INTERNATIONAL SCIENTIFIC JOURNAL

MATERIALS SCIENCE. NON-EQUILIBRIUM PHASE TRANSFORMATIONS

PUBLISHER:

SCIENTIFIC TECHNICAL UNION OF MECHANICAL ENGINEERING

108, Rakovski Str., 1000 Sofia, Bulgaria
tel. (+359 2) 987 72 90,
tel./fax (+359 2) 986 22 40,
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ISSN PRINT 2367-749X, ISSN WEB 2534-8477
YEAR III, ISSUE 1 / 2017

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CHARACTERISTIC PROPERTIES THE MOTION OF DISLOCATIONS DURING THE DEFORMATION OF SINGLE CRYSTALS

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ХАРАКТЕРНЫЕ ОСОБЕННОСТИ ДВИЖЕНИЯ ДИСЛОКАЦИЙ ПРИ ДЕФОРМИРОВАНИИ МОНОКРИСТАЛЛОВ

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Abstract. The motion of a dislocation in Aluminum is considered at room temperature with allowance for the Peierls relief. This study has been accomplished using the methods of mathematical modeling. It was shown by means of numerical experiment that the free path length of dislocation depends on the frequency of applied external elastic field. Here a hardening of crystal took place due to the dynamical losses. In the presence of resonant frequency external alternating elastic field the gradient of hardening curve growth, and therefore, the yield strength, is reduced. It was shown that the regularities of large-scale processes occurring in deformable body may be clarified by means of analyzing the micro processes.

KEYWORDS. THE PEIERLS RELIEF, FRENKEL-KONTOROVA DISLOCATION, COMPUTER SIMULATION, THE STRESS-STRAIN DEPENDENCE.

1.Introduction

The cold plastic strain is generally known to lead to significant interdependent changes in the shape, dimensions and physic-chemical and mechanical properties of wrought metals and alloys. The totality of phenomena due to the change of mentioned properties is called the strain hardening. Despite the abundance of conducted experimental and theoretical studies of this problem, the physical nature of hardening has not been completely elucidated to date. The experimental investigations at different states of stress witness that the parameter characterizing the hardening, i.e., the deformation resistance for cold deformation, is a non-linear function of the current value of accumulated strain. In descriptions of hardening phenomenon in the phenomenological theories the mentioned dependence is approximated by some power function form $\sigma = K\varepsilon^n$.

Where K, n the hardening parameters which are determined from experimental data on tensile tests of this material, σ is the stress of deformation resistance [1]. From microscopic viewpoint, the plastic strain is the result of the motion of linear defects – the dislocations. Owing to the translational symmetry of a crystal the potential energy of dislocations is a periodical function of coordinates. For this reason, a periodical force acting from the distorted lattice on dislocation in the process of sliding is described by a sinusoidal potential corresponding to the crystal relief (the Peierls relief)

The microstructure and mechanical properties of technically pure ultrafine Al obtained by means of equal-channel angular pressing in 4,2–295 K temperature range have been examined in [2]. The heightened interest to aluminum is due to the fact that it is at the basis of the class of materials for aviation, space, and cryogenic technologies.

The experiments showed notably diminishing of the yield point and of the growth gradient of strain hardening with application of ultrasound waves[3]. The motion within the Peierls relief (discreteness of the lattice) stimulates the emergence of dynamic losses as well [4]. So, an analysis of the motion of dislocations with due regard for resistance of medium in the form of internal friction in the presence of ultrasound is an urgent problem.

2. Results

In the present work the motion of dislocations in aluminum with allowance for Peierls relief is considered. For description of dislocation phenomena we used the one-dimensional Frenkel-Kontorova model. The motion of dislocations is assumed to have the thermal activation mechanism [5]. In aluminum the Peierls potential barrier is of the order of $4{*}10^{-15}$ erg [6]. At $\Omega \sim 10^{12}$Hrz frequency the duration of voltage pulse is comparable to the time of dislocation transition to neighboring valley.

For description of mechanisms of internal friction and hardening we have derived in homogeneous sine-Gordon equation with friction and periodic external elastic stress $\sigma(t) = \sigma_0 e^{i\Omega t}$ where $\sigma_0$is the amplitude of external action, Ω is the frequency.

If X axis is directed along the equilibrium position of a straight dislocation, then the equation for displacement of atoms from the equilibrium position will be:

$$m\ddot{y}_n = f_0 \sin\frac{2\pi y_n}{a} + k(y_{n+1} - y_n) - k(y_n - y_{n-1}) + F_{fr} + F_0 \sin[\Omega t] \qquad (1)$$

where y_n is the displacement of the n –th atom from the equilibrium position, m is the mass of atom,

$f_0 = \frac{mV_0{}^2 a}{2\pi(l_0)^2}$, where $l_0$is the parameter that increases with increasing spring stiffness and decreasing strength from the substrate, i.e., decreases with increasing Peierls barrier, $V_0$is the speed of sound, a is the lattice constant.

In dimensionless unit s$=\frac{V_0}{\omega}\tilde{x}$, $t = \frac{\tilde{t}}{\omega}$ then the equation assumes the form of inhomogeneous sine Gordon equation [7].

$$\ddot{\varphi}_n + \sin\varphi_n - \varphi^0{}_n + \beta\varphi_n = \gamma \sin\frac{\Omega t}{\omega}, \qquad (2)$$

$$\omega^2 = \frac{2\pi f_0}{ma} V_0 = a\sqrt{\frac{k}{m}} \beta = \frac{\mu_0}{m\omega} \gamma = \frac{2\pi F_0}{ma\omega^2}$$

$\mu_0$is the coefficient that characterizes the friction, $\varphi_n$is the displacement of n –th atom from the equilibrium position.

A numerical experiment has been conducted for three dislocations that at the initial time are in the origin of coordinates. If in the equation (2) only the friction is taken into account, then the dislocation stops in time, if the frequency and friction – then after passing of some distance, the dislocation is stopped and vibrates in the attained position by changing its shape. In the absence of supplemental external influence both the dislocations remain in the same state even after elimination of the cause initiating their appearance [8]. For comparison, the third dislocation makes free sliding (Figure 1).

Now investigate the dependence of free path length of the dislocation on the frequency of external elastic filed. It follows from the numerical experiment that the dislocations while starting from the same point are stopped in time, the free path lengths of dislocations being different depending on the frequency of external variable field .At a certain frequency the free path length has the greatest value. Now construct a graph of free path length of the dislocation versus the frequency of elastic field by passing HF sound of~10^{12}Hrz with coefficients 0.06,0.08,0.1,0.25, 0.5,1,1.5, 2,2.5 respectively through the crystal. (in Figure 2.).

It is seen in Figure 2 that at a certain frequency the free path length of dislocation is maximum. It is obvious that the formation of no collapsing double kink corresponds to this value of frequency, as a result of which the dislocation passes to the next valley of potential relief during the time of positive part of the external elastic field [5]. This frequency also determines the starting stress. This result proves that under the above conditions the motion of dislocations in alumimum has a thermally activated mechanism.

Figure 1.Motion of dislocations at successive instants of time: (1) free sliding; motion with allowance for friction force (thick curve), motion with allowance for friction force and variable elastic field.

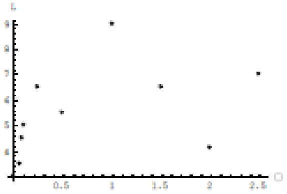

Figure 2.Dependence of free path length of dislocations on frequency of variable elastic field

The dependences σ(ε) have been constructed in the presence and absence of resonant frequency. Prior to that we constructed the dependences σ(x). In the presence of external mechanical frequency the dependence σ(x) has a form shown in Figure 3.

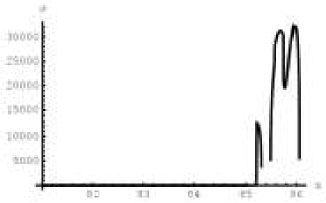

Figure 3. Dependence of stress on coordinate in the vicinity of dislocation (with external variable elastic field)

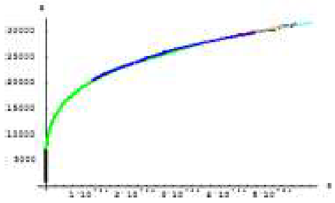

Figure 4. The stress-strain dependence in the vicinity of dislocation (with external variable elastic field)

Respectively, the dependence σ(ε) in the ranges of monotonous growth of function σ(x) is seen in Figure 4.

The dependence of stress on coordinate in the absence of external frequency is shown in Figure 5.The maximum stress is seen to be realized near the dislocation line and decreases with distance from that. The oscillations in this case are presumably due to the periodical Peierls potential.

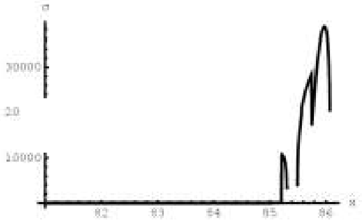

Figure 5. Dependence of stress on coordinate in the vicinity of dislocation (in the absence of variable elastic field)

Comparing dependences of tension on coordinate in the neighborhood of dislocation to the external variable elastic field and without it (Figure 3, Figure 5), we conclude that the resonance external field reduces Payerls's barriers.

Comparative dependences of tension on coordinate for a resonant frequency and nearby frequencies are simulatived (for obviousness descriptive reasons plots are given for slightly displaced instants (Figure 6.))

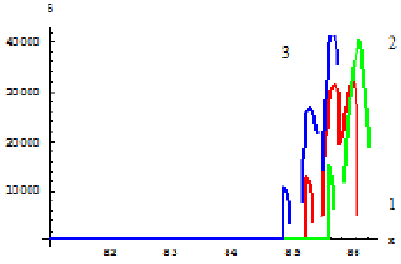

Figure 6. Dependences of tension on coordinate for a resonant frequency (1) and nearby frequencies (2), (3).

Dependence of dislocation rate on coordinate the vicinity of Peierls barrier is shown in Fig. 7. It is seen in Fig. 7 that the dislocation gets over the Peierls barrier really at variable speed. Such a character of dislocation travel is possible only in case of changeableresistance of medium to dislocation motion. At slowing down of dislocation, i.e., increasing of the medium resistance, a macro scale deformation hardening is the case.

In the region of third rise in the dependence of stress on coordinate (Figure 5) (motion from the valley to the potential relief) the dislocation rate decreases, and increases on the slope (potential relief–the next valley).

Based on this fact it is assumed that there is a microplasticity region around the dislocation. Actually, in the range of monotonous dependence of stress on coordinate, the numerical experiment in the absence of external elastic field gives the following dependence of stress on strain(Figure 8).

The slope of monotone increasing curve $\left({}^{d\sigma}/_{d\varepsilon}\right) = \theta$ is called the hardening coefficient [9]. In fcc crystals (including also aluminum) 3 sections are distinguished, in which various mechanisms of strain and hardening are effective [8].

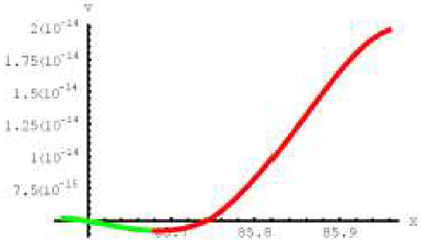

Figure 7. Dependence of dislocation rate on coordinate the vicinity of Peierls barier

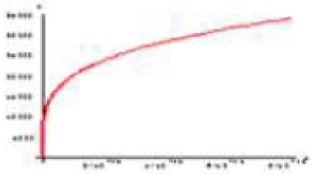

Figure 8. Dependencies of stress on strain in the absence of external field

We have obtained the dependence of hardening coefficient on coordinates in the absence and presence of external field: Fig.9 (thin line corresponds – resonance frequency application, the bold-to the absence of frequency). From a numerical experiment (Fig.9) it is visible that existence of a resonant frequency reduces hardening coefficient.

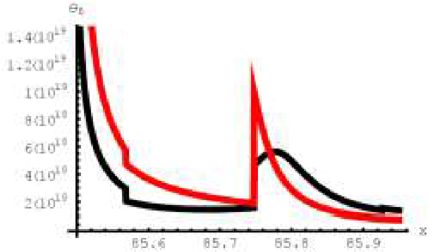

Figure.9. Dependencies of hardening coefficient on coordinates in the vicinity of dislocation

Dislocation moves irregular in Payerls's relief at room temperature, being slowed down before Payerls's barrier and accelerating after overcoming a barrier. The area of microplasticity is implemented in the vicinity of dislocation. The external variable elastic field changes the free path length of dislocation, and depending on frequency it is possible to regulate a free path length. Fixing of dislocation after passing of some distance speaks about hardening. The existence of a resonant frequency reduces hardening coefficient.

3 sections are distinguished, in which various mechanisms of strain and hardening are effective.

The dislocation structure changes in each stage. Resonant frequency reduces hardening coefficient. Hardening in this case is caused by dissipation of energy when driving dislocation in Payerls's relief.

At low temperatures, the movement of dislocations through Peierls barriers carried out by tunneling of kinks[10]. On the macro level, there is softening of crystal.From sine-Gordon equation and the stress-strain dependence [11]

$\sigma = a_0 \varepsilon^{a_1} \zeta^{-a_2} \exp^{-a_3 \theta}$, a_0, a_1, a_2, a_3 – constants of the material, ζ - the rate of deformation, θ - the temperature , by the numerical experiment we find the strain -stress plots (constants taken for aluminum).

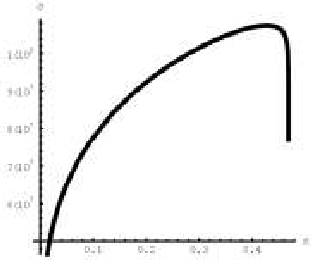

Figure 10. Strain- stress dependence at $\theta = 0^0 C$, high Peierls barrier .

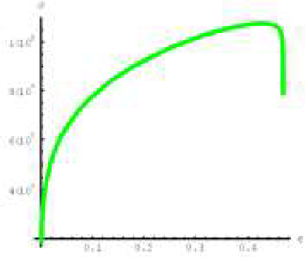

Figure 11. Strain- stress dependence , $\theta = 10K$, low Peierls barrier

As can be seen from the figures, the curves is similar: the tunneling on the microscale (Figure 10.) corresponds to the softening on makroscale (Figure 11.).

3. CONCLUSION

Dislocation moves irregular in Payerls's relief at room temperature, being slowed down before Payerls's barrier and accelerating after overcoming a barrier.

The resonance external elastic field reduces Payerls's barriers. The free path length of dislocation is maximum at a certain frequency of elastic field.

The effect of high Peierls barrier is similar to the effect of low temperatures or in other words at lower temperatures the Peierls barrier decreases.

Thus, the results of this investigation of micro characteristics at the motion of a dislocation explain the macrolevel behavior of moving dislocations. The assumption that a microplasticity is formed in the vicinity of dislocation is justified because the results of macro scale regularities agree with known experimental data.

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