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Microscopic constitutive equations for plastic deformation of an alloy system

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A theoretical expression for an average velocity of mobile dislocations is derived by incorporating dynamic effects and thermal activation process. Combined with constitutive equation for mobile dislocation density,a stress- strain curve is calculated. The anomalies due to normal-superconducting transitions are qualitatively reproduced.

1. Introduction

Among various quantities characterizing dislocations behavior, central quantities are density N_m and average velocity $\overline{v}$ of mobile dislocations. It was shown by Johnston and Gilamnn [1] that the semi-empirical knowledge of these quantities enable one to draw a stress-strain curve by substituting them into a constitutive equation given by

$$\frac{d\tau_a}{dy_c} = \left(1 - \frac{l_0 \cdot f_s \cdot N_m \cdot b \cdot \overline{v}}{S_c}\right) \cdot \frac{f_s \cdot K}{A}, \quad (1)$$

where y_c, l_0 and A are, respectively, the displacement, initial dimension and cross sectional area of a sample, f_s the Schmid factor, S_c the crosshead speed and K is the rigidity of the machine-sample combined system.

Haasen and Alexander [2], then, proposed an equation describing the evolution and devolution of mobile dislocations density, N_m, in the following differential form;

$$\frac{dN_m}{dy} = \frac{1}{S_c} \cdot B_m \cdot \tau_{eff} \cdot N_m \cdot \overline{v}, \quad (2)$$

where B_m is a materials parameter specifying the multiplication rate. Noticeable in the above equation is the fact that the work hardening due to multiple dislocations is well incorporated by *feed back* effect through effective stress τ_{eff} given as

$$\tau_{eff} = \tau_{app} - \frac{\mu \cdot b \cdot N_m^{\frac{1}{2}}}{\beta}, \quad (3)$$

where μ and β are, respectively, the rigidity of a sample and the Taylor factor. The second term represents long range back stress field created by multiple dislocations which function to suppress further multiplications.

In order to consolidate the theoretical basis for the stress-strain relationship, one needs to elucidate microscopic mechanism of determining the average dislocation velocities, $\overline{v}$. The purpose of the present brief article is to derive the constitutive equation for $\overline{v}$ to be combined with eqs. (1) and (2) in order to draw a stress-strain curve. A particular emphasis is placed on the cryogenic temperature for which *dynamic effects* induce various intriguing anomalies.

2. Theoretical Model

We start with the string model [3] to describe a moving dislocation motion which is given as

$$m \cdot \frac{\partial^2 y}{\partial t^2} + B_d \cdot \frac{\partial y}{\partial t} - \Gamma \cdot \frac{\partial^2 y}{\partial x^2} = \tau_{eff} \cdot b, \quad (4)$$

where m is the mass of a dislocation, t the time, x and y are the space coordinates in the directions of extension and motion of a dislocation line, respectively, B_d is the damping constant due to various media such as electrons, phonons etc., Γ the line energy per unit length, b the Burgers vector and τ_{eff} represents effective stress which is the difference between the applied stress τ_{app}

and internal stress τ_{in} caused by other dislocations. The leading two terms represent *inertia* and *damping* of a moving dislocation which are termed *dynamic effects* manifested at cryogenic temperatures, while the third term together with the effective force describes static mechanical equilibrium condition. The solution of the above second order partial differential equation under the boundary conditions, $y(0,t) = y(\overline{L},t) = 0$, and initial conditions, $y(x,0) = 0$ and $\partial y/\partial t = v_0$ is given as

$$y = \frac{b \cdot \tau_{eff}}{2\Gamma}\left(\overline{L} - x\right)x - \frac{4\tau_{eff} \cdot b \cdot \overline{L}^2}{\pi^3 \Gamma} \cdot \exp\left(-\gamma t\right) \sin\left(\frac{\pi x}{\overline{L}}\right) \cdot \cos\left[\omega_0 \left(1 - \frac{\gamma^2}{\omega_0^2}\right)^{\frac{1}{2}} t\right], \quad (5)$$

where v_0 is the initial velocity, $\overline{L}$ the average separation of obstacles along a dislocation line and γ and ω are measures of the damping defined as $\gamma = B_d/2m$ and $\omega_0 = \left(\pi/\overline{L}\right)\left(\Gamma/m\right)^{1/2}$. It is noted that the second term of eq.(5) is the dynamic contribution which modifies a solution of the static equilibrium equation given by the first term.

It is noted that a dislocation overcomes an obstacle with the aid of thermal assist even at cryogenic temperatures [4]. The thermal activation process has been successfully described within a framework of Eyring's rate theory and the activation energy, ΔG^*, is written as

$$\Delta G^* = G_0 - W_d \quad (6)$$

where G_0 is the interaction energy between an obstacle and a dislocation and W_d is the work performed by a dislocation. The difficulty, however, stems from the fact that the thermal activation process is a stochastic process while the dislocation motion described by eq.(4) is fully deterministic process. An incorporation of these two characters in a single theoretical framework claims a sophisticated statistical mechanical approach [5], which is beyond the scope of the present study. Following Suzuki's prescription [6], we circumvent this difficulty by averaging a force on an obstacle, $F(t)$, originating from a line tension of a vibrating dislocation line during a relaxation time:

$$\frac{1}{1/\gamma^*}\int_0^{\frac{1}{\gamma^*}} F\left(t\right)dt \approx \frac{1}{1/\gamma^*}\int_0^{\frac{1}{\gamma^*}} 2\Gamma\left(\frac{dy(t)}{dx}\right)_{x=0} dt. \quad (7)$$

One can readily show that the equation (7) is reduced to $\tau_{eff} \cdot \overline{L} \cdot b \cdot \overline{Y_m}$ in which the product of the first three terms is nothing but the force exerted on an obstacle by a dislocation in the static equilibrium state. Hence, $\overline{Y_m}$ defined as

$$\overline{Y_m} = 1 + \frac{e^z}{1/\gamma}\int_0^{\frac{1}{\gamma}} e^{-zt}dt \cong 1 + 0.6e^{-z}, \quad (8)$$

where z given as $\left(\pi\gamma\right)/\omega_0$ specifies the magnitude of the dynamic effects. The larger the deviation of $\overline{Y_m}$ from unity is more significantly the dynamic effects are realized. By confining our attention to a *point – like* obstacle of which width is specified by d ($d << \overline{L}$), the work performed by a dislocation in eq.(6) is given as $W_d = \tau_{eff}\overline{L}bd\overline{Y_m}$. Thereby, the thermal activation process is incorporated in the description of a vibrating dislocation motion.

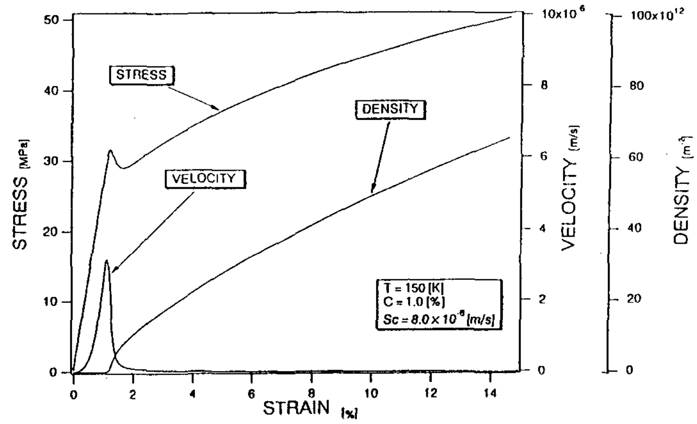

Figure 1: Stress-Strain curve calculated for $T = 150K$, $C = 1.0\%$, and $S_c = 8.0 \times 10^{-6}[m/sec.]$. Average velocity and density of mobile dislocations are also demonstrated. The other parameters are tabulated in Table 1.

The estimation of $\overline{L}$ claims a *statistical* problem, since the averaging process of the separation of obstacles *along* a dislocation critically depends on the curvature of a dislocation line which is a function of various parameters such as the stress, concentration of obstacles, line tension etc. Friedel [7] demonstrated that, in the limit of dilute solid solution containing only single type of point obstacles, $\overline{L}$ is given as

$$\overline{L} = \left[\frac{2b\Gamma}{C}\right]^{\frac{1}{3}} \cdot \tau_{eff}^{-\frac{1}{3}}, \quad (9)$$

where C is the concentration of the obstacle. The validity of the application of Friedel's statistics to the present case in which both dynamic effects and thermal activation process are involved is still open to questions. Yet, our preliminary analysis[8] suggests that the obtained results are not seriously hampered within the range of the employed conditions which will be demonstrated in the next section.

initial cross sectional area of a specimen	:	$A = 7.5\times10^{-6}[m^2]$
initial length of a specimen	:	$l_0 = 2.0 \times 10^{-2}[m]$
stiffness of the testing system	:	$K = 5.0 \times 10^3[Pa \cdot m]$
Schmid factor	:	$f_s = 0.4$
Burgers vector	:	$b = 2.8635 \times 10^{-10}[m]$
Boltzman constant	:	$k = 1.3806 \times 10^{-23}[J/K]$
Debye frequency	:	$\nu_D = 4.43 \times 10^{12}[1/sec]$
strength of an obstacle	:	$G_0 = 3.701 \times 10^{-20}[J]$
mass of a dislocation per unit length	:	$m = 2.214 \times 10^{-16}[kg/m]$
constant specifying the multiplication rate of dislocations	:	$B_m = 2.5 \times 10^{-5}$
shear modulus of a specimen	:	$\mu = 2.8 \times 10^{10}[Pa]$
parameter characterizing the interaction between dislocations	:	$\beta = 1.613$
damping constant	:	$B_d = 5.0 \times 10^{-6}[N \cdot sec \cdot m^{-2}]$

Table 1: Parameters for the calculation

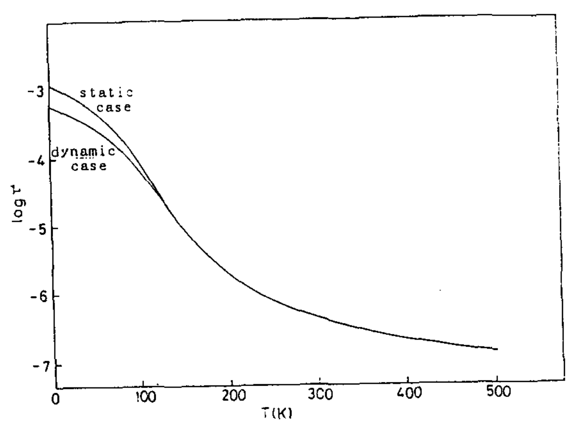

Figure 2: Temperature dependency of the effective stress with and without dynamic effects.

Unlike the case of *viscous* motion, the rate process of *spurt – like* motion is determined by the activation frequency, $\dot{P}+$, at an obstacle defined as

$$\dot{P}+ = \frac{P}{t_w}, \tag{10}$$

where P is the number of obstacles interacting with mobile dislocations given as

$$P = \frac{N_m}{\overline{L}} \tag{11}$$

and t_w is the waiting time at an obstacle which is related to the activation energy of eq.(6) by

$$\frac{1}{t_w} = \nu \exp\left(-\frac{\Delta G^*}{kT}\right). \tag{12}$$

With the Debye frequency, ν_D, the trial frequency ν is further expressed as $\nu = \left(b/2\overline{L}\right)\nu_D$.

In the spirit of Friedel statistics, the area swept out by a dislocation line which overcomes an obstacle is equivalent to the average area, $L_s^2 \left(= b^2/C\right)$, occupied by an obstacle in a slip plane. Then, the microscopic strain rate, $\dot{\epsilon}$, is expressed as

$$\dot{\epsilon} = \dot{P}+ \left(L_s\right)^2 b. \tag{13}$$

Substitution of eqs.(10)-(12) into the above equation yields

$$\dot{\epsilon} = \frac{N_m}{\overline{L}}\nu \exp\left(-\frac{\Delta G^*}{kT}\right)\left(L_s\right)^2 b. \tag{14}$$

From the above equation, the average velocity, $\overline{v}$, is deduced as

$$\overline{v} = \left(\frac{L_s^2}{\overline{L}}\right)\left(\frac{b \cdot \nu_D}{2\overline{L}}\right)\exp\left(-\frac{\Delta G^*}{k \cdot T}\right). \tag{15}$$

Note that, in the deduction of $\overline{v}$, viscous nature and spurt-like nature are not clearly distinguished, which remains to be settled in the future investigation.

3. Results and Discussions

Among various results obtained [8], we reproduce three major results. Listed in Table 1 are the parameters employed in the calculations. The materials constants such as b, ν_D, m, μ simulate aluminium matrix and all other parameters are relevant to standard testing conditions. The strength of an obstacle, G_0, is estimated based on the elastic interaction between Al and Mg.

A typical stress-strain curve obtained in the present model is demonstrated in Fig. 1 together

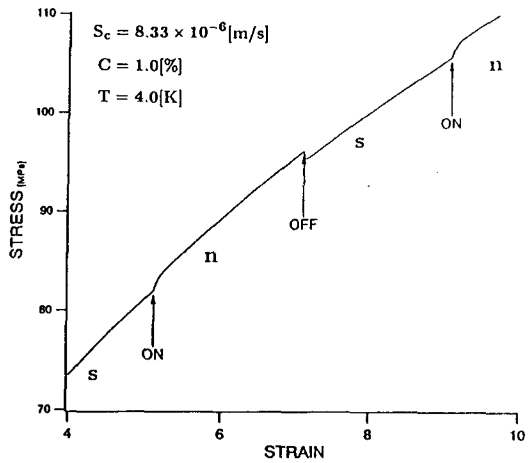

Figure 3: Simulation of a stress-strain curve during the cyclic variation of superconducting-normal transition.

with $\overline{v}$ and N_m. One sees that $\overline{v}$ increases drastically at the yielding and that the monotonous increase of N_m causes work hardening. We also confirmed that the deformation stress increases with increasing C and S_c and with decreasing T.

Shown in Fig. 2 are the temperature dependances of effective stress with and without $(\overline{Y_m} = 1)$ introducing the dynamic effects. The concentration of obstacles and a crosshead speed are fixed. The overall dependency for both cases indicates a typical thermal activation behavior. However, one notices that a single curve split into two curves in the low temperature region and less stress is required with dynamic effects. This indicates that the thermal activation and dynamic effects are complementary each other and the loss of thermal activation energy can be compensated by the dynamic effects under a fixed strain rate.

Various anomalies have been reported [9] in the cryogenic temperature region. Among them, most striking one is the softening and hardening phenomena due to the cyclic transition between the superconducting and normal states. The physical origin is attributed to the phonon-electron coupling which modifies the damping constant, B_d, which is further ascribed to the increase (normal state) and decrease (superconducting state) of the effective number of conduction electrons. We attempt to simulate this behavior by introducing the cyclic variation to B_d between 1.3 $\times 10^{-5}[N \cdot sec/m^2]$ for the normal state and one third of it for the superconducting state. The resultant stress-strain curve demonstrated in Fig. 3 qualitatively reproduces the experimental tendency. The details of the relaxation behavior associated with the transitions will be reported in a forthcoming issue.

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