Generation of Ultrasonic Second and Third Harmonics Due to Dislocations. I*

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(Received 16 August 1965)

By representing the effective-tension term of a dislocation (string model) as a power series in displacement gradients, and retaining the first nonlinear term, expressions for the amplitudes of the second and third harmonics of an ultrasonic wave introduced into a solid containing mobile dislocations are obtained. In the case of the second harmonic, a lattice term, a dislocation term, and a cross term contribute to the amplitude and all three terms can be of comparable magnitude. In the case of the third harmonic, in a solid containing a reasonable density of mobile dislocations, the dislocation contribution to the amplitude is dominant and usually lattice effects can be neglected. Except in special circumstances, it is difficult to separate the three terms that contribute to the amplitude of the second harmonic, and dislocation dynamics, therefore, are more easily studied through the generation of third harmonics.

INTRODUCTION

WHEN a sinusoidal ultrasonic wave of a given frequency and of sufficient amplitude is introduced into a nonlinear or anharmonic solid, the fundamental wave will distort as it propagates, so that the second, third, and higher harmonics of the fundamental frequency will be generated. In many solids the nonlinearity of the stress-strain relation (deviation from Hooke's law) may arise from two causes. One is the anharmonicity of the lattice which is a characteristic of all solids, and the other is the contribution of the nonlinear part of the stress-strain relation for dislocation displacement; this cause applies to solids in which glide motion of dislocations is produced by small stresses, i.e., to most metals. The remainder of this discussion refers to the cases for which both contributions are present.

Generation of the second harmonic in 2*S* aluminum (the main cause for this case may be attributed to the lattice anharmonicity) has been reported by Breazeale and Thompson.[1] On the other hand, the dislocation contribution to the generation of second harmonics in high-purity aluminum single crystals was demonstrated by Hikata *et al.*[2,3] It should be emphasized here, however, that for the generation of the second harmonic the stress-strain relation must be nonlinear, as well as not symmetric with respect to displacement gradients. In the case of dislocations, therefore, the displacement from the equilibrium position should be different for equal positive and negative values of stress. This condition may be achieved, for example, by applying a static bias stress in addition to the ultrasonic wave, assuming that the dislocations are straight at the outset. The static bias stresses usually required for this purpose are in the range 10^5–10^6 dyn/cm^2; these stresses have no measurable effect on the coefficients of the anharmonic terms of the lattice.[2–4]

In the case of the third harmonic, however, the condition of nonsymmetry is not required. A symmetric (nonlinear) stress-strain relation is sufficient to generate the third harmonic; in other words, the bias stress is no longer necessary for dislocations to generate the third harmonic. In the case of the second harmonic, the absolute value of the thermal expansion coefficient is a measure of the lattice contribution,[5] and in the cases studied so far, the lattice contribution and the dislocation contribution were found to be of comparable magnitude. Thus, in order to study experimentally either lattice or dislocation anharmonicity it is necessary to separate the two effects. On the other hand, the lattice contribution to the third harmonic is found to be a factor of 10 or more smaller than the dislocation contribution to the third harmonic (the dislocation contribution is comparable for the second and the third harmonic). Therefore, by investigating the third harmonic, it should be possible to obtain detailed information on dislocation motion under stress without the complications of the lattice contribution.

In Refs. 2 and 3, the generation of the second harmonic has been analyzed on the assumption that the increase of potential energy of a dislocation is proportional to the increase of its length. Although the analysis was successful in explaining most of the experimental results, the effect that the dislocation oscillation is damped was not taken into account. Under the same assumption Suzuki *et al.*[4] have treated the problem using the vibrating-string analogy for dislocations and have incorporated the effect of dislocation damping on the amplitude of the second harmonic generated in the specimen. In the following analysis, the latter treatment is extended to the case of the third harmonic with some modifications and refinements.

* This work has been supported, in part, by the Research and Technology Division, Air Force Command, U. S. Air Force.

[1] M. A. Breazeale and D. O. Thompson, Appl. Phys. Letters 3, 77 (1963).

[2] A. Hikata, B. B. Chick, and C. Elbaum, Appl. Phys. Letters 3, 195 (1963).

[3] A. Hikata, B. B. Chick, and C. Elbaum, J. Appl. Phys. 36, 229 (1965).

[4] T. Suzuki, A. Hikata, and C. Elbaum, J. Appl. Phys. 35, 2761 (1964).

[5] J. M. Ziman, *Electrons and Phonons* (Clarendon Press, Oxford, England, 1960), p. 152.

EQUATION OF MOTION

When a stress wave is propagated along a solid containing dislocations, the dislocations will oscillate causing additional local displacement and strain in the solid. If one denotes the longitudinal displacement of an infinitesimal element of a solid in the x direction by u, then

$$u=u_l+u_d,$$

where u_l is the displacement of the lattice, and u_d is the displacement due to the dislocation motion. The one-dimensional form of the equation of motion for the displacement u in the x direction is given by

$$\rho\frac{\partial^2 u}{\partial t^2}=\rho\frac{\partial^2}{\partial t^2}(u_l+u_d)=\frac{\partial\sigma}{\partial x}, \tag{1}$$

where ρ is the density of the undeformed material, σ is the applied stress, and t denotes time. It is convenient for us to use the differentiated form (with respect to x) of Eq. (1)

$$\rho\frac{\partial^2}{\partial t^2}\left(\frac{\partial u_l}{\partial x}+\frac{\partial u_d}{\partial x}\right)=\frac{\partial^2\sigma}{\partial x^2}. \tag{2}$$

Thus, the problem is now reduced to expressing $\partial u_l/\partial x$ and $\partial u_d/\partial x$ as a function of stress σ and to solve Eq. (2) with respect to σ. In the present case, however, a sinusoidal wave of frequency ω is introduced at one end of the specimen (at $x=0$). As the wave propagates, the wave form will be distorted due to the nonlinearity of the solid. Therefore, at a distance x, the stress σ should be expressed in terms of the harmonics of the fundamental wave, i.e.,

$$\sigma=A_0+A_1\cos(\omega t-kx)+A_2\cos2(\omega t-kx-\delta_2)+A_3\cos3(\omega t-kx-\delta_3), \tag{3}$$

where A_0 is a static bias stress, A_1, A_2, and A_3 are the amplitudes of the fundamental, the second, and the third harmonic waves, respectively, $2\delta_2$ and $3\delta_3$ are the phase angles of the second and the third harmonics relative to the fundamental wave, respectively, and k is the wave vector. It is assumed here that dispersion is negligible. The boundary conditions are

at $x=0$,
$A_1=A_{10}$ (the amplitude of the induced fundamental wave),
$A_2=A_3=0$.

Since the nonlinearity considered here is not expected to be large, one can assume that

$$A_2, A_3\ll A_1.$$

Thus, if one expresses both sides of Eq. (2) in terms of the harmonics, a comparison of the sine and cosine terms of the corresponding frequencies will provide sets of equations which determine the amplitudes of the harmonics.

EXPRESSION FOR $\partial u_l/\partial x$

The one-dimensional relation between stress σ and displacement gradient $\partial u_l/\partial x$ of a solid, correct to the square terms is given by[6]

$$\sigma=E_1\frac{\partial u_l}{\partial x}+a\left(\frac{\partial u_l}{\partial x}\right)^2, \tag{4}$$

where E_1 is the second-order elastic constant and a is a combination of the second- and third-order elastic constants. Thus,

$$\begin{aligned}\frac{\partial u_l}{\partial x}&=\frac{1}{E_1}\sigma-\frac{a}{E_1{}^3}\sigma^2+\cdots\\
&=\frac{A_0}{E_1}-\frac{a}{E_1{}^3}\left(A_0{}^2+\frac{A_1{}^2}{2}\right)+\left[\frac{A_1}{E_1}-\frac{a}{E_1{}^3}(2A_0A_1+A_1A_2\cos2\delta_2)\right]\cos(\omega t-kx)\\
&\quad-\left[\frac{a}{E_1{}^3}A_1A_2\sin2\delta_2\right]\sin(\omega t-kx)+\left[\frac{A_2}{E_1}\cos2\delta_2-\frac{a}{E_1{}^3}\left(2A_0A_2\cos2\delta_2+\frac{A_1{}^2}{2}\right)\right]\cos2(\omega t-kx)\\
&\quad+\left[\frac{A_2}{E_1}\sin2\delta_2-\frac{a}{E_1{}^3}2A_0A_2\sin2\delta_2\right]\sin2(\omega t-kx)+\left[\frac{A_3}{E_1}\cos3\delta_3-\frac{a}{E_1{}^3}(2A_0A_3\cos3\delta_3+A_1A_2\cos2\delta_2)\right]\cos3(\omega t-kx)\\
&\quad+\left[\frac{A_3}{E_1}\sin3\delta_3-\frac{a}{E_1{}^3}(2A_0A_3\sin3\delta_3+A_1A_2\sin2\delta_2)\right]\sin3(\omega t-kx).\end{aligned} \tag{5}$$

EXPRESSION FOR $\partial u_d/\partial x$

The linear case of small-amplitude dislocation oscillations under the influence of an externally applied oscillatory stress was treated, using the string analogy, by Koehler[7] and later by Granato and Lücke.[8] In these

[6] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity* (Pergamon Press, Inc., New York, 1959), p. 115.
[7] J. S. Koehler, *Imperfections in Nearly Perfect Crystals* (John Wiley & Sons, Inc., New York, 1952).
[8] A. Granato and K. Lücke, J. Appl. Phys. **27**, 583 (1956).

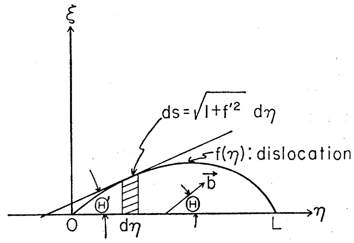

FIG. 1. Bowed-out dislocation $\xi=f(\eta)$. η axis coincides with the straight-line configuration of the dislocation before bowing out. **b**, Burgers vector.

treatments[7,8] the line energy is assumed to be independent of the position and orientation of a dislocation. In fact, however, even in an isotropic material, the line energy of an edge dislocation differs significantly from that of a screw dislocation.[9–12] It follows that, in general, the line energy of a bowed-out dislocation (under an external stress) is not constant along the dislocation line. In the case of an anisotropic solid, the energy difference between edge and screw dislocations could be quite large as pointed out by Foreman,[10] and deWit and Koehler.[11]

The present study is concerned with nonlinear effects for which the assumption of small displacement amplitudes does not apply. Under such conditions, one has to take into account the effects of both the variation of the line energy along dislocations and the higher order terms in $(\partial\xi/\partial\eta)$ (for definitions of ξ and η see Fig. 1).

In order to obtain the equation of motion of dislocations, one has to establish first the differential equation determining the equilibrium configuration of dislocations under the influence of a static stress. For this purpose, we follow the calculation carried out by Leibfried[12] and extend it to the nonlinear case by retaining the higher order terms of $(\partial\xi/\partial\eta)$ in the expansion of the energy expression [see Eqs. (10) and (11)].

The line energy of a dislocation (per unit length) in an isotropic material has been calculated and is given by

$$W_e=\frac{\mu b^2}{4\pi}\frac{1}{1-\nu}\ln\frac{R}{R_c} \tag{6}$$

for edge dislocations and

$$W_s=(\mu b^2/4\pi)\ln(R/R_c) \tag{7}$$

for screw dislocations. Here μ is the shear modulus, ν is Poisson's ratio, b is the absolute value of the Burgers vector, R_c is an effective core radius (in the order of b), and R is an effective external radius. Typically, R/R_c is about 10^4 and the logarithm therefore is in the order of 10. Since W is only logarithmically dependent on R/R_c, the exact value of R/R_c is usually thought to be of minor importance.

In the string model, a line segment ds of a dislocation line has an energy $V_L ds$ with

$$V_L=W_e(b_\perp^2/b^2)+W_s(b_{\parallel}^2/b^2)=W_e(1-m\cos^2\theta). \tag{8}$$

Here, $b_\perp$ and $b_{\parallel}$ are the components of the Burgers vector **b** perpendicular and parallel to the segment, and θ is the angle between **b** and d**s** (Fig. 2), and

$$m=(W_e-W_s)/W_e. \tag{9}$$

In the following we will refer to a straight dislocation line along the η axis as the original and stable position. The dislocation motion is governed by the change in energy caused by deviations from the straight line. The slip plane is taken as the $\xi\eta$ plane and the dislocation line is defined by $\xi=f(\eta)$ (Fig. 1). Then, by using Eq. (8) the following is obtained:

$$V=\int d\eta\, W_e[(1+f'^2)^{1/2}\times\{1-m\cos^2(\Theta-\Theta')\}-(1-m\cos^2\Theta)].$$

Here, $f'=\partial\xi/\partial\eta$, and $\Theta-\Theta'=\theta$ is the angle between the line segment and Burgers vector, and the meaning of Θ and Θ' is explained in Fig. 1. Introducing $\tan\Theta'=f'$ we obtain

$$V=\int d\eta\, W_e\left[(1+f'^2)^{1/2}\left\{1-\frac{m}{1+f'^2}(\cos^2\Theta+2f'\sin\Theta\cos\Theta+f'^2\sin^2\Theta)\right\}-(1-m\cos^2\Theta)\right]. \tag{10}$$

The integrand of (10) can be expanded in powers of f'. If one keeps terms up to the fourth power in f', the result is given by

$$V=\int d\eta\, W_e[-2mf'\sin\Theta\cos\Theta+\tfrac{1}{2}(1+m\cos^2\Theta-2m\sin^2\Theta)f'^2+f'^3\sin\Theta\cos\Theta-\tfrac{1}{8}(1+3m\cos^2\Theta-4m\sin^2\Theta)f'^4]. \tag{11}$$

If the dislocation is pinned at $\eta=0$ and $\eta=L$, the deviations from the straight configuration should be the same for equal positive and negative stresses. In other words, V should be symmetrical in terms of f'. Therefore, in Eq. (11) the terms containing f' and f'^3 should vanish.

The equilibrium condition for the line segment L can be obtained from a variational principle; i.e., the total energy $W=V-V_\tau$ should be an extremal, where

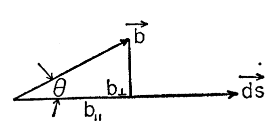

FIG. 2. Definition of $b_{\parallel}$ and $b_\perp$.

[9] R. M. Stern and A. Granato, Acta Met. **10**, 92 (1962).
[10] A. J. E. Foreman, Acta Met. **3**, 322 (1955).
[11] G. de Wit and J. S. Koehler, Phys. Rev. **116**, 1113 (1959).
[12] G. Leibfried, Oak Ridge National Laboratory Progress Report No. ORNL 2829, 1959 (unpublished).

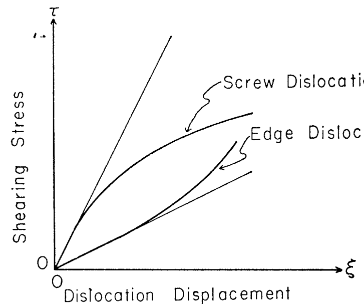

FIG. 3. Stress-displacement relationship of screw and edge dislocations (schematic); straight lines give linear approximation.

V_τ is the work done by the external force and given by

$$V_\tau=\tau b\int_0^L f(\eta)d\eta,$$

and τ is the resolved shear stress in the glide plane and in the slip direction. The equilibrium condition becomes

$$\delta W=\delta(V-V_\tau)=0,$$

or, according to the Euler-Lagrange equation,

$$\frac{d}{d\eta}\frac{\partial W}{\partial f'}-\frac{\partial W}{\partial f}=0.$$

The result is then

$$-f''W_e[(1+m\cos^2\Theta-2m\sin^2\Theta)-\tfrac{3}{2}(1+3m\cos^2\Theta-4m\sin^2\Theta)f'^2]=\tau b. \quad (12)$$

If one assumes that the line energies of edge dislocations and of screw dislocations are equal, i.e., $m=0$, then Eq. (12) becomes

$$-W_ef''(1-\tfrac{3}{2}f'^2)=\tau b,$$

which is the case treated in Refs. 2–4, and 13. If one assumes further that the higher order term is negligible, the equation reduces to

$$-W_ef''=\tau b,$$

which is the case of the linear approximation treated by Granato and Lücke.[8] Even in an isotropic material, m is not equal to zero, and is given by

$$m=\nu=\tfrac{1}{3}\quad (\nu,\ \text{Poisson's ratio}).$$

Thus, for an edge dislocation ($\Theta=\pi/2$), Eq. (12) reduces to

$$-\tfrac{1}{3}W_ef''(1+\tfrac{3}{2}f'^2)=\tau b$$

or, since $W_e/3\approx\frac{1}{2}\mu b^2$,

$$-\tfrac{1}{2}\mu b^2f''(1+\tfrac{3}{2}f'^2)=\tau b. \quad (13)$$

For a screw dislocation ($\Theta=0$),

$$\left.\begin{array}{l}-(4/3)W_ef''(1-(9/4)f'^2)=\tau b,\\ -2\mu b^2f''(1-(9/4)f'^2)=\tau b.\end{array}\right\} \quad (14)$$

[13] A. Hikata, B. B. Chick, and C. Elbaum, U. S. Air Force Technical Report AFML-TR-65-56, 1965 (unpublished).

Equations (13) and (14) reveal two important features: (a) The linear term of Eq. (13), $-\frac{1}{2}\mu b^2f''$, is $\frac{1}{4}$ of the linear term of Eq. (14), $-2\mu b^2f''$. This means that for a small applied stress, the displacement of an edge dislocation is approximately four times larger than that of a screw dislocation. Therefore, for a small oscillatory stress, it is expected that the contribution from edge dislocations is predominant for the quantities such as attenuation and velocity change, provided that the density and loop length of the two types of the dislocations are similar.[9,12] (b) The nonlinear term in Eq. (13), $-\frac{3}{2}f'^2$ is negative, while that of Eq. (14), $+(9/4)f'^2$ is positive. This means that, the stress-displacement relation for edge dislocations is hardening (as the applied stress increases, a larger stress increment is necessary to produce a given amount of displacement), while the stress-displacement relation for screw dislocations is softening (see Fig. 3). Of course, the deviation from a linear stress-displacement relationship, whether it is softening or hardening, is the source of the harmonic generation.

The nonlinear relation between a static stress and the dislocation displacement of a pinned dislocation leads to the following equation of motion of a dislocation under the influence of combined static and oscillatory stresses:

$$A\frac{\partial^2\xi}{\partial t^2}+B\frac{\partial\xi}{\partial t}-C\left[\left(\frac{\partial^2\xi}{\partial\eta^2}\right)-C'\left(\frac{\partial\xi}{\partial\eta}\right)^2\left(\frac{\partial^2\xi}{\partial\eta^2}\right)\right]=bR\sigma, \quad (15)$$

where

σ is given by Eq. (3),
$A=\pi\rho b^2$ (effective mass of dislocation per unit length),
B is the damping coefficient,
$C=W_e(1+m\cos^2\Theta-2m\sin^2\Theta)$,

$$C'=\frac{3}{2}\frac{(1+3m\cos^2\Theta-4m\sin^2\Theta)}{(1+m\cos^2\Theta-2m\sin^2\Theta)},$$

m and Θ are the quantities defined in the previous section,
b is the Burgers vector,
R is the resolving shear factor converting the axial stress to the shear stress in the slip plane and in the slip direction.

The terms $A(\partial^2\xi/\partial t^2)$ and $B(\partial\xi/\partial t)$ represent the inertia force and frictional force of a dislocation per unit length, respectively. The nonlinear differential Eq. (15) can be solved approximately by iteration. First, utilizing the Fourier expansion of $bR\sigma$, one obtains a solution ξ_1 for the linear approximation of Eq. (15) (i.e., the equation without the nonlinear term),

$$\xi_1=\xi_{10}+\xi_{11}+\xi_{12}+\xi_{13}, \quad (16)$$

where

$$\xi_{10}=\frac{4bRA_0L_0^2}{\pi^3C}\sum_0^\infty\frac{1}{(2n+1)^3}\sin\frac{(2n+1)\pi\eta}{L_0},$$

$$\xi_{11}=\frac{4bRA_1}{A\pi}\sum_0^\infty\frac{1}{2n+1}\frac{1}{S_n^{1/2}}\times\sin\frac{(2n+1)\pi\eta}{L_0}\cos(\omega\tau-kx-\delta_{1n}),$$

with

$$S_n=(\omega_n^2-\omega^2)^2+(\omega d)^2,$$

$$\omega_n=(2n+1)(\pi/L_0)(C/A)^{1/2},$$

$$\tan\delta_{1n}=\omega d/(\omega_n^2-\omega^2),$$

$$d=B/A,$$

$$\xi_{12}=\frac{4bRA_2}{A\pi}\sum_0^\infty\frac{1}{2n+1}\frac{1}{M_n^{1/2}}\times\sin\frac{(2n+1)\pi\eta}{L_0}\cos2(\omega t-kx-\delta_2-\delta_{2n})$$

with

$$M_n=\{\omega_n^2-(2\omega)^2\}^2+(2\omega d)^2,$$

$$\tan2\delta_{2n}=\frac{2\omega d}{\omega_n^2-(2\omega)^2},$$

$$\xi_{13}=\frac{4bRA_3}{A\pi}\sum_0^\infty\frac{1}{2n+1}\frac{1}{T_n^{1/2}}\times\sin\frac{(2n+1)\pi\eta}{L_0}\cos3(\omega t-kx-\delta_3-\delta_{3n}),$$

with

$$T=\{\omega_n^2-(3\omega)^2\}^2+(3\omega d)^2,$$

$$\tan3\delta_{3n}=\frac{3\omega d}{\omega_n^2-\omega^2}.$$

In the following analysis, only the first terms ($n=0$) of each infinite series are taken into account.[14] Inserting $\xi=\xi_1+\xi_2$ into Eq. (15), where ξ_2 is the iterated solution, and retaining those nonlinear terms containing only ξ_1, one obtains the equation

$$A\frac{\partial^2\xi_2}{\partial t^2}+B\frac{\partial\xi_2}{\partial t}-C\frac{\partial^2\xi_2}{\partial\eta^2}=-CC'\left(\frac{\partial\xi_1}{\partial\eta}\right)^2\left(\frac{\partial^2\xi_1}{\partial\eta^2}\right)$$
$$=\frac{CC'}{4}\left(\frac{\pi}{L_0}\right)^4\left(\sin\frac{3\pi\eta}{L_0}+\sin\frac{\pi\eta}{L_0}\right)\{A_0P+A_1Q\cos(\omega t-kx-\delta_{10})$$
$$+A_2K\cos2(\omega t-kx-\delta_2-\delta_{20})+A_3J\cos3(\omega t-kx-\delta_3-\delta_{30})\}^3,\quad(17)$$

where

$$P=\frac{4bRL_0^2}{\pi^3C},\quad Q=\frac{4bR}{A\pi S_0^{1/2}},\quad K=\frac{4bR}{A\pi M_0^{1/2}},$$

and

$$J=\frac{4bR}{A\pi T_0^{1/2}}.$$

Neglecting the term $\sin(3\pi\eta/L_0)$[15] and retaining the terms up to the third harmonic in the right-hand side of Eq. (17), one obtains the solution ξ_2,

$$\xi_2=\xi_{20}+\xi_{21}+\xi_{22}+\xi_{23},\quad(18)$$

where

$$\xi_{20}=h\sin\frac{\pi\eta}{L_0}\frac{L^2}{\pi^2C}[A_0^3P^3+\tfrac{3}{2}A_0PA_1^2Q^2],$$

$$h=\frac{CC'}{4}\left(\frac{\pi}{L_0}\right)^4,$$

$$\xi_{21}=h\sin\frac{\pi\eta}{L_0}\frac{1}{AS_0^{1/2}}[\{\tfrac{3}{4}A_1^3Q^3+3A_0^2P^2A_1Q\}\cos(\omega t-kx-2\delta_{10})+3A_0PA_1QA_2K\cos(\omega t-kx-2\delta_2-2\delta_{20})],$$

[14] The displacement of the modes corresponding to $n>0$ decreases very rapidly with increasing n and may be neglected for the purposes of this calculation.

[15] When the term $\sin(3\pi\eta/L_0)$ is retained various parts of the solution are multiplied by numerical factors of order unity.

$$\xi_{22}=h\sin\frac{\pi\eta}{L_0}\frac{1}{AM_0^{1/2}}[\tfrac{3}{2}A_0PA_1^2Q^2\cos2(\omega t-kx-\delta_{10}-\delta_{20})+3A_0^2P^2A_2K\cos2(\omega t-kx-\delta_2-\delta_{20})],$$

$$\xi_{23}=h\sin\frac{\pi\eta}{L_0}\frac{1}{AT_0^{1/2}}[\tfrac{1}{4}A_1^3Q^3\cos3(\omega t-kx-\delta_{10}-\delta_{30})+3A_0^2P^2A_3J\cos3(\omega t-kx-\delta_3-2\delta_{30})$$
$$+3A_0PA_1QA_2K\cos3(\omega t-kx-\tfrac{1}{3}(\delta_{10}+2\delta_2+2\delta_{20}+3\delta_{30}))].$$

Thus, after one iteration, one obtains for the solution of Eq. (15),

$$\xi=\xi_1+\xi_2, \tag{19}$$

where ξ_1 and ξ_2 are given by expressions (16) and (18).

Once ξ is obtained in terms of η, $\partial u_d/\partial x$ can be calculated by the following relation:

$$\frac{\partial u_d}{\partial x}=\frac{Nbq}{L_0}\int_0^{L_0}\xi\,d\eta, \tag{20}$$

where N is the effective dislocation density and q is a factor converting the shear strain to the longitudinal strain.

AMPLITUDE OF THE SECOND AND THIRD HARMONIC

Inserting the expressions (3), (5), and (20) into Eq. (2) and equating separately the sine and cosine terms of each harmonic, the following relations are obtained:

$$(d^2A_1/d_x^2)-k^2A_1=-\rho\omega^2[(A_1/E_1)-(a/E_1^3)(2A_0A_1+A_1A_2\cos2\delta_2)+gQA_1\cos\delta_{10}$$
$$+hg(1/AS_0^{1/2})\{(\tfrac{3}{4}A_1^3Q^3+3A_0^2P^2A_1Q)\cos2\delta_{10}+3A_0PA_1QA_2K\cos2(\delta_2+\delta_{20})\}], \tag{21}$$

$$2k(dA_1/dx)=-\rho\omega^2[-(a/E_1^3)A_1A_2\sin2\delta_2+A_1Qg\sin\delta_{10}+h(g/AS_0^{1/2})$$
$$\times\{(\tfrac{3}{4}A_1^3Q^3+3A_0^2P^2A_1Q)\sin2\delta_{10}+3A_0PA_1QA_2K\sin2(\delta_2+\delta_{20})\}], \tag{22}$$

$$(d^2A_2/dx^2)\cos2\delta_2-4k(dA_2/dx)\sin2\delta_2-4k^2A_2\cos2\delta_2$$
$$=-4\rho\omega^2[(A_2/E_1)\cos2\delta_2-(a/E_1^3)(2A_0A_2\cos2\delta_2+(A_1^2/2))+A_2Kg\cos2(\delta_2+\delta_{20})$$
$$+h(g/AM_0^{1/2})\{\tfrac{3}{2}A_0PA_1^2Q^2\cos2(\delta_{10}+\delta_{20})+3A_0^2P^2A_2K\cos2(\delta_2+2\delta_{20})\}], \tag{23}$$

$$(d^2A_2/dx^2)\sin2\delta_2+4k(dA_2/dx)\cos2\delta_2-4k^2A_2\sin2\delta_2$$
$$=-4\rho\omega^2[(A_2/E_1)\sin2\delta_2-(a/E_1^3)(2A_0A_2\sin2\delta_2)+KA_{2}g\sin2(\delta_2+\delta_{20})$$
$$+h(g/AM_0^{1/2})\{\tfrac{3}{2}A_0PA_1^2Q^2\sin2(\delta_{10}+\delta_{20})+3A_0^2P^2A_2K\sin2(\delta_2+2\delta_{20})\}], \tag{24}$$

$$(d^2A_3/dx^2)\cos3\delta_3-6k(dA_3/dx)\sin3\delta_3-9k^2A_3\cos3\delta_3$$
$$=-9\rho\omega^2[(A_3/E_1)\cos3\delta_3-(a/E_1^3)(2A_0A_3\cos3\delta_3+A_1A_2\cos2\delta_2)+JA_{3}g\cos3(\delta_3+\delta_{30})+h(g/AT_0^{1/2})$$
$$\times\{\tfrac{1}{4}A_1^3Q^3\cos3(\delta_{10}+\delta_{30})+3A_0^2P^2A_3J\cos3(\delta_3+2\delta_{20})+3A_0PA_1QA_2K\cos(\delta_{10}+2\delta_2+2\delta_{20}+3\delta_{30})\}], \tag{25}$$

$$(d^2A_3/dx^2)\sin3\delta_3+6k(dA_3/dx)\cos3\delta_3-9k^2A_3\sin3\delta_3$$
$$=-9\rho\omega^2[(A_3/E_1)\sin3\delta_3-(a/E_1^3)(2A_0A_3\sin3\delta_3+A_1A_2\sin2\delta_2)+JA_{3}g\sin3(\delta_3+\delta_{30})+h(g/AT_0^{1/2})$$
$$\times\{\tfrac{1}{4}A_1^3Q^3\sin3(\delta_{10}+\delta_{30})+3A_0^2P^2A_3J\sin3(\delta_3+2\delta_{20})+3A_0PA_1QA_2K\sin(\delta_{10}+2\delta_2+2\delta_{20}+3\delta_{30})\}], \tag{26}$$

where

$$g=2Nbq/\pi.$$

In Eqs. (21) and (22), the terms containing A_2 are much smaller than the terms containing A_1; furthermore, in the present study the term containing A_1^3 is negligible compared with the term containing A_1. These terms are, therefore, neglected. After these approximations one obtains as the solutions of Eqs. (21) and (22),

$$A_1=A_{10}e^{-\alpha_1x}, \tag{27}$$

with

$$\alpha_1=(\rho\omega^2g/2k)[Q\sin\delta_{10}+(3h/AS_0^{1/2})A_0^2P^2Q\sin2\delta_{10}], \tag{28}$$

$$k^2-\alpha_1^2=\rho\omega^2\left[\frac{1}{E_1}-\frac{2a}{E_1^3}A_0+g\left\{Q\cos\delta_{10}+\frac{3h}{AS_0^{1/2}}A_0^2P^2Q\cos2\delta_{10}\right\}\right], \tag{29}$$

where A_{10} is the amplitude of the induced oscillatory stress at $x=0$.

The expression (28) represents the attenuation of the fundamental wave. Since $k=\omega/v$ and $v=(E/\rho)^{1/2}$ (v is the velocity of sound in the material), the first term of the expression (28) can be written

$$\alpha_{10}=4NE_1b^2qR\omega^2d/vA\pi^2S_0, \tag{30}$$

which agrees with Granato and Lücke's[6] results. The second term of the expression (28) represents the effect of bias stress on the attenuation. Although it increases with the square of the bias stress, its contribution to the attenuation turns out to be negligible in the stress range of interest here.

From Eq. (29), one can derive the velocity change of $\Delta v/v$ of the fundamental wave,

$$(\Delta v/v)\cong(a/E_1^2)A_0-\tfrac{1}{2}E_1g\{Q\cos\delta_{10}+(3h/AS_0^{1/2})A_0^2P^2Q\cos 2\delta_{10}\}. \tag{31}$$

From Eqs. (23) and (24), the amplitude A_2 of the second harmonic can be obtained;

$$A_2=\left\{\frac{a}{2E_1^3}\sin 2\delta_2-\frac{3}{2}\frac{hg}{AM_0^{1/2}}A_0PQ^2\sin 2(\delta_2-\delta_{10}-\delta_{20})\right\}\frac{\rho\omega^2}{k}A_{10}^2\frac{e^{-2\alpha_1x}-e^{-\alpha_2x}}{\alpha_2-2\alpha_1}, \tag{32}$$

with

$$\alpha_2=(\rho\omega^2g/k)\{K\sin 2\delta_{20}+(3h/AM_0^{1/2})A_0^2P^2K\sin 4\delta_{20}\}, \tag{33}$$

where the following relation should also be satisfied:

$$d^2A_2/dx^2=[4k^2-4\rho\omega^2\{(1/E_1)-(2a/E_1^3)A_0+Kg\cos 2\delta_{20}+(3hg/AM_0^{1/2})A_0^2P^2K\cos 4\delta_{20}\}]A_2$$
$$+4\rho\omega^2\{(a/2E_1^3)\cos 2\delta_2-\tfrac{3}{2}(hg/AM_0^{1/2})A_0PQ^2\cos 2(\delta_2-\delta_{10}-\delta_{20})\}A_1. \tag{34}$$

If one compares the expression for α_2 [Eq. (33)] and that of the fundamental wave α_1 [Eq. (28)], it is easily seen that α_2 is equivalent to the attenuation of an independent wave propagating with a frequency 2ω. This means that since dispersion is assumed to be negligible, the following relation between k and α_2 should also hold,

$$4k^2-\alpha_2^2=4\rho\omega^2[(1/E_1)-(2a/E_1^3)A_0+g\{K\cos 2\delta_{20}+(3h/AM_0^{1/2})A_0^2P^2K\cos 4\delta_{20}\}]. \tag{35}$$

Substituting the expressions (32) and (35) into (34), one obtains the following relation for the phase angle δ_2 between the fundamental and the second harmonic wave:

$$\tan 2\delta_2\cong\frac{a/2E_1-(3h/AM_0^{1/2})A_0PQ^2\cos 2(\delta_{10}+\delta_{20})}{(3h/AM_0^{1/2})A_0PQ^2\sin 2(\delta_{10}+\delta_{20})}. \tag{36}$$

If one neglects the dislocation contribution to the second harmonic, the phase angle becomes,

$$2\delta_2=\pi/2.$$

On the other hand, if one neglects the lattice contribution, $2(\delta_2-\delta_{10}-\delta_{20})$ is very close to $\pi/2$. Thus, one can express the amplitude of the second harmonic with reasonable accuracy as follows:

$$A_2=\frac{\rho\omega^2}{k}[X^2+Y^2-2XY\cos 2(\delta_{10}+\delta_{20})]^{1/2}\times A_{10}^2\frac{e^{-2\alpha_1x}-e^{-\alpha_2x}}{\alpha_2-2\alpha_1}, \tag{37}$$

where

$$X=a/2E_1^2,$$
$$Y=48Nb^4R^3qC'A_0/\pi^2A^3S_0M_0^{1/2}L_0^2,$$

furthermore, in the case where $\omega_0\gg 4\omega$, the factor

$$\cos 2(\delta_{10}+\delta_{20})$$

can be replaced by

$$(\omega_0^2/S_0M_0^{1/2})(\omega_0^4-5\omega^2d^2).$$

From Eqs. (25) and (26), the following expressions for the amplitude A_3 and the attenuation α_3 of the third harmonic can be obtained:

$$A_3=-\frac{3}{8}\frac{\rho\omega^2g}{k}\frac{hQ^3A_{10}^3\sin 3(\delta_3-\delta_{10}-\delta_{30})}{AT_0^{1/2}}\frac{e^{-3\alpha_1x}-e^{-\alpha_3x}}{\alpha_3-3\alpha_1}, \tag{38}$$

$$\alpha_3=\frac{3}{2}\frac{\rho\omega^2g}{k}\left\{J\sin 3\delta_{30}+\frac{3h}{AT_0^{1/2}}A_0^2P^2J\sin 6\delta_{30}\right\}, \tag{39}$$

where the following relation should also be satisfied:

$$\frac{d^2A_3}{dX^2}=\left[9k^2-9\rho\omega^2\left\{\frac{1}{E_1}-\frac{2a}{E_1^3}A_0+g\left(J\cos 3\delta_{30}+\frac{3h}{AT_0^{1/2}}A_0^2P^2J\cos 6\delta_{30}\right)\right\}\right]A_3$$
$$-[(9/4)\rho\omega^2(gh/AT_0^{1/2})Q^3\cos 3(\delta_3-\delta_{10}-\delta_{30})]A_1^3. \tag{40}$$

As in the case of the second harmonic, expression (39) indicates that the third harmonic generated in the solid attenuates in the same manner as an independent wave of frequency 3ω introduced into the solid. This leads to the following condition determining the phase angle $3\delta_3$ between the fundamental and the third harmonic wave:

$$\tan 3(\delta_3-\delta_{10}-\delta_{30})=6k/(\alpha_3+3\alpha_1).$$

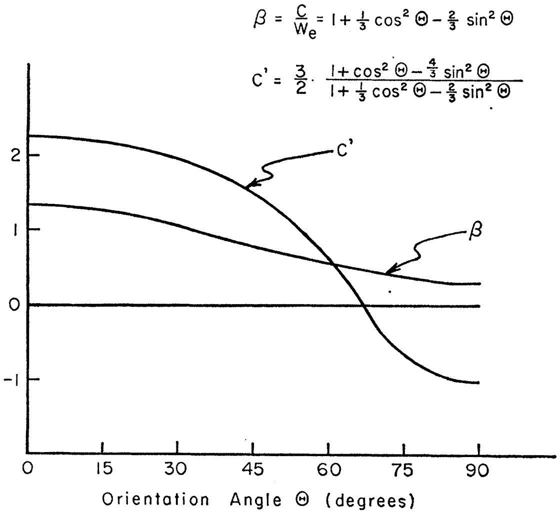

FIG. 4. Variation of the factors β and C' with orientation angle Θ.

Since the right-hand side of the above equation is a very large quantity, $3(\delta_3-\delta_{10}-\delta_{30})$ is positive and very close to $\pi/2$. Thus, one can express the amplitude of the third harmonic with reasonable accuracy as follows,

$$A_3=\frac{12\rho\omega^2Nb^4qR^3CC'A_{10}{}^3}{kA^4S_0{}^{3/2}T_0{}^{1/2}L_0{}^4}\frac{e^{-3\alpha_1x}-e^{-\alpha_3x}}{\alpha_3-3\alpha_1}. \quad (41)$$

It should be emphasized that expression (41) represents the contribution of dislocations only to the third harmonic and that the lattice contribution is neglected.

DISCUSSION

In the following, several significant consequences of the above expressions are presented:

(a) There are two contributions to the second harmonic, one arising from the lattice anharmonicity which is represented by the first term of the expression (37), the other arising from the nonlinear dislocation motion which is represented by the second term of the expression. In addition, the existence of the phase angle $2(\delta_{10}+\delta_{20})$ between the two components leads to the cross term in expression (37). The factor Y is a function of dislocation density, of bias stress (internal or external), and of loop length (which in turn depends on bias stress), while X is independent of the bias stresses in the range considered here and is a constant for a given solid and mode of wave propagation. In general, a separation of the two contributions is quite difficult because of the cross term in expression (37). Under certain circumstances, either X or Y is dominant and the cross term is unimportant. A separation of the two terms is also possible, of course, when $2(\delta_{10}+\delta_{20})\approx(\pi/2)$ (δ_{10} and δ_{20} depend on loop length).

In the case of the third harmonic, the lattice contribution does not appear in the expression (41). This is simply because the terms in powers higher than the square of the displacement gradient are not taken into account in the expression (4). Although for the lattice part the magnitude of the cubic term relative to the linear and the square terms is not known at present, it is reasonable to assume that in most solids the lattice contribution to the third harmonic is negligible, at least near room temperature, where the temperature dependence of the thermal expansion coefficient is small. Thus, the third harmonic observable near room temperature can be considered to be predominantly due to the nonlinear motion of dislocations.

(b) The amplitudes of the second and third harmonic are proportional, respectively, to the square and cube of the amplitude of the fundamental wave as long as the dislocation loop lengths remain constant.

(c) At $x=0$, the amplitude of the harmonics is zero. As the fundamental wave propagates along the x axis, it starts generating the harmonics. However, both fundamental and harmonic waves suffer attenuation. The resulting initial build-up followed by a decay of the amplitude of the second and third harmonics as a function of propagation distance x are represented, respectively, by

$$(e^{-2\alpha_1x}-e^{-\alpha_2x})/(\alpha_2-2\alpha_1) \quad (42)$$

and

$$(e^{-3\alpha_1x}-e^{-\alpha_3x})/(\alpha_3-3\alpha_1). \quad (43)$$

Each factor has a maximum at a distance $(x_2)_{\max}$ and $(x_3)_{\max}$ given by the following relations

$$(x_2)_{\max}=\frac{\ln(2\alpha_1/\alpha_2)}{2\alpha_1-\alpha_2}\quad(\text{cm}), \quad (44)$$

$$(x_3)_{\max}=\frac{\ln(3\alpha_1/\alpha_3)}{3\alpha_1-\alpha_3}\quad(\text{cm}). \quad (45)$$

(d) Since C appears in the factors S_0, M_0, and T_0, the magnitude and the sign of the harmonics depend on the values of C and C', which are, of course, a function of

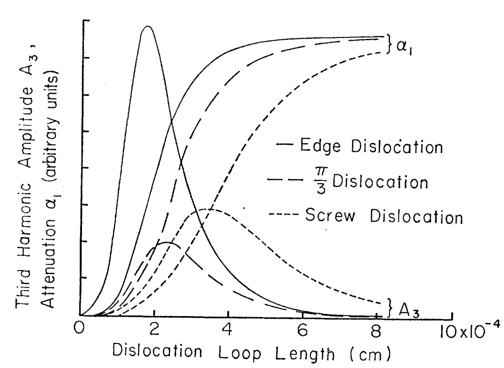

FIG. 5. Amplitude of the third harmonic A_3 and attenuation of the fundamental wave α_1 for edge, screw, and $\pi/3$ dislocations as a function of loop length. (Arbitrary units for A_3 and α_1.)

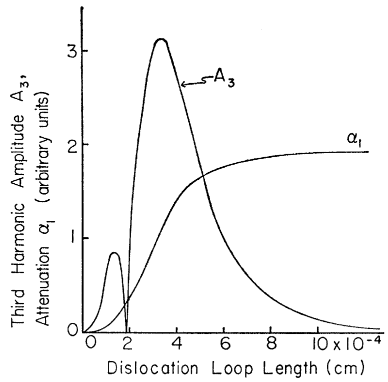

FIG. 6. Amplitude of the third harmonic A_3 and attenuation of the fundamental wave α_1 averaged over the range $0 \leq \Theta \leq 90°$. (Arbitrary units for A_3 and α_1.)

the orientation angle Θ. In Fig. 4, the factors

$$\beta = C/W_e = 1+m-3m\sin^2\Theta$$

and

$$C' = -\frac{3}{2}\frac{(1+3m-7m\sin^2\Theta)}{(1+m-3m\sin^2\Theta)}$$

are plotted as a function of Θ, taking $m=\nu=\frac{1}{3}$ (ν is Poisson's ratio). As can be seen, C' changes its sign at approximately $\Theta=67.5$ deg. This means that the harmonics generated by the dislocations whose orientation angles (see Fig. 4) are in the range $0<\Theta<67.5$ deg are opposite in sign to the harmonics generated by the dislocations whose orientation angles are in the range $67.5°<\Theta<90°$. In the case of the second harmonic, the applied static stress A_0 is, in fact, a parameter to indicate the degree of deviation of a bowed out dislocation from its straight-line configuration. Therefore, regardless of whether the static stress is tension or compression, the absolute value $|A_0|$ should be used in evaluating the expression (37). Thus, except for the factor C', the quantities that appear in the dislocation contribution are all positive. The contribution of the dislocations may be of the same or opposite sign as the lattice term, depending on the relative signs of X and Y, as well as on the sign of $(\omega_0^4-5\omega^2d^2)$—see Eq. (37). In the case of the third harmonic, the absolute value should be used in evaluating the expression (41).

The factor β(as well as C) also depends on the angle Θ. The larger the value of C, the smaller is the corresponding dislocation displacement for a given stress, as discussed in the previous section. Since the amplitude of the harmonics depends strongly on the dislocation displacement, it is expected that the dislocations with smaller C values will generate larger harmonics, if other factors are identical.

In all cases the dislocation contribution depends not only on loop length but also on orientation, i.e., the angle Θ. Therefore, the expression (41) should be calculated using appropriate distributions of both dislocation orientation and loop length. Since the information on the distribution of orientation and loop length is very scarce, in the following, the Θ and loop-length-dependent part of the amplitude A_3 (disregarding the attenuation factor)

$$CC'/S_0^{3/2}T_0^{1/2}L_0^4 \tag{46}$$

is calculated numerically for edge, screw, and $\pi/3$ dislocations as a function of loop length L_0, for a single loop and using the following values, $A=7.6\times10^{-15}$ g cm^{-1}, $B=5\times10^{-4}$ dyn sec cm^{-2}, $\omega=2\pi\times10^7$ sec^{-1}, $W_e=1.2\mu b^2$, $\mu=3\times10^{11}$ dyn cm^{-2}, $b=3\times10^{-8}$ cm. The results are given in Fig. 5. As can be seen, the maximum amplitude of the third harmonic arising from edge dislocations is considerably larger than that arising from screw or $\pi/3$ dislocations. In this figure, the attenuation of the fundamental wave α_1 is also plotted for the three types of dislocations. In each case, the loop length for the maximum amplitude of the third harmonic coincides approximately with the loop length corresponding to the inflection point in the attenuation curve. The maximum of the third harmonic, therefore, corresponds approximately to the transition between underdamped and overdamped behavior. The condition determining the loop length for the maximum amplitude A_3 is given by

$$\omega_0/\omega \simeq 1.12(d/\omega)^{1/2}. \tag{47}$$

In plotting Fig. 5, the absolute values are taken for the third-harmonic amplitude A_3. As mentioned earlier, the amplitude A_3 for dislocations whose orientation angles Θ are in the range $0<\Theta<67.5°$ are opposite in sign to those whose orientation angles are in the range $67.5°<\Theta<90°$. Therefore, cancellations of amplitude A_3 will take place when the dislocations in the two ranges operate simultaneously. To see this effect, a simple average of the expression (46) over the range $0\leq\Theta\leq90°$ was calculated as a function of loop length using the same numerical values as given above. The results are shown in Fig 6. The cancellation occurs approximately at the loop length of 1.9×10^{-4} cm. Whether this effect becomes significant or not depends, of course, on the orientation distribution of dislocations.

In view of the difficulties in separating the lattice and dislocation contributions in the case of the second harmonic, dislocation dynamics are studied more easily through the generation of third harmonics. It should also be emphasized that in order to study lattice anharmonicity by means of second-harmonic generation, it is necessary to eliminate the dislocation contribution.