International Journal of Emerging Technology and Advanced Engineering
Website: www.ijetae.com (ISSN 2250-2459, ISO 9001:2008 Certified Journal, Volume 5, Issue 11, November 2015)

An Analysis of the Phenomenon of Strain Hardening of Single Crystals

Arakelyan M. M.

Yerevan State University, Faculty of Physics, Department of Solid State Physics, 1 Al. Manoogian, Yerevan 0025, Armenia.

***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 microprocesses.**

***Keywords*—Aluminum, dislocations, Peierls relief, hardening, Frenkel-Kontorova model, sine-Gordon equation.**

I. Introduction

The cold plastic strain is generally known to lead to significant interdependent changes in the shape, dimensions and physico-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 of $\sigma = K\varepsilon^n$ form, where the hardening parameters K, n are determined from experimental data on tensile tests of this material, σ being 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). It is evident that the higher is the potential barrier, the larger are the external forces required for sliding of dislocations. In case of $\sigma > \sigma_p$ (σ is the applied stress, σ_p is the Paierls stress) the motion of dislocations corresponds to the classical case, but at $\sigma < \sigma_p$ the motion of dislocations is due to the thermoactivated surmounting of potential barriers accomplished by way of fluctuational initiation of inflections (breaks) of the dislocation line in sliding plane. At very low temperatures and stresses the motion of dislocations may be realized by means of quantum tunneling under the Peierls barriers [2].

It is known that for pure single crystals in case of strain rate of 10^{-6} 1/s, the stresses required for initiation of plastic strain (starting stresses) may be a few tenths of N / mm^2. This is obviously due to the fact that in the presence of thermal fluctuations even the minimum loads may cause a directional displacement of dislocations, and, hence, a plastic strain.

Experimentally it was established that to a given threshold stress there corresponds a definite constant velocity of motion of dislocation rather than their acceleration, as it should have followed from the Newton's second law. This effect may be due to the fact that the travel of dislocation in the plane of sliding should be hindered by some force that increases with the travel speed. This force is usually referred to as the internal friction force that is responsible for dissipation of elastic energy. One of causes of internal force is the interaction of moving dislocation with the lattice Peierls relief, with impurity atoms etc.

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.

IJETAE
EXPLORING RESEARCH AND INNOVATIONS

International Journal of Emerging Technology and Advanced Engineering
Website: www.ijetae.com (ISSN 2250-2459, ISO 9001:2008 Certified Journal, Volume 5, Issue 11, November 2015)

At present the accuracy and performance capabilities of experimental technique permit to observe the motion of separate dislocations in a crystal and explain the mechanism of dislocation travel in more detail. In case of low density of dislocations (10^2 - 10^3 cm^{-2}) in aluminum, when the interaction between them is negligible, the dislocations are observed as straight lines along crystallographic directions with small indices, that is indicative of the influence of the Peierls barrier [3].

The experiments showed notably diminishing of the yield point and of the growth gradient of strain hardening with application of ultrasound waves . This is because the sound vibrations facilitate the passage of both the grain barriers, and the ones that are due to the crystal structure. The mobility of dislocations may be affected by vibrations of dislocation segments, macroscopic viscosity of metals at plastic strain etc. The amplitude-independent internal friction is also observed at passage of high frequency ultrasound [4]. The motion within the Peierls relief (discreteness of the lattice) stimulates the emergence of dynamic losses as well. 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.

II. THEORETICAL FRAMEWORK

In the present work the motion of dislocations in aluminum with allowance for Peierls relief is considered. Owing to the presence of Peierls relief during the motion of dislocation in a crystal, its configuration and elastic energy experience periodic changes giving rise to dynamic losses, as the periodical variations of dislocation configuration and nonuniformity of its motion lead to emission of elastic waves by the dislocation, i.e., to the internal friction.

In general, from the dislocational viewpoint an analysis of hardening phenomenon is a complicated problem. Consequently, for description of dislocation phenomena we used the one-dimensional Frenkel-Kontorova model. In this model the action of neighboring atoms in the upper layer is represented by springs, and the action of the substrate – by a periodic sine wave. This model has some advantages in comparison with other ones: in this model the discrete approach is used, here pursuant to the experiment the Peierls energy decreases with increasing dislocation width, the Peierls stress is also consistent with experimental data in order of magnitude, $\sigma_p \sim 10^{-4}\mu - 10^{-2}\mu$, $\mu -$ is the shear modulus of crystal [3].

The motion of dislocations is assumed to have the thermal activation mechanism. The mathematical modeling of dislocation motion in the periodic field in the framework of adopted model allows to obtain information about the characteristics and mobility of dislocations [5]. Thus, the time of dislocation transition to the neighboring valley of potential relief is changed depending on external field frequency. Accordingly, the free path of dislocation must change. The time of loaded state changes with decreasing frequency. If the load action time is less than the formation time of critical size double kink, the dislocation will have no time to go to the neighboring valley of potential relief and the remaining double kinks will annihilate. Otherwise, the dislocation will move into the next valley and its free path will increase [5]. The dynamics of individual dislocations in silicon single crystals at loading with periodical pulse-loads commensurate with the time of dislocation transition to the next valley has been experimentally studied in [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 inhomogeneous sine-Gordon equation with friction and periodic external elastic stress $\sigma(t) = \sigma_0 e^{i\Omega t}$, where σ_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:

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

where y_n -is the displacement of the n-th atom from the equilibrium position, m is the mass of atom, $f_0 = \frac{m(v_0)^2 a}{2\pi (l_0)^2}$, 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.

International Journal of Emerging Technology and Advanced Engineering
Website: www.ijetae.com (ISSN 2250-2459, ISO 9001:2008 Certified Journal, Volume 5, Issue 11, November 2015)

In dimensionless units $x = \frac{v_0}{\omega}\tilde{x},\ \ t = \frac{t}{\omega}$ the equation assumes the form of inhomogeneous sine Gordon equation

$$\ddot{\varphi}_n + \sin\varphi_n - \varphi_n'' + \beta\dot{\varphi}_n = \gamma \sin\frac{\Omega t}{\omega}, \qquad (2)$$

$\omega^2 = \frac{2\pi f_0}{ma}, v_0 = a\sqrt{\frac{k}{m}}, \beta = \frac{\mu_0}{m\omega}, \gamma = \frac{2\pi F_0}{ma\omega^2}$, μ_0 is the coefficient that characterizes the friction, φ_n is the displacement of the n-th atom from the equilibrium position in angular units.

The resulting equation admits analytical solutions in particular cases. In more complex cases, approximate solutions of inhomogeneous sine - Gordon equation are obtained using the perturbation method (e.g., [7]). And we investigate the solutions of inhomogeneous sine-Gordon equation numerically.

III. Results And Discussion

The modeling was carried out using Mathematics Routine. In case of external frequency of 10^{12} Hrz the time scale is $2,5*10^{-6}$.

The displacement and deformation in the Frenkel-Kontorova model are known to have the form (Fig. 1) (numerical experiment).

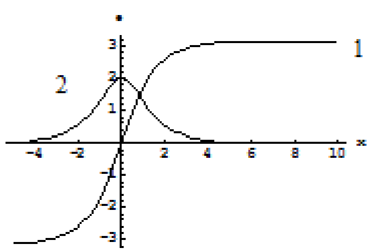

Figure 1. Displacement (1) and strain (2) field for dislocations in the Frenkel-Kontorova model

As is seen in the plot, the strain (bell-shaped curve) has the character of soliton localized on the dislocation line.

A numerical experiment has been conducted for three dislocations that at the initial time are in the origin of coordinates. One of these moves the frictional force is taken onto account, the other – when the frictional force and variable elastic field are taken into account, and the third one executes the free sliding.

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]. Such an infinite relaxation time is due to the friction force acting on the dislocation from the Peierls relief or point obstacles. For comparison, the third dislocation makes free sliding (Fig.2).

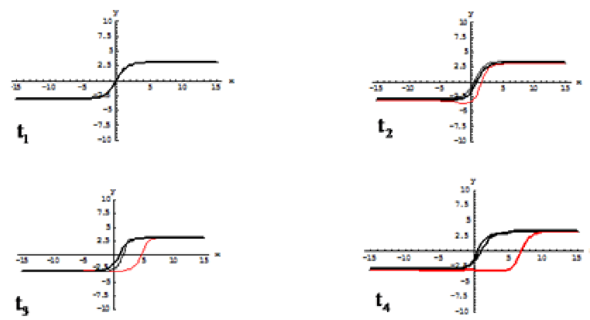

Figure 2. Motion of dislocations at successive instants of time: (1) free sliding; motion with allowance for friction force (thick curve), motion with allowance for friction force and variable elastic field.

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 (Fig.3).

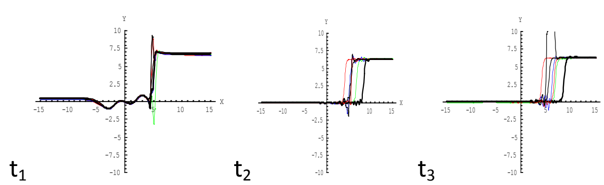

Figure 3. The free path lengths of dislocation for different frequencies

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. (Fig.4.)

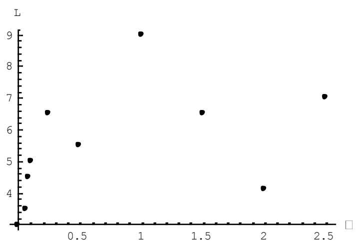

Figure 4. Dependence of free path length of dislocations on frequency of variable elastic field

It is seen in Fig.4 that at a certain frequency the free path length of dislocation is maximum. It is obvious that the formation of noncollapsing double kink corresponds to the 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 aluminum has a thermally activated mechanism.

According to [1] the dependence of stress on strain in ductility macroscale is as follows:

$$\sigma = k\varepsilon^n,\ n = \ln\left(1+\delta\right),\ \ k = \sigma_b * e^n n^{-n}, \qquad (3)$$

Where σ is the stress, ε - the accumulated strain, σ_b - tensile strength, δ - relative tensile strain.

The dependences $\sigma(\varepsilon)$ have been constructed in the presence and absence of resonant frequency. Prior to that we constructed the dependences $\sigma(x)$. In the presence of external mechanical frequency the dependence $\sigma(x)$ has a form shown in Fig.5

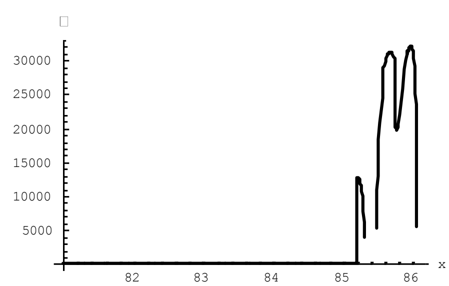

Figure 5. Dependence of stress of coordinate in the vicinity of dislocation (with external variable elastic field)

Respectively, the dependence $\sigma(\varepsilon)$ in the ranges of monotonous growth of function $\sigma(x)$ is seen to be in Fig.6.

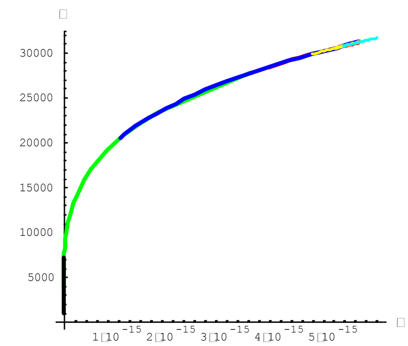

Figure 6. The stress-strain dependence (in the presence of external variable elastic field)

The dependence of stress on coordinate in the absence of external frequency is shown in Fig. 7. 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. The motion of dislocation with due regard for the potential relief of crystal proceeds as follows: a double kink is formed on the dislocation under the influence of thermal activation, and further travel of kinks in different directions occurs at very small stresses. Thus, the sliding event is a stage wise process. But how the dislocation rate is changed in this case?

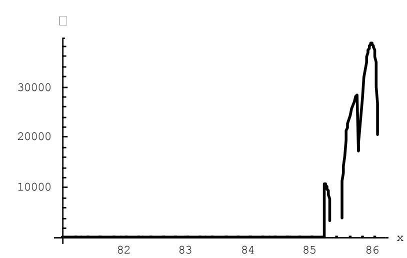

Figure 7. Dependence of stress on coordinate in the vicinity of dislocation (in the absence of variable elastic field)

In the region of third rise in the dependence of stress on coordinate (Fig.7) (motion from the valley to the potential relief) the dislocation rate decreases, and increases on the slope (potential relief – the next valley). The corresponding graph is shown in Figure 8.

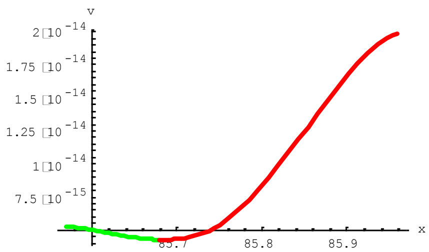

Figure 8. Dependence of dislocation rate on coordinate in the vicinity of Peierls barrier

It is seen in figure 8 that the dislocation gets over the Peierls barrier really at variable speed. Such a character of dislocation travel is possible only in case of changeable resistance 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. Based on this fact it is assumed that there is a micro plasticity region around the dislocation. So, one can assume that in the plasticity state realized in the vicinity of dislocation the stress-strain dependence for aluminum is determined by formula (3), where the value $\sigma_b = 73.5*10^7\ dn/sm^2$ (Al) is used. 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 (Fig.9).

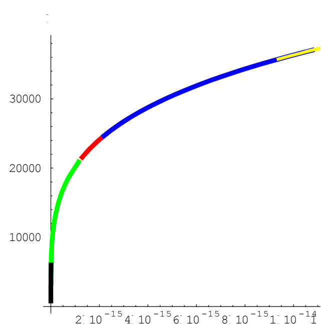

Figure 9. Dependencies of stress on strain in the absence of external field

The slope of monotonically increasing curve $(d\sigma / d\varepsilon) = \theta$ 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].We have obtained the dependence of hardening coefficient on coordinates in the absence and presence of external field (Fig.10).

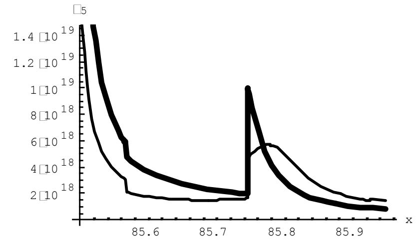

Figure 10. Dependence of hardening coefficient on coordinates in the vicinity of dislocation (thin line corresponds to the case of resonance frequency application), the bold line – to the absence of trequency

As is seen in Fig.10, to each 3 clearly distinguished sections there correspond different dependences of hardening coefficient on coordinate. In the presence of resonant ultrasound the dependence of hardening coefficient on coordinates is changed, the hardening coefficient being reduced.

The hardening in this case is apparently due to the dissipation of energy at the motion of dislocation in the Peierls relief.

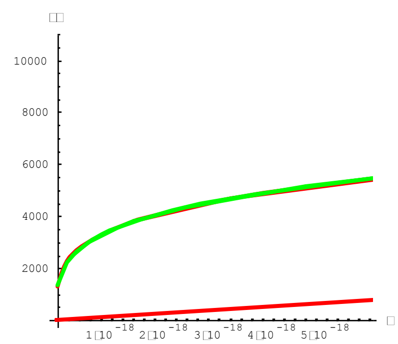

Figure 11. Dependencies of stress on strain in the absence (the upper curve) and presence of variable elastic field

In Fig.11 the curves of stress-strain dependences in the presence and absence of sound are given.

It is seen in the figure 11 that in the presence of sound the gradient of the growth of hardening curve decreases, and, hence, the yield stress is decreased.

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

For instance, let us examine the plot of the dependence of stress versus the coordinate (Fig.7)

International Journal of Emerging Technology and Advanced Engineering
Website: www.ijetae.com (ISSN 2250-2459, ISO 9001:2008 Certified Journal, Volume 5, Issue 11, November 2015)

If x in the (2) equation changes from 85.9 to 85,905 (top of the barrier), then the stress -to- strain dependence takes on the form (Fig.12). I.e., at over-barrier motion of dislocation the dependence of stress on strain demonstrates an elastic behavior.

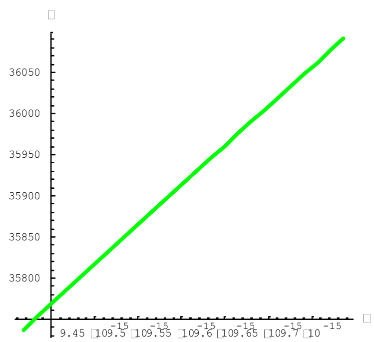

Figure 12. The dependence of stress on the strain in case of over-barrier motion

When x changes from 86 to 86.1(region of slope on $\sigma(x)$ curve), then the dependence of stress on strain as shown in Fig. 13 has a plasticity range.

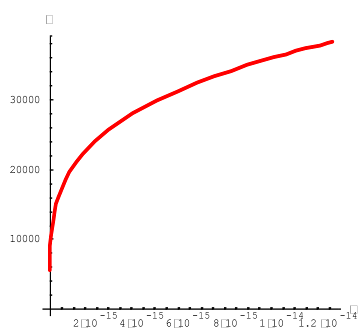

Figure 13. Dependencies of stress on strain in the region of monotone dependence in $\sigma(x)$ plot

So, one can conclude that in overcoming the Peierls barrier the dislocation at the micro level periodically passes from the micro plasticity to the elasticity regions.

IV. CONCLUSION

In aluminum, at room temperature the motion of dislocation in the Peierls relief is uneven by slowing down in front of the Peierls barrier and speeding after overcoming that. In the vicinity of dislocation a region of microplasticity is realized. At the application of external variable elastic field the free path length of dislocation is changed, it being controllable as a function of the frequency (of the field). The pinning of dislocation after passage of some distance is an indication of crystal hardening .In the presence of external elastic field the gradient of hardening curve growth decreases, implying that the yield stress will also decrease. 3 sections clearly differ in the dependence of hardening coefficient on coordinate that are characterized by different mechanisms of strain and hardening. The dislocation structure is changed at each stagewise. The hardening coefficient is reduced in the presence of resonant frequency. In this case the hardening is due to the dissipation of energy during the motion of dislocation in the Peierls relief.

REFERENCES

[1] Hosford W.F., Caddell R.M.. Metal Forming. Cambridge , 2007.

[2] Estrin Yu.Z., Isaev N.V., Grigorova T.V., Pustovalov V.V., Fomenko V.S., Shumilin S.E., Braude I.S., Malykhin S.V., Reshetnyak M.V., Yanechek M.. Low Temperature Plastic Strain of Ultrafine Aluminum. Physics of Low Temperatures. Vol. 34, N 8, (2008), 842-851.

[3] Hirth J., Lothe J.. Theory of dislocations.New York, 1972.

[4] Alshits V.I., Indenbom V.L.. Dynamic braking of dislocations. Uspekhi Fizi`eskikh Nauk, Vol. 115, Is. 1, (1975) 3-39.

[5] Nikitenko V.I., Farber B.Ya., Iunin Yu.L.. On the Possibility of Experimental Study of Formation Kinetics and Mobility of Kinks on Dislocation Line. Pis'ma v JETF, Vol.41, Is.3, (1985), 103-105.

[6] Melik-Shakhnazarow W.A., Mirzoeva I.I., Naskidashvili, I.,A.,"Tunneling of the dislocation kink in aluminium". Pis'ma v JETF, 43(5), (1986) 247-249.

[7] Fogel M.B., Trullinger S.E., Bishop A.R., Krumhansl J.A.Phys.Rev.v.15, N3, (1977) 1578-1592.

[8] Malygin G.A.. The Processes of Self-Organization of Dislocations and the Plasticity of Crystals. Uspekhi Fizi`eskikh Nauk, Vol.169, N 9, (1999) 979-1010.

[9] Orlov A.N.. Introduction to the Theory of Defects in Crystals. Moscow, 1983.