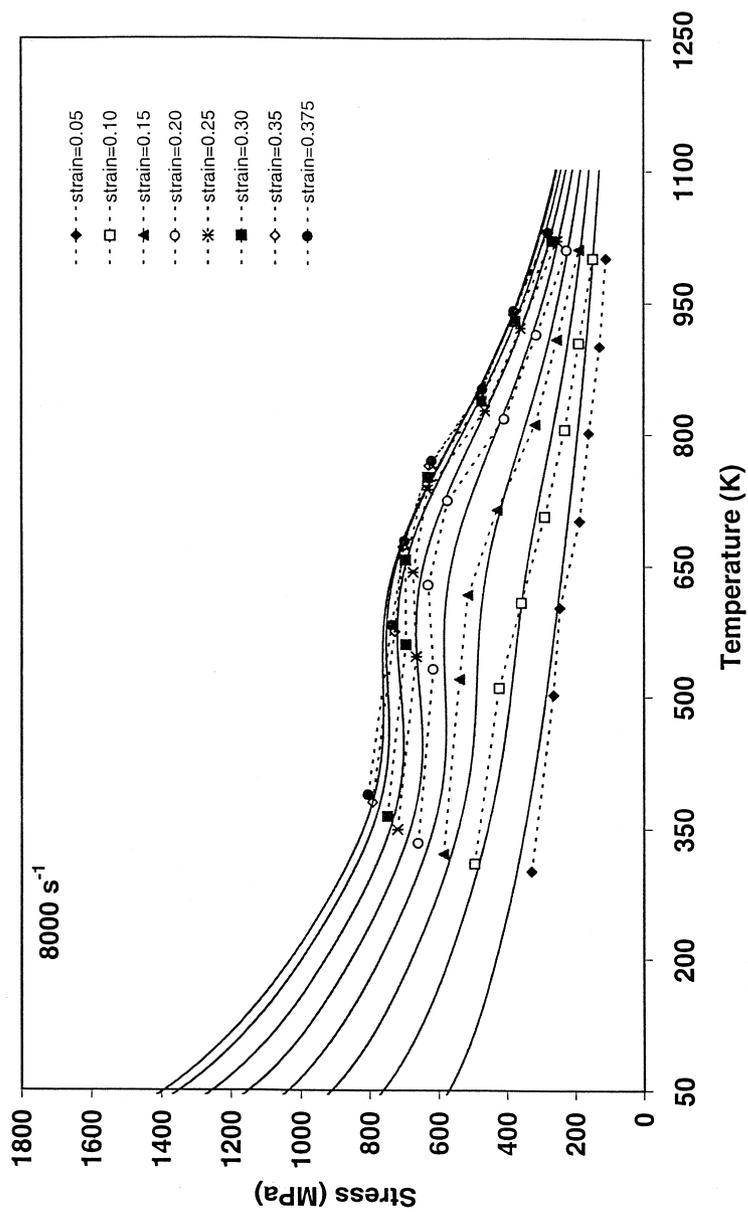


Fig. 5. Flow stress vs temperature curves of CP-Ti at indicated plastic strains (dotted lines: experimental; solid lines: theoretical).

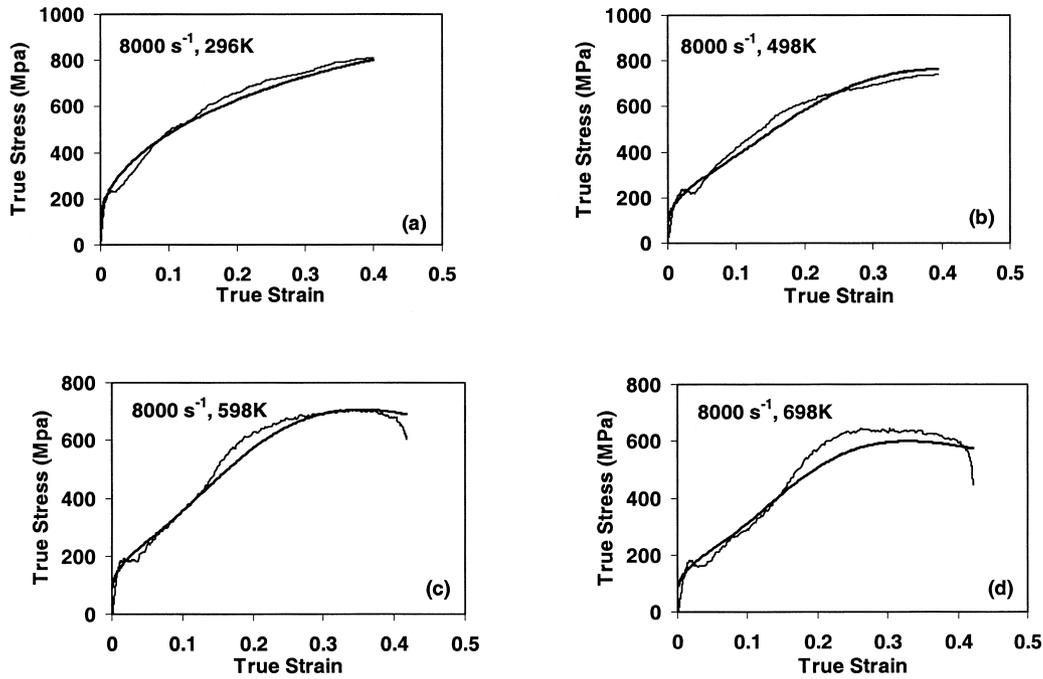


Fig. 6. Experimental (thin solid) and model (thick solid) stress-strain curves.

being held at dislocation forests. The increase in the concentration of the dislocation core atmosphere is a result of the diffusion of the existing core atmosphere along with the dislocation, and the new solutes which are encountered and captured by the dislocation. Due to the increase in the core atmosphere density, both the total thermal activation

energy and the mechanical threshold stress are increased, as they are modeled through equations (8) and (9). Hence the driving stress needed to move the dislocations increases, leading to the dynamic strain aging.

Because a strong interaction force between dislocations and solutes exists in the dislocation core

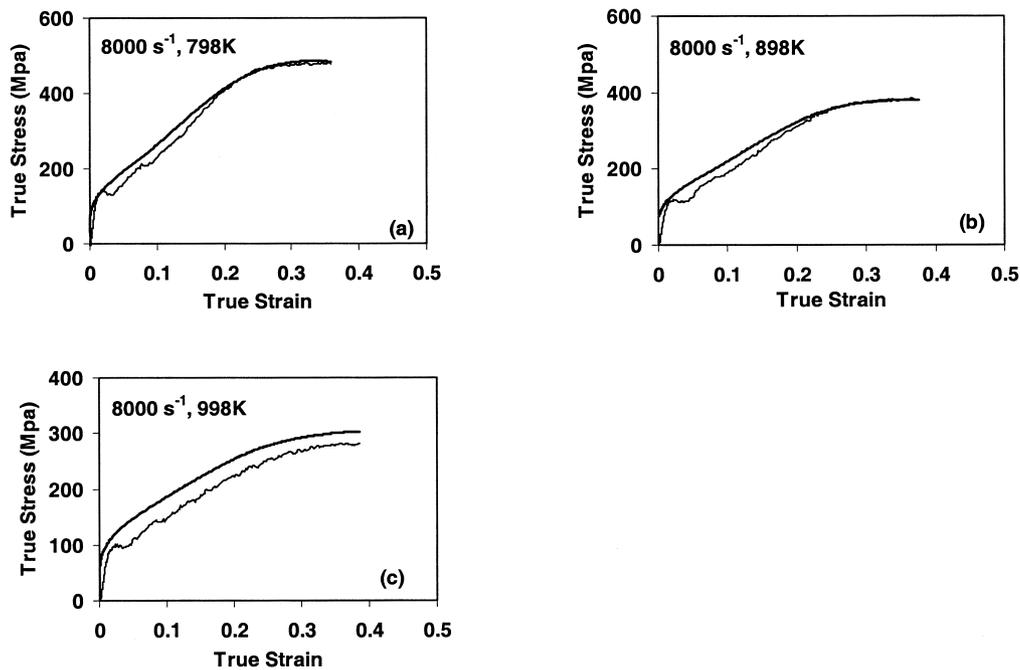


Fig. 7. Experimental (thin solid) and model (thick solid) stress-strain curves.

area, the diffusion of the core atmosphere becomes significant at much lower temperatures than possible for the solute atoms situated outside the core area, provided that the resolved shear stress on the dislocations is high enough. Because the force exerted on each of the solutes is inversely dependent on the concentration of the core atmosphere, the mobility of the core atmosphere is a decreasing function of the solute concentration. The required temperature for the dynamic strain-aging effect due to the core atmosphere diffusion, shifts to higher values when the concentration of solutes is increased. It is possible for the dynamic strain aging to occur due to both the core diffusion and the volume diffusion of the solute atmosphere outside the core area, when the solute concentration is high. But the mobility of the core atmosphere is still higher than that of the outside atmosphere. The model seems to provide a good explanation of the phenomenon that the observed temperature for the appearance of dynamic strain aging is always much lower than that calculated based on the volume diffusion, for almost all materials. To explain this discrepancy, various mechanisms are proposed in the literature, including production of voids by straining [22], and drainage of solutes from forest dislocations through pipe diffusion [23]. Here we have proposed a different mechanism that seems to provide a natural and straightforward explanation for the observed data.

To be able to observe the dynamic strain-aging effect which is caused by the core atmosphere diffusion, the solute concentration must be very low. Otherwise, diffusion may occur at both the core and outside of the core. According to our model, the dynamic strain-aging effect becomes significant only under high applied stress conditions, because only then is the directional diffusion of the core atmosphere guaranteed to occur during a relatively long deformation history. This is in accord with the experimental observations. Under dynamic deformation conditions, the observed unusual dynamic strain-aging effect is more pronounced than the corresponding effect under quasi-static deformation conditions, simply because the former has higher applied stresses. The research efforts for the dynamic strain-aging effect of titanium are usually focused on high-temperature and quasi-static loading conditions, because it is usually assumed that the diffusion of solutes is a slow high-temperature process [14]. From the experimental results reported in [1], it is seen that the dynamic strain-aging effect at lower temperatures is not very pronounced. That is why the phenomenon has been observed only recently at high strain rates [1].

4.2. Associated phenomena

4.2.1. Increased workhardening rate.. An import-

ant underlying mechanism for workhardening is the increase in the density of dislocations. The flow stress, τ , is usually assumed to be proportional to the square root of the total dislocation density ρ_t ,

$$\tau = \tau_0 + \alpha' \mu b \sqrt{\rho_t}, \quad (33)$$

where τ_0 and α' are constants and μ is the shear modulus. The direct effect of the point defect drag is to cause an increase in the concentration of the core solute atmosphere. This increase of the core atmosphere results in an increase in the rate of workhardening and the total thermal activation energy required for the dislocation to break away from the core atmosphere, as is predicted by the model.

The drag of the point defects results in extra resistance to the motion of dislocations. Therefore, the applied stress must be increased to further plastically deform the material at a constant imposed strain rate. But the increase of the applied stress due to this extra resisting force activates the dislocation sources that are inactive at lower stresses. Therefore, an increased multiplication of dislocations results.

The results of the interrupted tests in [1], at the temperature of 600 K and a strain rate of 2200 s^{-1} , support the above argument. After unloading at a 24.5% strain, and reloading at the unloading temperature, the flow stress is observed to be lower than that of the continued adiabatic loading. During the interrupted test, the sample undergoes a temperature cycle from the test temperature to room temperature and then again to the test temperature. During this temperature cycle, the sample is partially annealed. The higher the temperature rise, the greater is the annealing. Therefore, the yield stress at the reloading temperature of 630 K (which is the temperature at the unloading state) is lower than that of the isothermal response at 600 K.

Transmission electron microscopy (TEM) studies [24] have indicated that an increased workhardening rate in the dynamic strain-aging region of temperatures and strain rates is caused by an enhancement of the dislocation multiplication rate due to the locking of mobile dislocations, rather than by the dragging of the point defect atmospheres. This seems to be a commonly accepted [25] point of view.

The occurrence of intensified acoustic emission concurrent with the dynamic strain-aging deformation has been noted in the literature [26]. During deformation under the dynamic strain-aging conditions, high-frequency acoustic emission is regularly detected. Attempts have been made to correlate this phenomenon with dislocation multiplication events [27, 28].

Due to the saturation property of the core atmosphere, one may expect that the workhardening rate should increase to a maximum value with increasing

temperature, and then decrease to normal values. The effect of the point defect drag is only of significance at an appropriate combination of the mobility between the dislocations and the point defects. One may also expect that the point defect drag effect that takes place at a relatively low temperature has a more pronounced effect on the rate of workhardening. When the temperature is not high, the process of the annihilation of dislocations through cross slip is not significant. Most of the extra dislocations that are generated because of the drag effect, are accumulated. This results in a significant increase in the rate of workhardening. When the temperature is high enough, the dislocations generated in the process of the point defect drag are partially annihilated through the dynamic recovery process. Therefore, the increase of the rate of workhardening is less significant than that at lower temperatures.

4.2.2. Critical strain for occurrence of dynamic strain aging. A critical strain must be attained for the dynamic strain aging to appear. An explanation for this is that a certain vacancy population is needed to enhance the mobility of the solute atoms [22], because, generally speaking, plastic deformation increases the density of vacancies in the material. On the other hand, plastic deformation also causes an increase in the total dislocation density. Hence, the density of the mobile dislocations also increases, resulting in a reduced average velocity of the mobile dislocations. The model of Kubin and Estrin [29] deals with the critical strain in terms of the strain dependence of both mobile and forest dislocation densities. Hence, the strain dependence of the parameter Ω is calculated; see equation (28). At low strains, the increase in the mobile dislocation density is predominant and Ω increases with increasing strain. Once the mobile dislocation density has saturated, the strain dependence of Ω is determined by the increase in the forest dislocation density, or by the decrease in the average length of the dislocation segments, l . Therefore, critical strains must be achieved before the appearance and disappearance of the dynamic strain aging.

The model proposed in this paper deals with the critical strain in an alternative way. According to our model, the critical strains relate to the saturation behavior of the dislocation core atmosphere. The concentration of the core atmosphere depends on both the mobility of the solute atoms in the dislocation core and the extent of the bowing-out of the dislocation segment. Both of these are determined by the stress resolved on the dislocation. At low strains, the applied stress level is low. Therefore, the dislocation is unable to undergo large bowing-out to capture more solute atoms. The concentration of the core atmosphere therefore does not vary and the dynamic strain aging is not observed. When the applied stress is suitably large,

which occurs at larger strains, the process of capturing solute atoms by dislocation cores becomes significant. Therefore, a critical strain is achieved before the appearance of the dynamic strain aging. But with the increasing plastic strain, the dislocation density increases, and consequently the average length of the dislocation segments becomes shorter. It hence becomes more difficult for a dislocation segment to bow out. Also, because of the increased total dislocation density, more solute atoms have stable positions within the existing dislocation cores. Hence, there are fewer free solute atoms to be captured by mobile dislocations. Therefore, at large strains, the dynamic strain aging eventually disappears. For this, a critical strain must be reached.

The models based on the deformation-generated vacancies and mobile dislocations have been criticized in the literature, on both theoretical and experimental grounds [30]. The present model provides an alternative mechanism that does not rely on the above assumptions and is based on a clear physical reasoning.

4.2.3. Thermal hardening phenomenon. An increase in the temperature increases the mobility of solute atoms. It also makes it easier for the dislocation segments to adjust their equilibrium configuration and to bow out to a greater extent. Hence, more solute atoms are captured by the dislocation segments. The higher the concentration of the core atmosphere, the greater the resistance to the movement of the dislocations. A temperature rise, however, reduces the resistance of the obstacles, while an increase in the concentration of the core atmosphere increases the resistance to the dislocation motion. When the strengthening effect due to the increase in the core atmosphere concentration dominates the thermal softening effect, a thermal hardening is manifested.

Once the core atmosphere is saturated, a further rise in temperature no longer can lead to an increase in the core atmosphere concentration, and the usual thermal-softening behavior is attained. With a decrease in the flow stress due to thermal softening, the core atmosphere concentration is also decreased, because of the stress dependence of the saturation value of the core atmosphere concentration. The material returns to its normal behavior at high temperatures, as no change in the core atmosphere concentration can then occur.

5. SUMMARY AND CONCLUDING REMARKS

From the preceding analysis, the following summary and conclusions are obtained.

1. A new constitutive model that combines the concepts of athermal long-range and thermally activated short-range barriers, with the model of a "trough" [2] for the thermally activated break-

away of dislocations from the core atmosphere, is established. The variation of the core atmosphere concentration is included in the model, based on the strong interaction force between dislocations and point defects in the core area. The final product is a unified model which accurately predicts the response of commercially pure titanium, over a broad range of strain rates and temperatures, with the effect of dynamic strain aging included.

2. According to the model, different mechanisms are dominant in different temperature ranges, in controlling the mechanical behavior of metals. At high temperatures, the flow stress stems mainly from the athermal resistance to the dislocation motion. At low temperatures, besides the athermal resistance, the thermal resistance to the dislocation motion contributes to the flow stress. In an intermediate temperature range, if the metal contains solute atoms, the mobility of the solute atoms changes the properties of the local obstacles to the motion of dislocations. The thermal activation energy and the mechanical threshold stress then vary with the dislocation core atmosphere concentration. Dynamic strain aging is the macroscopic manifestation of the solute mobility.
3. A new mechanism is proposed for the interpretation of the dynamic strain aging observed in commercially pure titanium at high strain rates and high temperatures. It is based on the concept that the solute atoms in the dislocation core, i.e. the core atmosphere, diffuse directionally with the movement of the dislocation, under the interaction force between the dislocation and solute atoms, and that the dislocation captures new solutes during its bowing-out adjustment of its equilibrium position while waiting at the forest dislocation barriers. An increase in the concentration of the core solute atmosphere results from this process, leading to an increase in the thermal activation energy, mechanical threshold stress and the workhardening rate.
4. It is the dynamic strain-aging effect due to the interaction between the moving dislocations and the mobile dislocation core atmosphere (here mainly the interstitial atoms of oxygen, nitrogen and carbon) that is responsible for the anomalous behavior of this commercially pure titanium. Because the force exerted on each of the core solutes by the dislocation is inversely proportional to the concentration of the core solute atmosphere, this kind of dynamic strain aging can only be observed at low solute concentrations.

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