ABSTRACT

A THEORETICAL STUDY OF DISLOCATION EFFECTS
ON THE STATIC AND DYNAMIC MODULI OF CRYSTALS

by David H. Y. Yen

The relation between the static and dynamic moduli of a perfect crystal is derived from the laws of thermodynamics. However, if a crystal contains impurities, this relation is much more complicated. In this paper, the effects due to dislocations are studied.

The nonlinear stress-dislocation strain law derived by Granato and Lucke to account for a strain amplitude dependent internal friction is used to define the change of effective static modulus. The stress-dislocation strain law depends on the distribution function of dislocation loop lengths. A different distribution function is suggested and a different stress-dislocation strain law derived. Numerical results of the changes of static and dynamic moduli are obtained by using both stress-dislocation laws. The results are also compared and discussed.

A THEORETICAL STUDY OF DISLOCATION EFFECTS ON THE STATIC AND DYNAMIC MODULI OF CRYSTALS

By

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LIST OF SYMBOLS

A: Effective mass per unit length of dislocation

B: Damping force per unit length of dislocation

C: Effective tension in dislocation

G: True shear modulus

I: Unit matrix

L_N: Network length of dislocation; average value of L_N's

L_C: Length of dislocation segment separated by impurities; average value of L_C's

$N(l)dl$: Distribution function of dislocation loops

Q: $\frac{8a^2 \Lambda L_c^2 3!}{\pi^4 C}$

Q': Slope of the $\sigma - \varepsilon_{dis}$ curve

T: Temperature

Z: Distance between an impurity and dislocation axis

a : Atomic spacing; Burger's vector of dislocation

c_{ij} : Elastic contant matrix

c_p: Specific heat capacity

$\bar{f}$: Cottrell's force

q: $\frac{\mathcal{L}}{L_c}$

r: Ratio of internal friction to change of dynamic modulus

s_{ij} : Elastic compliance matrix

k: wave number

v: Velocity of stress wave propagation

α_i, α_j : Changes of strains $\varepsilon_i, \varepsilon_j$ with temperature

γ : L_N/L_c

LIST OF SYMBOLS CONTINUED

ε': Difference in atomic radii of solute atom and solvent atom divided by the atomic radius of the solvent atom

ε_{el}: Elastic strain

ε or ε_{total}: Total strain

ε_{dis}: Dislocation strain

ε_N : Strain at which the stress-dislocation strain relation starts to be nonlinear

σ : Stress component

σ_N : Stress at which the stress-dislocation strain relation starts to be nonlinear

ν : Poisson's ratio

ω : Frequency

Λ : Dislocation density

Γ : $\frac{\pi^2 f}{4aL_c}$

$\mathcal{L}$: Characteristic length of dislocation determined by

ξ : Dislocation displacement

CHAPTER I

INTRODUCTION

In the study of theory of elasticity, the generalized Hooke's Law is postulated after the concepts of stress and strain are introduced and formalized. It is well known that this generalized Hooke's Law, being the starting point of traditional elasticity, has the form of a 6 by 6 square matrix for a completely anisotropic medium, i.e., the constants c_{ij} between stress and strain components in the following system of equations

$$\sigma = \sum_{j=1}^{6} c_{ij}\, e_j \qquad (i = 1, 2, \cdots 6) \qquad (1-1)$$

take up 36 independent values. However, depending upon the existence of a strain-energy function and the symmetry properties of a specific material, this number of independent elastic constants is greatly reduced. In the simplest case for a material which possesses complete isotropy, there are only two independent elastic constants.

Because in engineering design the values of these elastic constants are at least equally as important as the mathematical theory of the strength of materials itself, the measurement of elastic constants of materials has had a long history. Results of such measurements on various materials by previous researchers have been reviewed and summarized in the papers by Hearmon (1946;1956)[1,2] and by Huntington (1958).[3]

According to the ways these measurements are made, the elastic constants have the names of static and dynamic constants. In the former case the modulus is obtained by directly measuring the stresses and strains, while in the latter case measurements may be made, for example, by using resonance techniques to obtain the velocity of stress wave propagation through the material; therefrom the elastic constants are calculated.

Static methods give the isothermal constants, in the sense that the temperature is kept constant during the measurement; while dynamic methods give the adiabatic constants, implying that during the measurement heat neither flows in nor flows out. For a perfect crystal, these two constants are related by the following equation

$$[S_{ij}]_{static} - [S_{ij}]_{dynamic} = \frac{\alpha_i \alpha_j T}{\rho c_p} \qquad (1\text{-}2)$$

where $[S_{ij}]$, the elastic compliances matrix is defined as the inverse of the elastic constants matrix, i.e.,

$$[c_{ij}][S_{ij}] = I \qquad (1\text{-}3)$$

Equation (1-3) can therefore be written as

$$[c_{ij}]^{-1}_{static} - [c_{ij}]^{-1}_{dynamic} = \frac{\alpha_i \alpha_j T}{\rho c_p} \qquad (1\text{-}4)$$

Here $\alpha_i \alpha_j$ are the changes of strains $\epsilon_i \epsilon_j$ with temperature T, ρ is the density, and c_p the specific heat capacity. It is seen from equation (1-4) that the static and dynamic constants are directly related by the thermodynamic properties of the material.

For a crystal which is other than perfect, it is expected that the imperfections will affect the relationship between static and dynamic constants in equation (1-4). While the meaning of the expression "imperfections in crystals" has many implications, namely the following six primary types of imperfections:

(a) phonons

(b) electrons and holes

(c) excitons

(d) vacant lattice sites and interstitial atoms

(e) foreign atoms in either interstitial or substitutional positions

(f) dislocations

and the following three transient imperfections

(g) light quanta

(h) changed radiations

(i) unchanged radiations,

it is only the effects of dislocations and those which interact with dislocations during their motions under the action of stresses that will be studied in what follows.

In 1941, Read[4] first suggested that dislocation motion under applied stress might contribute to the observed strain and give rise to that portion of the internal friction in metals which cannot be explained by other mechanisms. There have been a great number of theoretical as well as experimental investigations since Read's suggestion on the effects of impurities, and of cold work and annealing of the specimens. Among them, Koehler (1952) made a theoretical study of the influence of dislocations and impurities on the damping and the elastic constants of metal single crystals by using the idea that the motion of a dislocation under an oscillating stress can be considered analogous to the motion of a damped vibrating string. By the method of successive approximations Koehler solved the differential equations of motion and was thereby able to express the internal frition loss and change of elastic modulus as a function of frequency. He also derived expressions for the strain-amplitude dependent internal friction loss and change of elastic modulus by using the idea that the dislocation line would break away from the impurity atoms at large strain amplitudes.

Koehler's vibrating string model was further developed by Granato and Lücke (1956)[6], who solved the differential equations of motion in a much more general way, making it possible to consider the dependence of the internal friction loss and change of elastic modulus on the loop length for all frequencies.

The vibrating-string model, as developed by Granato and Lücke, leads to two types of loss and change of modulus. The first type is a dynamic one due to the damping of the vibrating dislocation segments, and is strain-amplitude independent. The second type is due to the fact that during the loading and unloading parts of the stress cycle, points on the stress-dislocation strain diagram do not follow the same path, thus giving rise to a hysteresis loop. For low frequencies, the kilocycle range, the stress-dislocation strain relationship is independent of frequency, and so are the internal friction loss and change of elastic modulus.

As this paper is not primarily concerned with the internal friction and change of elastic modulus in various materials as functions of frequency, amplitude, and the degree of impurity, but rather with the static and dynamic elastic constants in a dislocation-containing crystal, a review of the various theories on the internal friction and change of elastic constants will not given here. However, it is interesting to note that in order to account for a strain-amplitude dependent internal friction loss and change of elastic modulus, a hysteresis loop in the stress-dislocation strain diagram was suggested in the Granato and Lücke development by extending the idea of breakaway first used by Koehler. It was found that both the internal friction and the change of dynamic constant are directly proportional to the area of the hysteresis loop on the stress-dislocation strain diagram, with the two proportionality constants being of the same order of magnitude.

The static modulus of a crystal is obtained from the stress-strain curve under static loading. Theoretically, the load is applied to the specimen in a time of length infinity. Under this type of loading one can not expect to have the same stress-dislocation strain relation as obtained before, as judged from a theoretical point of view, since the impurities will not pin the dislocations in the way suggested, but follow the applied stress in a diffusion process.

However, as the diffusion process is an extremely slow one, while in actual practice the static loading and unloading is always accomplished in a finite length of time, it is reasonable to assume that diffusion of impurities will not occur in actual cases. Under this assumption, the string model and idea of breakaway can still be applied.

The stress-dislocation strain loop is dependent on the magnitude of the maximum stress. The path of a point on the loop is non-linear during the increasing-stress portion of the cycle due to successive breakaways of the dislocation line from impurities. But the path during decreasing stress is linear since the entire bowed-out dislocations come back to their original position as single loops. This linear portion occurring during unloading will be used to define the effective static modulus, which is dependent on the maximum stress as mentioned above.

In the following chapter, both the effective static modulus and the dynamic modulus as a function of the maximum stress, and,hence a function of the hysteresis loop, will be studied and compared numerically. Furthermore, as the hysteresis loop in the stress-dislocation strain diagram also depends on the distribution function of dislocation loops (i.e., the number of loops for a given length l as a function of l) under each stress, it is expected that a different distribution of dislocation lines from the one used by Granato and Lücke will affect the hysteresis loop and hence the relationships between the static and dynamic modulus. In the Granato and Lücke theory, the initial distribution of loop lengths L_c(the lengths determined by impurity atoms) is an exponential function, while in the final stage the lengths have a delta function distribution with L_n, the network length, equal to a constant. There remains the contradiction that in the initial distribution of L_c there are lengths greater than L_n. For this reason, an alternate assumption is made about the distribution of loop lengths after the breakaway from impurities occurs, and the consequent results are studied and compared.

CHAPTER II

THEORY

In this chapter, a brief summary of the vibrating string model of dislocation movement under stress, as developed by Granato and Lücke, will be given in Section 1. Section 2 covers the derivations of the functional dependencies of the distribution of dislocation loop lengths on stress suggested by Granato and Lücke, as well as those suggested by the author of this paper. In Section 3, the stress-dislocation strain laws as consequences of the derivations of Section 2 will be given. The definition of static effective modulus and its relation to the dynamic modulus as a result of the stress-dislocation strain hysteresis loop will be given and discussed in Section 4.

Section I The Vibrating String Model

It is known that a crystal contains dislocations in the form of a three-dimensional network. If the crystal contains a large enough concentration of impurity atoms, which interact with the dislocation lines through the so-called Cottrell mechanism, there are two characteristic dislocation lengths in the model. They are : The network length L_n, and the Length L_c which is caused by the pinning action of the loops by the impurities. In general, both L_n and L_c have distribution functions which again are functions of the applied load and other work conditions.

When a shearing stress σ is applied to the crystal, two kinds of strain will occur: The elastic strain ε_{el}, which would be the only strain we could have if the crystal were "perfect"; and a dislocation strain ε_{dis} due to the recoverable motion of the dislocations under the action of stress σ, i.e.,

$$\varepsilon = \varepsilon_{el} + \varepsilon_{dis} \tag{2-1}$$

The shearing stress σ and shearing strains are related by the wave equation,

$$\frac{\partial^2 \sigma}{\partial x^2} - \rho \frac{\partial^2 \varepsilon}{\partial t^2} = 0 \tag{2-2}$$

where x is the direction of stress amplitude, and ρ the density.

We also have the Hooke's Law

$$\varepsilon_{el} = \frac{\sigma}{G} \quad \left(= \frac{1}{c_{44}} \cdot \sigma \right) \tag{2-3}$$

where G is the true shear modulus.

The dislocation strain, ε_{dis}, caused by a loop of length l in a cube of edge L is given by

$$\varepsilon_{dis} = \frac{\bar{\xi} l a}{L^3} \tag{2-4}$$

where $\bar{\xi}$ is the average displacement of a dislocation of length l, and a the Burger's vector.

$\bar{\xi}$ is given by:

$$\bar{\xi} = \frac{1}{l}\int_0^l \xi(y)\,dy \qquad (2\text{-}5)$$

with y being the coordinate in the dislocation line as shown in Figure 1.

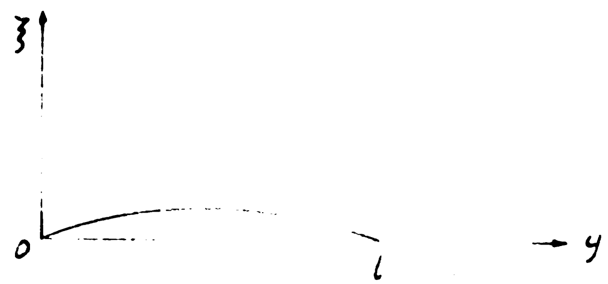

Fig. 1 A bowed-out dislocation

Now, if Λ is the total length of moveable dislocation line in a unit cube, then

$$\epsilon_{dis} = \bar{\xi}\Lambda a = \frac{\Lambda a}{l}\int_0^l \xi(y)\,dy \qquad (2\text{-}6)$$

The equation of the vibrating string model for the displacement of the dislocation under stress is

$$A\frac{\partial^2 \xi}{\partial t^2} + B\frac{\partial \xi}{\partial t} - C\frac{\partial^2 \xi}{\partial y^2} = a\sigma \qquad (2\text{-}7)$$

where $\xi = \xi(x, y, t)$

A = effective mass per unit length = $\pi \rho a^2$
B = damping force per unit length
C = tension in the string = $2 G a^2 / \pi (1-\nu)$
ν = Poisson's ratio

and the boundary conditions as shown in Figure 1 are

$$\begin{cases} \xi(x, 0, t) = 0 \\ \xi(x, l, t) = 0 \end{cases} \qquad (2\text{-}8)$$

To summarize, we have the following system of two simultaneous partial differential equations:

$$\frac{\partial^2 \Gamma}{\partial x^2} - \frac{\rho}{G}\frac{\partial^2 \Gamma}{\partial t^2} = \frac{A}{la}\int_0^l \frac{\partial^2 \xi}{\partial t^2}\, dy$$

$$A\frac{\partial^2 \xi}{\partial t^2} + B\frac{\partial \xi}{\partial t} - C\frac{\partial^2 \xi}{\partial y^2} = a\Gamma \qquad (2\text{-}9)$$

together with the boundary conditions (2-8). The solutions are

$$\Gamma = \Gamma_0 e^{-\alpha x} e^{i\omega(t - \frac{x}{v})} \qquad (2\text{-}10)$$

and

$$\xi = \frac{4a\Gamma}{\pi A}\sum_{n=0}^{\infty} \frac{1}{(2n+1)} \sin\frac{(2n+1)\pi y}{l} \frac{e^{-i\delta_n}}{[(\omega_n^2 - \omega^2)^2 + (\omega d)^2]^{1/2}} \qquad (2\text{-}11)$$

where $d = \frac{B}{A}$, $\omega_n = (2n+1)\frac{\pi}{l}\left(\frac{C}{A}\right)^{1/2}$, $\delta_n = \tan^{-1}\frac{\omega d}{\omega_n^2 - \omega^2}$

with

$$\alpha(\omega) = \frac{\omega}{2v}\,\frac{\Lambda \Delta_0 \gamma^2}{\pi}\,\frac{\omega d}{[(\omega_0^2 - \omega^2)^2 + (\omega d)^2]} \qquad (2\text{-}12)$$

$$v(\omega) = v_0\left[1 - \frac{\Lambda \Delta_0 \eta^2}{2\pi} \frac{(\omega_0^2 - \omega^2)}{[(\omega_0^2-\omega^2)^2+(\omega d)^2]}\right] \tag{2-13}$$

if only the first term of the above series for ξ is used, i.e.

$$\xi = \frac{4aC}{\pi A} \sin \frac{\pi y}{l} \frac{e^{-i\delta_0}}{[(\omega_0^2-\omega^2)^2+(\omega d)^2]} \tag{2-10)'$$

in which $v_0 = \sqrt{\frac{G}{\rho}}$ $\quad \Delta_0 = \frac{8Ga^2}{\pi^3 C}$ $\quad \eta^2 = \frac{\pi^2 C}{A}$.

Using the notations $D = \omega/d$ and $\Omega = \omega/\omega_0$, the change of dynamic modulus is given by

$$\frac{\Delta G}{G} = \frac{2(v_0 - v)}{v_0} = \frac{\Delta_0 \Lambda L^2}{\pi}\left[\frac{(1-\Omega^2)}{(1-\Omega^2)^2 + \Omega^2/D^2}\right] \tag{2-14}$$

as $L^2 = l^2 = \frac{\eta^2}{\omega_0^2}$. This gives the dependence of the change of dynamic modulus on frequency.

Section II Distribution of Loop Length as a Function of Stress

It can be shown that for frequencies in the kilocycle range, the expression

$$\frac{e^{-i\delta_0}}{[(\omega_0^2-\omega^2)^2+(\omega d)^2]^{1/2}}$$

is essentially $\frac{1}{\omega_0^2} = \frac{l^2 A}{\pi^2 C}$ as $\omega \ll \omega_0$ and $\delta_0 \to 0$, therefore,

$$v(\omega) = v_0\left[1 - \frac{\Lambda \Delta_0 \eta^2}{2\pi} \frac{(\omega_0^2 - \omega^2)}{[(\omega_0^2-\omega^2)^2+(\omega d)^2]}\right] \qquad (2\text{-}13)$$

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is essentially $\frac{1}{\omega_0^2} = \frac{l^2 A}{\pi^2 C}$ as $\omega \ll \omega_0$ and $\delta_0 \to 0$, therefore,

$$\xi = \frac{4a\sigma l^2}{\pi^3 C} \sin \frac{\pi y}{l} \qquad (2\text{-}10)''$$

The force exerted by the dislocation line at any instant is

$$f = C(\phi_1 - \phi_2) \qquad (2\text{-}15)$$

where

$$\phi = \frac{\partial \xi}{\partial y} = \frac{4a\sigma l}{\pi^2 C} \cos \frac{\pi y}{l}$$

Therefore,

$$f_{max} = C(\phi_1 - \phi_2)_{max} = \frac{4a\sigma(l_1 + l_2)}{\pi^2} \qquad (2\text{-}16)$$

By Cottrell's theory,[7] breakaway occurs when

$$f_{max} = \bar{f} = \frac{4G\epsilon' a^4}{Z^2} \qquad (2\text{-}17)$$

where ϵ' is the difference in atomic radii divided by the atomic radius of the solvent atom, and Z the distance between the impurity atom and the dislocation line.

So breakaway occurs when

$$l_1 + l_2 \geq \hat{l} = \frac{\pi^2 \bar{f}}{4a\sigma} \qquad (2\text{-}18)$$

Granato and Lücke assumed that the initial distribution of loop lengths is exponential, i.e.

$$N_i(l) = \frac{\Lambda}{L_c^2} e^{-\frac{l}{L_c}} dl$$

where L_c here means the average value of the L_c's. When the strain becomes very large, the loop lengths were assumed to have a delta function distribution. For intermediate strains, they assumed that the distribution function, denoted by $N'(l)dl$, consists of two parts, i.e., (1) an exponential part due to loops in networks which have not yet broken away; and (2) a delta function part due to the already broken away part,

$$N'(l)dl = \begin{cases} \dfrac{\Lambda}{L_c^2} e^{-l/L_c} J_1(\mathcal{L}, L_c, L_N)\, dl & 0 \le l < \mathcal{L} \\ \dfrac{\Lambda}{L_N} \delta(l - L_N)\, M\, dl & \mathcal{L} \le l < \infty \end{cases} \tag{2-19}$$

where L_n means the average of the L_n's and M is the fraction of network lengths in which the breakaway process has occurred; J_1 is determined by the condition that the length of line lost from the exponential distribution is gained by the delta function distribution.

Based on the idea of Koehler's statistical analysis concerning the breakaway of two adjoining lengths of a certain sum, and also considering the fact that the breakaway process is a catostrophic one within the network length, Granato and Lücke found M, for the early stages of the breakaway process, to be

$$M = (\gamma - 1)(q + 1)e^{-q} \quad (q = \mathcal{L}/L_c) \tag{2-20}$$

and J_1 is therefore

$$J_1 = 1 - M = 1 - (\gamma - 1)(q + 1)e^{-q} \tag{2-21}$$

Equations (2-19), together with (2-20) and (2-21), will be used in the next section for the derivation of the stress-dislocation strain law.

It is seen that in the above theory, the initial distribution of loop lengths is exponential, and ranges from zero to infinity, but in the final stage, all lengths have the same value L_n. As no loop reduces its length in the breakaway process, the loops which initially have lengths greater than L_n will always be greater than L_n. So the assumption made about the distribution in the final stage is doubtful. For this reason an alternate assumption is made below and the consequent results studied.

It is assumed that in the intermediate stage, the distribution $N'(l)dl$ is

$$N'(l)dl = \begin{cases} \dfrac{\Lambda}{L_c^2} e^{-l/L_c} J_2(\mathcal{L}, L_c, L_N)\,dl & 0 \le l < \mathcal{L} \\ \dfrac{\Lambda}{L_N^2} e^{-l/L_N}\,dl & \mathcal{L} \le l < \infty \end{cases} \qquad (2\text{-}22)$$

It is obvious from (2-22) that the author has assumed the same initial distribution as Granato and Lücke; but, different from them, the broken-away part is taken to be an exponential function in the L_n's. Physically this means that for each network length L_n which is greater than or equal to $\mathcal{L}$, the characteristic length, and which has several impurities distributed randomly along its length, there is always a chance to find two adjoining loops with a sum which is at least $\mathcal{L}$. The significance of this assumption will be further discussed later.

By requiring that $\int_0^\infty N'(l)\,dl = \Lambda$,

J_2 is found to be

$$J_2 = \frac{1 - \left(1 + \frac{l_c}{L_N}\right) e^{-\frac{l_c}{L_N}}}{1 - \left(1 + \frac{l_c}{L_c}\right) e^{-l_c/L_c}}$$

$$= \frac{1 - \left(1 + \frac{q}{\gamma}\right) e^{-q/\gamma}}{1 - (1 + q)\, e^{-q}} \qquad (2\text{-}23)$$

Equations (2-22) and (2-23) will also be used in the derivation of the stress-dislocation strain law.

Section III The Stress-Dislocation Strain Law

By (2-6) and (2-10)''

$$\epsilon_{dis} = \frac{\Lambda a}{l} \int_0^l \xi(y)\, dy$$

and

$$\xi = \frac{4 a \sigma L^2}{\pi^3 C} \sin \frac{\pi y}{l}$$

performing the integration, one obtains

$$\epsilon_{dis} = \frac{\Lambda a}{l} \; \frac{4 a \sigma l^2}{\pi^3 C} \; \frac{2l}{\pi}$$

$$= \frac{\Lambda\, 8\, a^2 l^2 \sigma}{\pi^4 C}$$

As $\sigma = \sigma_0 e^{-\alpha x} e^{i\omega(t - \frac{x}{v})}$, the in-phase part

By requiring that $\int_0^\infty N'(l)\,dl = \Lambda$,

J_2 is found to be

$$J_2 = \frac{1-\left(1+\frac{d}{L_N}\right)e^{-\frac{d}{L_N}}}{1-\left(1+\frac{d}{L_c}\right)e^{-d/L_c}}$$

$$= \frac{1-\left(1+\frac{q}{\gamma}\right)e^{-q/\gamma}}{1-(1+q)\,e^{-q}} \qquad (2\text{-}23)$$

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$$\epsilon_{dis} = \frac{\Lambda a}{l}\;\frac{4a\sigma l^2}{\pi^3 C}\;\frac{2l}{\pi}$$

$$= \frac{\Lambda\, 8\, a^2 l^2 \sigma}{\pi^4 C}$$

As $\sigma = \sigma_0 e^{-\alpha x} e^{i\omega(t-\frac{x}{v})}$, the in-phase part of ϵ_{dis} is

$$\epsilon_{dis} = \frac{\sigma_0 e^{-\alpha x} \Lambda 8 a^2 l^2}{\pi^4 C} \cos(\omega t - kx) \quad (2\text{-}24)$$

where $k = \frac{\omega}{v}$ and is the wave number. From the above equation one sees that the dislocation strain is directly proportional to the applied stress and is also a function of the loop length.

Neglecting the variation of stress over x, one obtains for the contribution of a single loop of length l to the dislocation strain

$$\left[\frac{8 a^2 \sigma_0}{\pi^4 C} \cos \omega t \right] l^3 = \psi l^3$$

The dislocation strain from the contribution of all loops is therefore

$$\epsilon_{dis}(\omega) = \int_0^{l_?} \psi l^3 N'(l)\, dl \qquad (2\text{-}25)$$

It has to be noted that the distribution function $N'(l)$ given by (2-19) and (2-22) is determined by the instantaneous value of the stress for the quarter cycle of increasing stress. For the quarter cycle of decreasing stress, the loops collapse elastically with no change in the distribution function. Denoting by $N_1'(l)$ and $N_2'(l)$ for the increasing and decreasing quarter cycles of stress, respectively, and remembering that

$$q = \frac{\alpha}{L_c} = \frac{\pi^2 f}{4 a L_c} \frac{1}{\sigma} = \frac{\Gamma}{q}$$

equation (2-19) can be written as

$$N'(l)\,dl = \begin{cases} N_1'(l)\,dl = \begin{cases} \dfrac{\Lambda}{L_c^2}\left[1-(\gamma-1)\left(\dfrac{\Gamma}{\sigma}+1\right)e^{-\frac{\Gamma}{\sigma}}\right]e^{-\frac{l}{L_c}}\,dl & 0 \le l < \mathcal{L} \\[2ex] \dfrac{\Lambda}{L_N}\,\delta(l-L_N)(\gamma-1)\left(\dfrac{\Gamma}{\sigma}+1\right)e^{-\frac{\Gamma}{\sigma}}\,dl & \mathcal{L} \le l < \infty \end{cases} \\[6ex] N_2'(l)\,dl = \begin{cases} \dfrac{\Lambda}{L_c^2}\left[1-(\gamma-1)\left(\dfrac{\Gamma}{\sigma_0}+1\right)e^{-\frac{\Gamma}{\sigma_0}}\right]e^{-\frac{l}{L_c}}\,dl & 0 \le l < \mathcal{L} \\[2ex] \dfrac{\Lambda}{L_N}\,\delta(l-L_N)(\gamma-1)\left(\dfrac{\Gamma}{\sigma_0}+1\right)e^{-\frac{\Gamma}{\sigma_0}}\,dl & \mathcal{L} \le l < \infty \end{cases} \end{cases} \quad (2\text{-}19)'$$

where $\Gamma = \dfrac{\pi^2 \bar{f}}{4 a L_c}$ and $\sigma = \sigma_0 \cos \omega t$

Substituting (2-19) into (2-25), one obtains

$$\epsilon_{dis} = \psi \Lambda L_c^2\, 3!\left[1 + e^{-q}\left\{\frac{\gamma^2(\gamma-1)(q+1)}{3!} - \left(\frac{q^3}{3!} + \frac{q^2}{2} + q + 1 + (\gamma-1)(q+1)\right)\right\}\right] \quad (2\text{-}26)$$

This simplifies to

$$\epsilon_{dis} = \Omega\left[1 + \frac{\gamma^3}{3!}\left(\frac{\Gamma}{\sigma}+1\right)e^{-\frac{\Gamma}{\sigma}}\right]\sigma \quad \begin{matrix}(2\text{-}27)\\ \text{(Formula I)}\end{matrix}$$

since q is taken in the range $0 \le q \le \gamma$ and no breakaway occurs for $q > \gamma$.

For the quarter cycle of decreasing stress,

$$\epsilon_{2\,dis} = Q\left[1+\frac{\gamma^3}{3!}\left(\frac{r}{r_0}+1\right)e^{-\frac{r}{r_0}}\right]\sigma \qquad \text{(2-27)} \quad \text{(Formula I)}$$

where $$Q = \frac{8a^2 \Lambda L_c^2\, 3!}{\pi^4 c}$$

Similarly, (2-22) can be written as

$$N'(l)\,dl = \begin{cases} N_1'(l)\,dl = \begin{cases} \dfrac{\Lambda}{L_c^2}\left[\dfrac{1-\left(1+\frac{r}{\gamma r_0}\right)e^{-r/\gamma r_0}}{1-\left(1+\frac{r}{r_0}\right)e^{-r/r_0}}\right]e^{-\frac{l}{L_c}}\,dl & 0 \le l < a \\ \dfrac{L}{L_N^2}\,e^{-\frac{l}{L_N}}\,dl & a \le l < \infty \end{cases} \\ N_2'(l)\,dl = \begin{cases} \dfrac{\Lambda}{L_c^2}\left[\dfrac{1-\left(1+\frac{r}{r_0}\right)e^{-r/r_0}}{1-\left(1+\frac{r}{r_0}\right)e^{-r/r_0}}\right]e^{-\frac{l}{L_c}}\,dl & 0 \le l < a \\ \dfrac{L}{L_N^2}\,e^{-\frac{l}{L_N}}\,dl & a \le l < \infty \end{cases} \end{cases} \qquad (2\text{-}22)'$$

Substituting (2-22) into (2-25) and performing the integration, one obtains

$$\begin{aligned} \epsilon_{1\,dis} = \psi \Lambda L_c^2\, 3!\Big[&\left\{1-e^{-q}\left(1+q+\frac{q^2}{2}+\frac{q^3}{3!}\right)\right\}\cdot \\ &\cdot\left\{\frac{1-\left(1+\frac{q}{r}\right)e^{-\frac{q}{r}}}{1-(1+q)\,e^{-q}}\right\}+ \\ &+\left(\frac{q^3}{3!\,r}+\frac{q^2}{2}+rq+r^2\right)e^{-\frac{q}{r}}\Big] \end{aligned} \qquad \text{(2-28)}$$

$$\epsilon_{2\,dis} = Q\left[1+\frac{\gamma^3}{3!}\left(\frac{r}{r_0}+1\right)e^{-\frac{r}{r_0}}\right]\sigma \qquad \text{(2-27) (Formula I)}$$

where $\quad Q = \dfrac{8a^2 \Lambda L_c^2\, 3!}{\pi^4 C}$

Similarly, (2-22) can be written as

$$N'(l)\,dl = \begin{cases} N_1'(l)\,dl = \begin{cases} \dfrac{\Lambda}{L_c^2}\left[\dfrac{1-(1+\frac{r}{r_0})e^{-r/r_0}}{1-(1+\frac{r}{r_0})e^{-r/r_0}}\right]e^{-\frac{l}{L_c}}\,dl & 0 \le l < l_c \\[2ex] \dfrac{l}{L_N^2}\, e^{-\frac{l}{L_N}}\,dl & \le l < \end{cases} \\[6ex] N_2'(l)\,dl = \begin{cases} \dfrac{\Lambda}{L_c^2}\left[\dfrac{1-(1+\frac{r}{r_0})e^{-r/r_0}}{1-(1+\frac{r}{r_0})e^{-r/r_0}}\right]e^{-\frac{l}{L_c}}\,dl & 0 \le l < \\[2ex] \dfrac{l}{L_N^2}\, e^{-\frac{l}{L_N}}\,dl & \le l < \end{cases} \end{cases} \qquad (2\text{-}22)'$$

Substituting (2-22) into (2-25) and performing the integration, one obtains

$$\begin{aligned}\epsilon_{1\,dis} = \psi \Lambda L_c^2\, 3!\Big\{&\left[1-e^{-q}\left(1+q+\frac{q^2}{2}+\frac{q^3}{3!}\right)\right]\cdot \\ &\cdot\left[\frac{1-(1+\frac{q}{r})e^{-\frac{q}{r}}}{1-(1+q)e^{-q}}\right] + \\ &+\left(\frac{q^3}{3!\,r}+\frac{q^2}{2}+rq+r^2\right)e^{-\frac{q}{r}}\Big\}\end{aligned} \qquad (2\text{-}28)$$

In the early stages $e^{-\frac{q}{r}} \gg e^{-q} \doteq 0$, so a first simplification gives

$$\epsilon_1\,dis = \psi \Lambda L_c^2\, 3!\Big[1 + \Big(\frac{q^3}{3!\,r} + \frac{q^2}{2} + r q + r^2\Big) e^{-\frac{q}{r}}\Big] \tag{2-29}$$

For cases where q is much larger than r, a further simplication is given by

$$\epsilon_1\,dis = Q\Big[1 + \frac{r^3}{3!\,\sigma_0^3}\, e^{-\frac{r}{\sigma_0}}\Big]\sigma$$

(2-30)
or
(Formula II)

$$\epsilon_2\,dis = Q\Big[1 + \frac{r^3}{3!\,\sigma_0^3}\, e^{-\frac{r}{\sigma_0}}\Big]\sigma$$

Some numerical results of the stress-dislocation strain laws, equations (2-27) and (2-30) will be given in the next chapter.

Section IV The Dependence of Changes in the Static and Dynamic Modulus on the Stress Amplitude

It is readily seen that both the stress-dislocation strain laws as given by equations (2-27) and (2-30) (referred to as Formula I and Formula II in the following analysis) have the following properties.

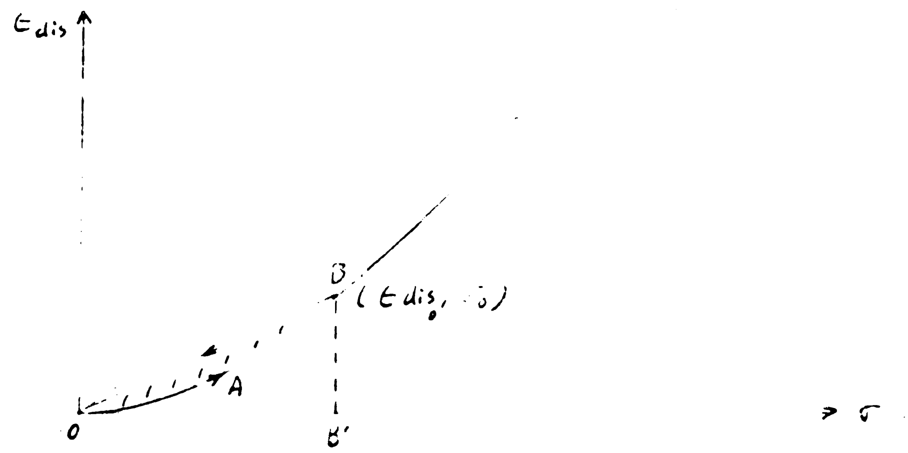


Fig. 2 A qualitative sketch of the stress-dislocation strain relationship

(1) When σ is small ϵ_{dis} is linearly proportional to σ, the proportionality constant being Q for Formula II. For Formula I, this linearity holds until $q = \gamma$.

(2) ϵ_{dis} increases rapidly (and nonlinearly) as σ increases. However, when σ becomes sufficiently large, the curve approaches the asymptote $\epsilon_{dis} = Q\left[1 + \frac{\gamma(\gamma-3)(\gamma+2)}{3!} \cdots\right]$ or $\epsilon_{dis} = Q[\gamma^2]\sigma$ respectively for the two theories.

(3) When the maximum stress σ_0 (the point B) is reached, and the quarter cycle of decreasing stress starts, the path will then be a straight line BO, determined by σ_0. The slope of this straight line will be used to define the change of the effective static modulus.

(4) The area OABO has been shown by Granato and Lucke to be proportional to the amplitude - dependent internal friction loss and the change of dynamic modulus. They also showed that the ratio of the internal friction to the change of dynamic modulus, called r by them, is a constant.

As the internal friction is given by the quotient of the area OABO divided by twice the area of the triangle OBB', the change of dynamic modulus can be obtained once r is known.

CHAPTER III
NUMERICAL RESULTS

In order to plot the stress-dislocation strain curves given by Formula (I) and Formula (II), the following numerical values were chosen for the parameters appeared in the equations. They apply to a 99.999% pure copper crystal, and are essentially the same as those used by Koehler[5] in his investigation.

$$a = 2.55 \text{ A} = 2.55 \times 10^{-8} \text{ cm}$$

$$\Lambda = 1.4 \times 10^{16} a = 3.5 \times 10^{8} \text{ cm/cm}^3$$

$$L_c = \frac{1}{1.2} \times 10^{3} a = 2.12 \times 10^{-5} \text{ cm}$$

$$\rho = 8.93 \text{ gram/cm}^3$$

$$\nu = 3.40$$

$$G = 4.53 \times 10^{11} \text{ dynes/cm}^2$$

$$A = 2.51 \times 10^{-14} \text{ gram/cm}$$

$$C = 3.90 \times 10^{-4} \text{ gram cm/sec}^2$$

$$Q = \frac{8 a^2 \Lambda L_c^2 \, 3!}{\pi^4 C} = 1.3 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$\bar{f} = 4 \times 10^{-6} \text{ dynes}$$

$$\Gamma = \frac{\pi^2 \bar{f}}{4 a L_c} = 1.8 \times 10^{7} \text{ dynes/cm}^2$$

Three different values of γ, i.e., $\gamma = 5$, $\gamma = 10$ and $\gamma = 50$ are used; and six curves are plotted up to the range of strains which is several times ε_N, ε_N being defined as the point where the stress-dislocation strain curves start to be nonlinear. On curves where no abrupt changes from "linear" to "nonlinear" can be found, the point $(\sigma_N, \varepsilon_N)$

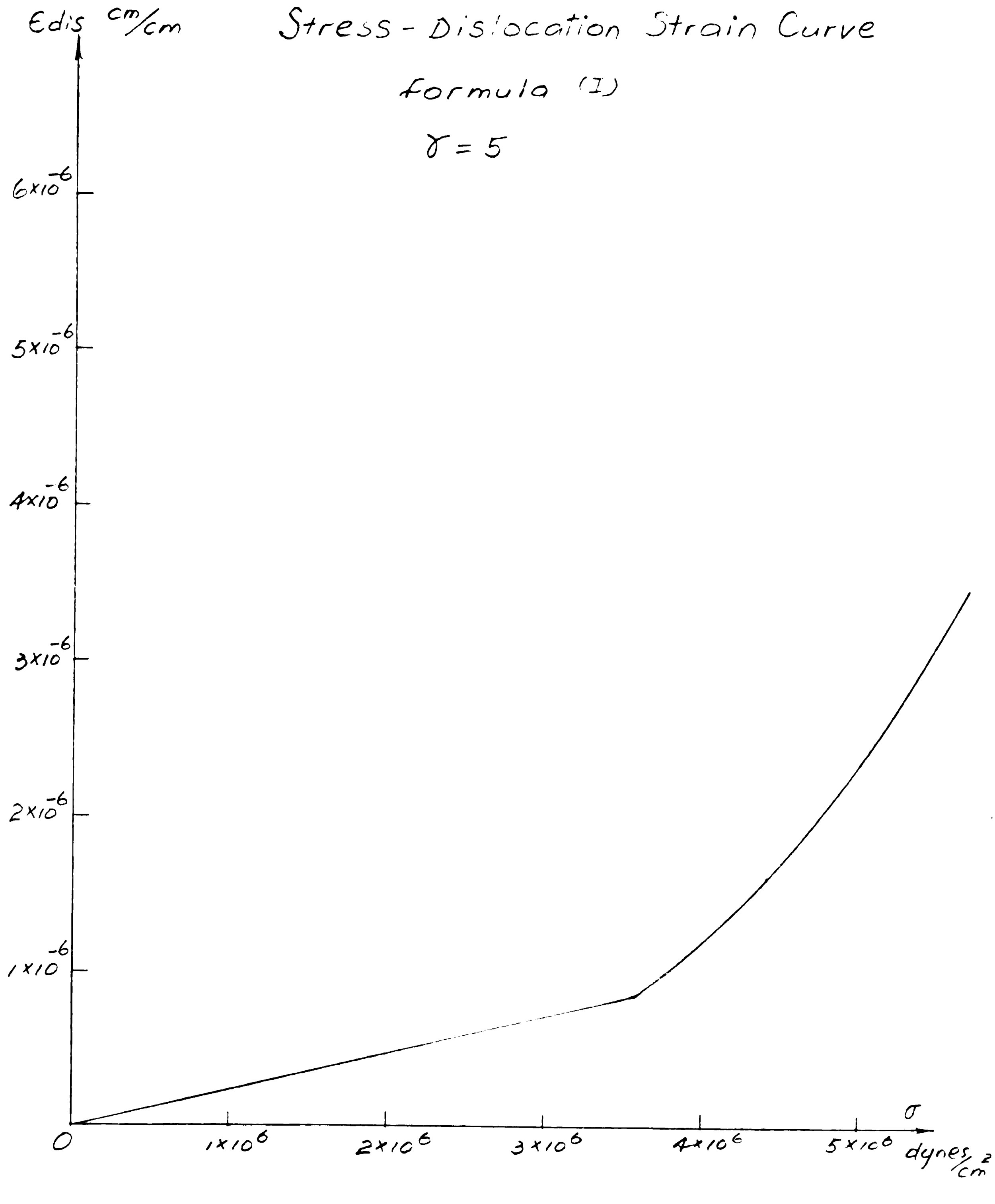
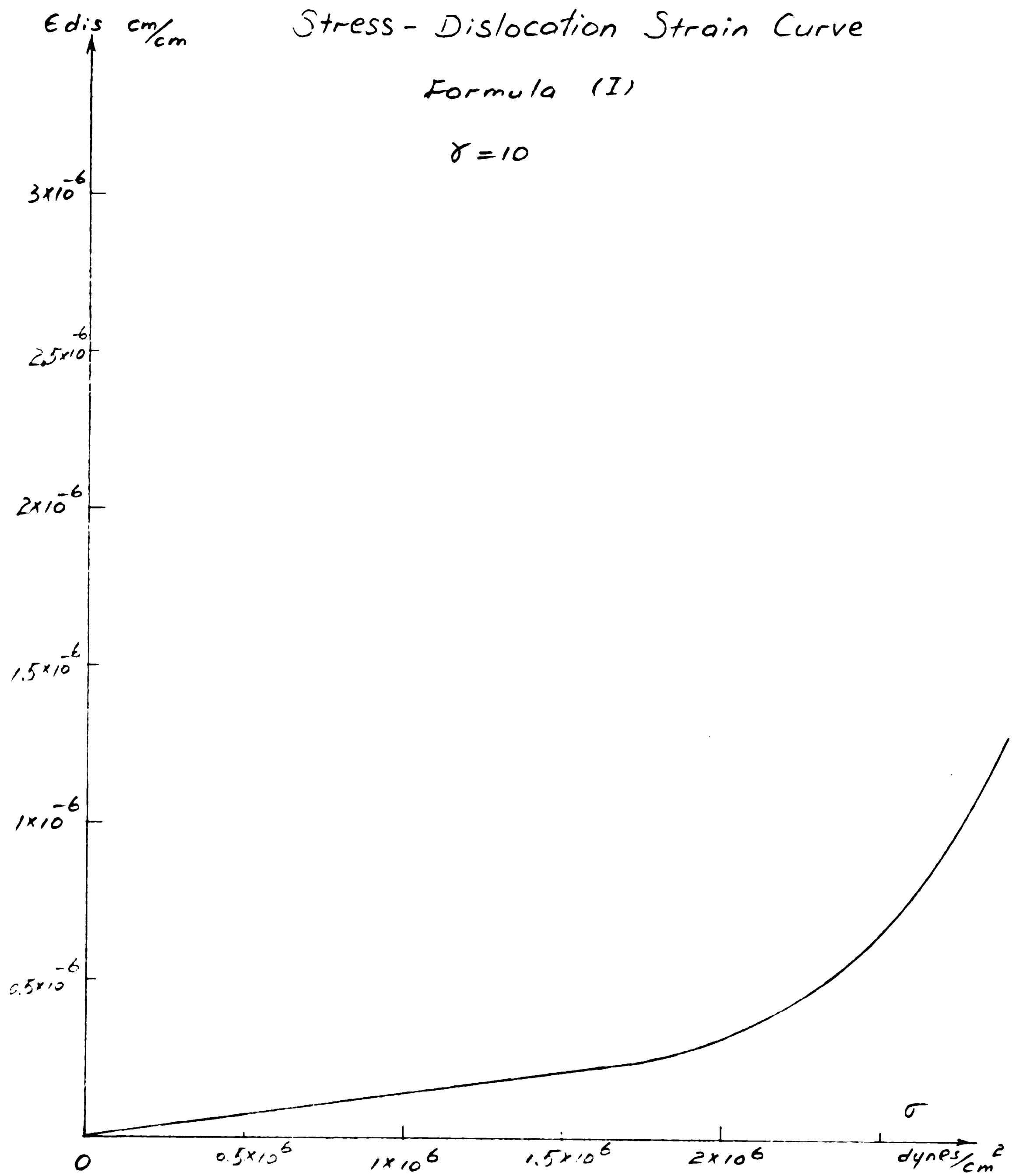
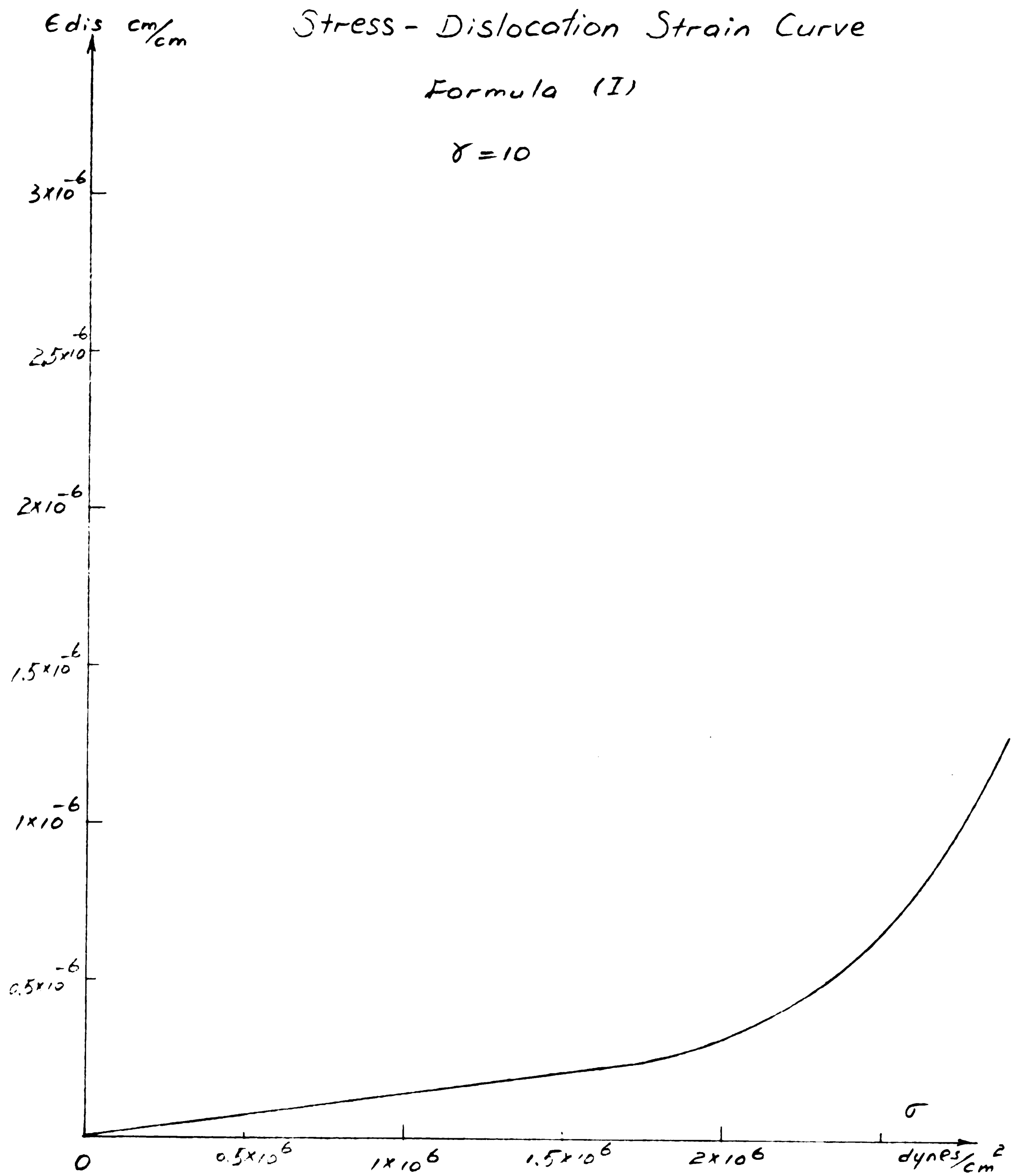

Edis cm/cm
Stress - Dislocation Strain Curve
formula (I)
γ = 5
6x10⁻⁶
5x10⁻⁶
4x10⁻⁶
3x10⁻⁶
2x10⁻⁶
1x10⁻⁶
O
1x10⁶
2x10⁶
3x10⁶
4x10⁶
5x10⁶
σ
dynes/cm²

Fig. 3



Stress - Dislocation Strain Curve
Formula (I)
γ = 10
Edis cm/cm
3x10⁻⁶
2.5x10⁻⁶
2x10⁻⁶
1.5x10⁻⁶
1x10⁻⁶
0.5x10⁻⁶
0
0.5x10⁶
1x10⁶
1.5x10⁶
2x10⁶
σ
dynes/cm²

Fig. 4



Edis cm/cm
Stress - Dislocation Strain Curve
Formula (I)
γ = 10
3x10⁻⁶
2.5x10⁻⁶
2x10⁻⁶
1.5x10⁻⁶
1x10⁻⁶
0.5x10⁻⁶
0
0.5x10⁶
1x10⁶
1.5x10⁶
2x10⁶
σ
dynes/cm²

Fig. 4

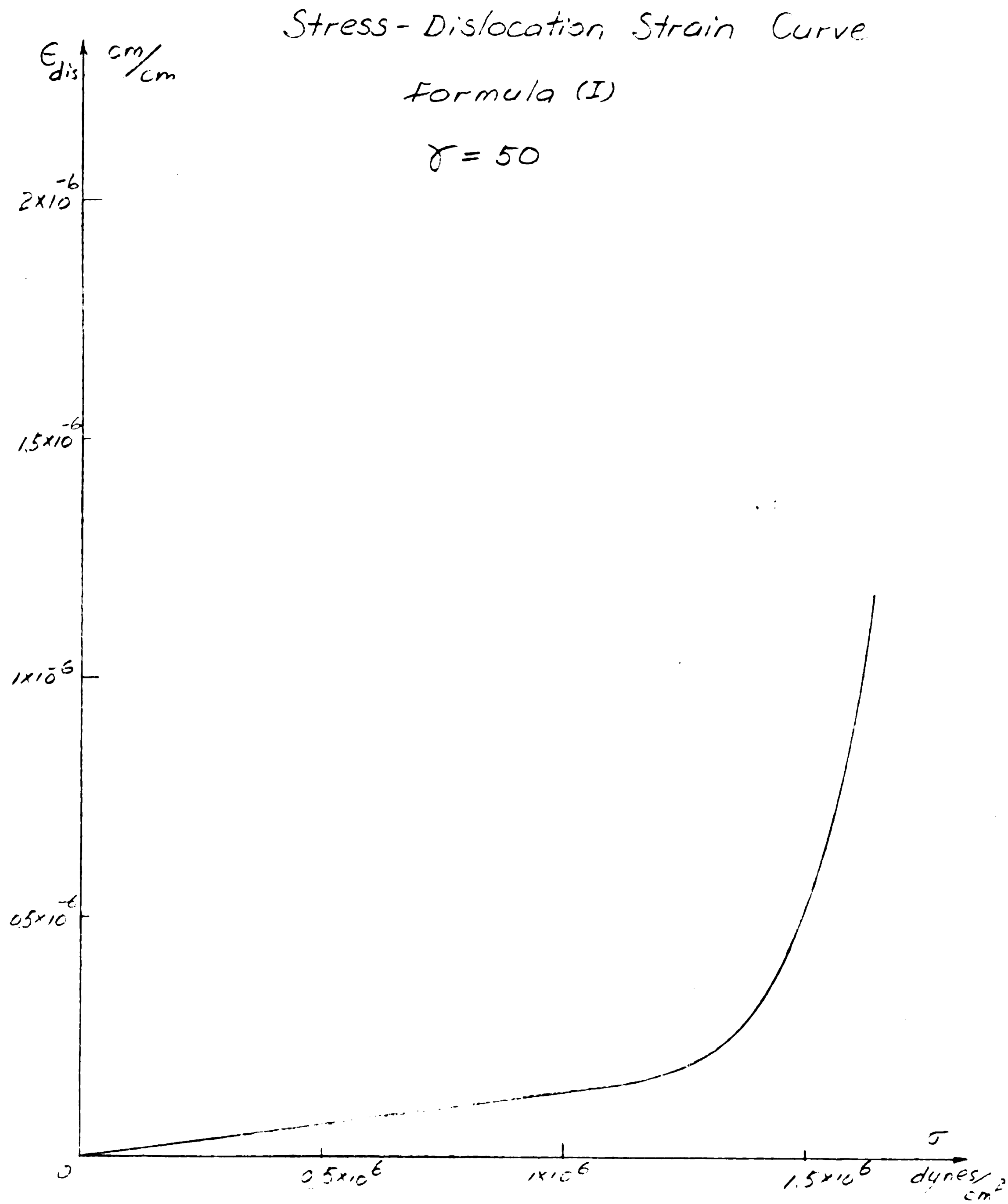

Stress - Dislocation Strain Curve
Formula (I)
γ = 50
ε dis cm/cm
2x10^-6
1.5x10^-6
1x10^-6
0.5x10^-6
0
0.5x10^6
1x10^6
1.5x10^6
σ
dynes/cm^2

Fig. 5

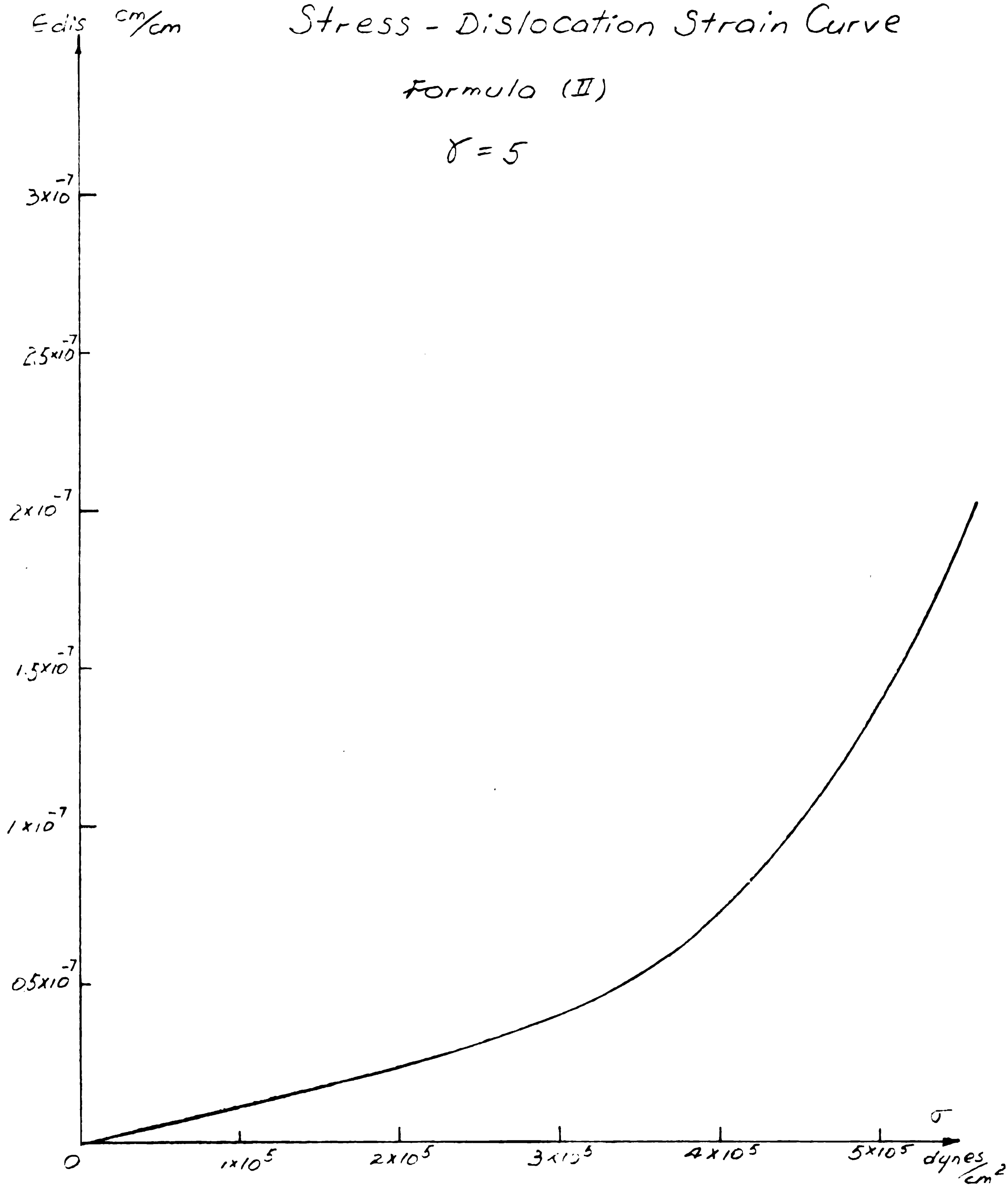
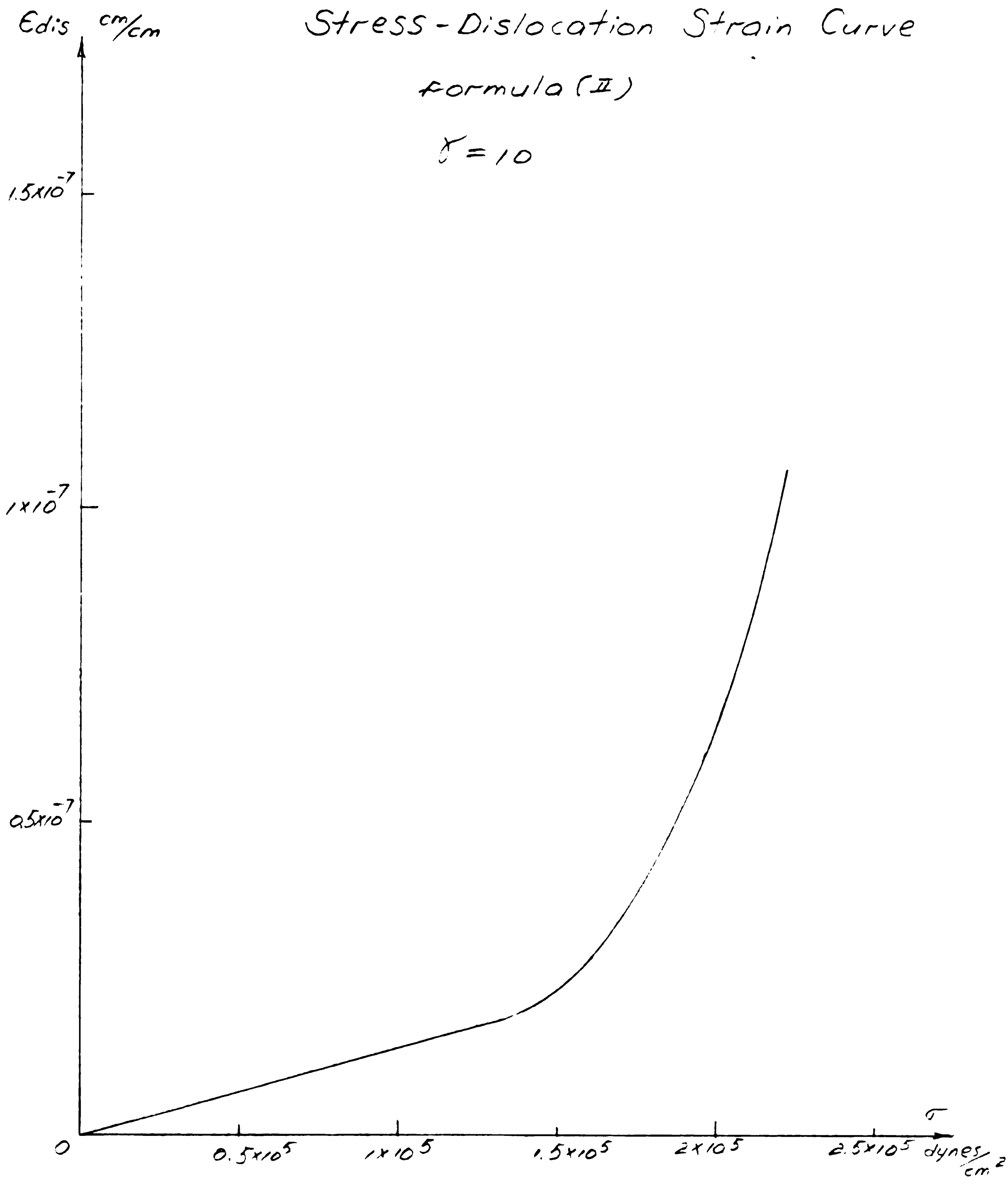
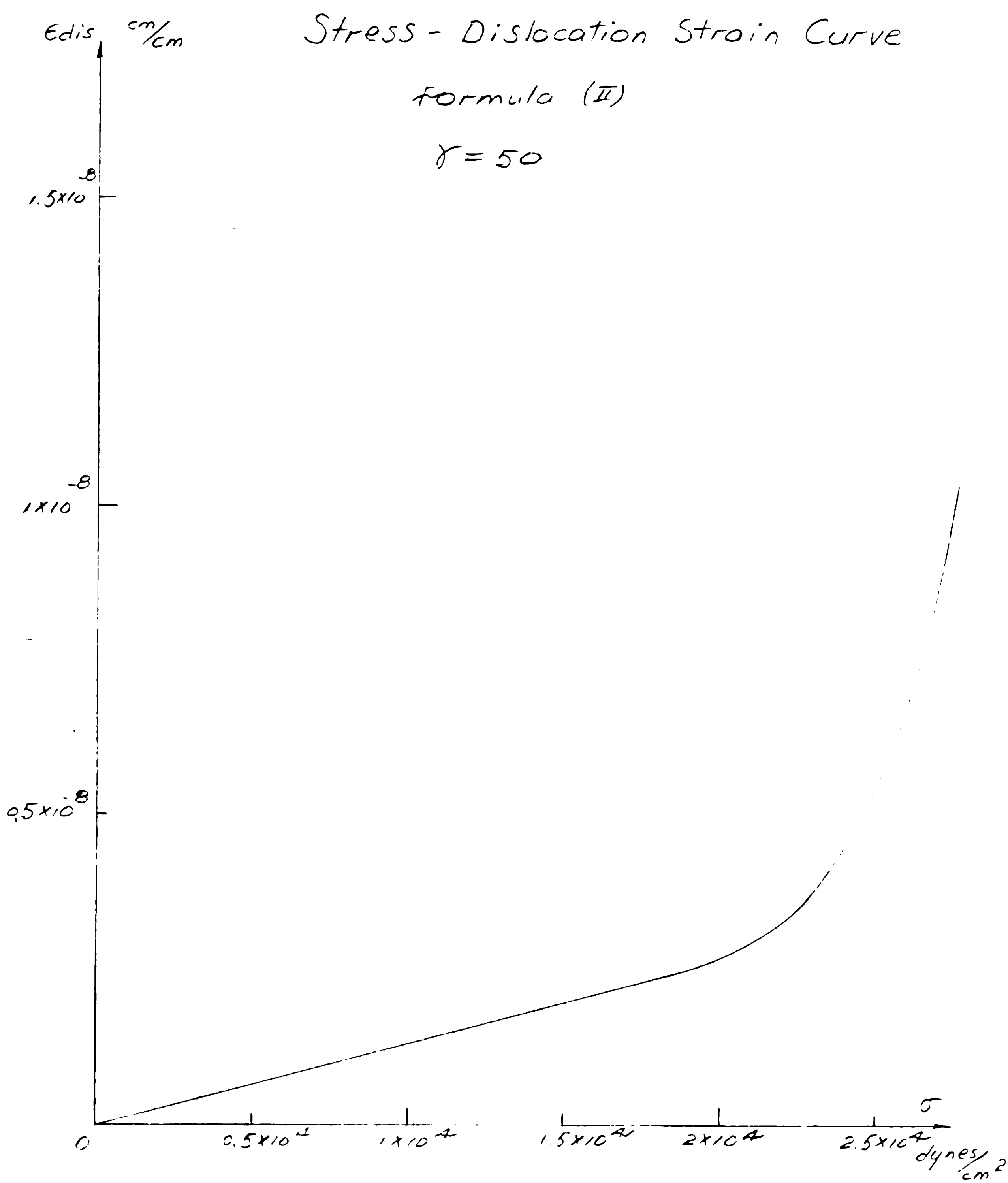

Stress - Dislocation Strain Curve
Formula (II)
γ = 5
ε dis cm/cm
3×10⁻⁷
2.5×10⁻⁷
2×10⁻⁷
1.5×10⁻⁷
1×10⁻⁷
0.5×10⁻⁷
0
1×10⁵
2×10⁵
3×10⁵
4×10⁵
5×10⁵
σ
dynes/cm²

Fig. 6



ϵ_{dis} cm/cm
Stress-Dislocation Strain Curve
formula (II)
$\gamma = 10$
1.5×10^{-7}
1×10^{-7}
0.5×10^{-7}
0
0.5×10^{5}
1×10^{5}
1.5×10^{5}
2×10^{5}
2.5×10^{5}
τ
dynes/cm²

Fig. 7



Edis cm/cm
Stress - Dislocation Strain Curve
formula (II)
γ = 50
1.5x10^-8
1x10^-8
0.5x10^-8
0
0.5x10^4
1x10^4
1.5x10^4
2x10^4
2.5x10^4
dynes/cm^2
σ

Fig. 8

is defined as the point at which the nonlinear effect contributes 1 % to the total strain. Values of $(\varepsilon_N, \sigma_N)$ are given in Table I.

Table I

Values of $(\varepsilon_N, \sigma_N)$ on the $\varepsilon_{dis} - \sigma$ Curves

Formula	γ	σ_N dynes/cm^2	ε_N cm/cm
I	5	3.6×10^6	8.6×10^{-7}
I	10	1.8×10^6	2.5×10^{-7}
I	50	1.1×10^6	1.5×10^{-7}
II	5	2.6×10^5	3.4×10^{-8}
II	10	1.3×10^5	1.8×10^{-8}
II	50	1.9×10^4	2.5×10^{-9}

It is seen from the above table that the $(\varepsilon_N, \sigma_N)$ points fall in ranges of different order.

For cases in which σ_{max} is smaller than σ_N, there is no amplitude-dependent change of dynamic modulus because the hysteresis loop has zero area. However, there is a change of static modulus determined by the slope of the straight portion and the true elastic modulus. This change is amplitude independent and has a constant value until σ_{max} is equal to σ_N. Table II gives this amplitude independent changes of static modulus.

Table II

Strain Amplitude Independent Changes of Static Modulus

Formula	γ	$(\Delta G/G)_{static}$
I	5	- 0.098
I	10	- 0.060
I	50	- 0.056
II	5	- 0.056
II	10	- 0.056
II	50	- 0.056

Results in the above Table were obtained as follows:

For a certain stress, the total strain is given by

$$\varepsilon_{total} = \varepsilon_{el} + \varepsilon_{dis} = \left(\frac{1}{G} + Q'\right)\sigma$$

where Q' is the slope of the straight portion of the hysteresis loop

$$\therefore G' = G + \Delta G = \frac{\sigma}{\varepsilon_{total}} = \frac{G}{1 + GQ'}$$

$$\left(\frac{\Delta G}{G}\right)_{static} = \frac{G' - G}{G} = -\frac{G Q'}{1 + G Q'} \qquad (3\text{-}1)$$

Taking $G = 4.53 \times 10^{11}$ dynes/cm²

and $Q' = Q = 1.3 \times 10^{-13}$ cm²/dyne

one obtains

$$\left(\frac{\Delta G}{G}\right)_{static} = -0.056$$

as given in rows 3 to 6. Results in the first two rows were obtained in a similar way.

The change of static modulus for strains greater than ε_N, but still in the early nonlinear range, is given in Table III. Points chosen are those with strains equal to $2\varepsilon_N$, $3\varepsilon_N$, and $4\varepsilon_N$, the calculations technique is similar to that described above.

Table III

Change of Static Modulus in the Early Nonlinear Range

Formula	γ	$(\Delta G/G)_{static}$ at $\varepsilon_{max} =$ ε_N	$2\varepsilon_N$	$3\varepsilon_N$	$4\varepsilon_N$	ε_N
I	5	- 0.098	- 0.182	- 0.226	- 0.262	8.6×10^{-7}
I	10	- 0.060	- 0.112	- 0.146	- 0.177	2.5×10^{-7}
I	50	- 0.056	- 0.113	- 0.153	- 0.188	1.5×10^{-7}
II	5	- 0.056	- 0.169	- 0.213	- 0.244	3.4×10^{-8}
II	10	- 0.056	- 0.197	- 0.246	- 0.290	1.8×10^{-8}
II	50	- 0.056	- 0.194	- 0.251	- 0.300	2.5×10^{-9}

The change of dynamic modulus, as explained in Chapter II, is given in Table IV at $\varepsilon_{max} = 2\varepsilon_N$, $3\varepsilon_N$ and $4\varepsilon_N$. The results were obtained by dividing the area of the hysteresis loop by ten times $\varepsilon_{max} \cdot \tau_{max}$. In this way, a factor of $r = 5$ (r being the ratio of the internal friction to the change of dynamic modulus) has been used.

Table IV

Change of Dynamic Modulus in the Early Nonlinear Range

Formula	γ	$(\Delta G/G)_{dynamic}$ at $\varepsilon_{max} =$				σ_N
		ε_N	$2\varepsilon_N$	$3\varepsilon_N$	$4\varepsilon_N$	
I	5	0	- 0.029	- 0.037	- 0.041	8.6 10
I	10	0	- 0.031	- 0.043	- 0.050	2.5 10
I	50	0	- 0.028	- 0.045	- 0.055	1.5 10
II	5	0	- 0.019	- 0.036	- 0.040	3.4 10
II	10	0	- 0.029	- 0.039	- 0.045	1.8 10
II	50	0	- 0.029	- 0.044	- 0.053	2.5 10

Results given in Table I through IV will be discussed in the next chapter.

CHAPTER IV

DISCUSSION AND CONCLUSIONS

Results obtained in Chapter III will be discussed first. It is seen from Table I that the two theories predict different orders of magnitude of stress. Whereas the Granato and Lucke theory predicts that the stress-dislocation strain relation starts to be nonlinear at stresses of the order 10^6 dynes/cm^2, the theory suggested is this paper gives results of the order 10^5 dynes/cm^2 for low values (low concentration of impurities) and of even lower order for high γ values. Also, results obtained by the present theory are seen to be more sensitive to the value assigned to γ than those obtained by the Granato and Lucke theory. It must be left to experiments to determine which theory gives the best results.

The numerical results given in Table II and III are left uncompared, since no experimental results are available. However, as one sees that some of the parameters involved in the equations are not well established, the values assigned to them are also questionable. In fact, the stress-dislocation strain law depends on two parameters, namely Q and Γ. Q in turn depends on Λ, L_c, and Γ on $\bar{f}$ and L_c. Therefore, a series of static measurements, with some of these parameters properly controlled, might yield information about their exact values. For instance, one might use neutron irradiation to produce interstitial atoms and lattice vacancies, which would pin the dislocations and thus reduce the average value of L_c''s .

As an example of the dependence of the results on the parameters, one can see that if a value for Q one tenth that previously assigned is used, results in Tables II and III will also be reduced by approximately a factor of 10.

Results given in Table IV are too large as compared with experimental results,[5] since the latter are in the order of 10^{-3} to 10^{-5}. The results given in Table IV are independent of Q when only the relation between change of dynamic modulus and stress amplitude is considered. However, these results depend on r , the ratio of internal friction and change of dynamic modulus, and the choice of $r = 5$ in the present case is rather arbitrary. Granato and Lücke concluded that r is of the order of unity in a detailed analysis, but experimental results indicate that r ranges from the order of unity to the order of ten.[5] The purer a specimen is, the greater the value r takes.

The significance of the suggested theory of the distribution of dislocation lengths will now be discussed. As indicated in Chapter II, the broken-away portion of the loop lengths has an exponential distribution e^{-l/L_N} for $\mathcal{L} \leq l < \infty$ This means that for network lengths not less than $\mathcal{L}$, the probability of finding two adjoining loops, separated by an impurity on a particular network loop, with a sum equal to or greater than $\mathcal{L}$, is one. Obviously this is a very good approximation for low γ values. This is because

γ is equal to the ratio of the average value of L_N to that of L_c. On the other hand, the Granato and Lücke theory will be a good approximation for high γ values, since then L_N is much larger than L_c, and in the initial distribution lengths greater than L_N can be neglected. In the present investigation, numerical results are compared for the cases $\gamma = 5$, $\gamma = 10$, and $\gamma = 50$; but just how good an approximation each theory gives is still in question.

Several other points should at least be mentioned. Throughout this paper, the terms "elastic constant" and "elastic modulus" have been used interchangeably; because in the present case only one shearing stress and shearing strain are used, the latter means the elastic shear modulus G and the former means c_{44}, with $G = c_{44}$. However, in general, though they are directly related, these two do not equal to each other.

If normal stress is used instead of shearing stress, i.e., the longitudinal wave instead of the transverse wave, an orientation factor taking account of the orientation relations between the direction of propagation of the longitudinal wave and the slip plane and slip direction has to be introduced. The effect of this orientation factor will not be discussed here, but can be found in Reference 6 in the Bibliography.

The use of the vibrating string model to account for the internal friction and change of elastic modulus in crystals due to dislocations is but one of several existing theories in the study of dislocation damping in crystals. However, as indicated by Niblett and Wilks[8] recently (1960), the vibrating string model generally gives a fairly satisfactory account of both the frequency dependent and amplitude dependent internal friction loss and change of dynamic modulus. It was also indicated that this theory enables one to take account of the effects on internal friction and change of dynamic modulus due to temperature, cold work or annealing, and impurities. The strain amplitude dependent part of the theory consists in the use of a nonlinear stress-dislocation strain law. This nonlinear relationship can be used to define the change of static modulus, which can be measured experimentally. Therefore, a combination of static and dynamic measurements furnishes a method of checking the current theories. Furthermore, the stress-dislocation strain law depends on several parameters such as Λ, the dislocation density, and L_c, the average length of dislocations between impurities, in different ways. By properly changing and controlling such parameters, and making both static and dynamic measurements, more information about the internal structure of a crystal can be obtained.

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