

Dislocation contribution to acoustic nonlinearity: The effect of orientation-dependent line energy

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Abstract

Dislocation dynamics (DD) simulations are used to investigate the emerging metal-fatigue detection technique of nonlinear ultrasonics. The acoustic nonlinearity parameter, β , is quantitatively predicted for a single dislocation bowing in its glide plane between pinning points under a quasi-static loading assumption using DD simulations. The existing model using a constant line energy assumption fails to capture the correct behavior of β for edge dislocations in materials with a nonzero Poisson's ratio. A strong dependence of β on the orientation of Burgers vector relative to the line direction of the dislocation is shown by the DD simulations. A new model using an orientation-dependent line energy is derived for the cases of initially-pure edge and screw dislocations. The model is shown to agree with the DD simulations over a range of Poisson's ratio and static stresses.

Key words: acoustic nonlinearity, fatigue, dislocation line energy

1. Background

Fatigue is a common failure mechanism of solid materials caused by progressive damage due to repeated loading. Unfortunately, maintenance of fatigue susceptible devices and detection of fatigue damage can be extremely expensive. Traditional nondestructive evaluation (NDE) techniques of metals rely on periodic inspections to detect the presence of macroscopic cracks. These tests often require taking the structure out of service and disassembling its components. Moreover, these evaluations are only able to detect the final stages in the fatigue life. In the high-cycle fatigue regime, the vast majority of the life is prior to the emergence of macrocracks [1].

Over the past few decades, a great deal of emphasis has been placed on developing methods to monitor damage evolution *in-situ*. A significant body of research on the use of embedded sensors to detect the

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presence of macrocracks has been amassed [2]. Being able to detect macro-cracks as they emerge can reduce costs and improve safety. However, it is still limited to detecting the ultimate stages of damage and cannot be used to monitor the early stages of the microstructural evolution.

Nonlinear ultrasonics is an emerging technique to detect the earliest stages of metal fatigue. An initially sinusoidal ultrasonic wave is passed through the material and the magnitude of the second harmonic response is measured. The results are commonly expressed in terms of the acoustic nonlinearity parameter, β , which can be defined in terms of experimentally measurable quantities as

$$\beta^{meas} = \frac{8A_1}{k^2 A_2^2 x}, \quad (1)$$

where k is the wave number, x is the propagation distance of the ultrasound, and A_1 and A_2 are the measured displacement amplitudes of the first and second harmonics, respectively. The importance of β can be easily illustrated in the one-dimensional nonlinear wave equation:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \left[1 - \beta \frac{\partial u}{\partial x} \right] \frac{\partial^2 u}{\partial x^2}, \quad (2)$$

where c is the infinitesimal-amplitude wave speed and $\partial u / \partial x$ is the displacement gradient. When β is zero, the equation reduces to the linear wave equation.

β is found to grow in magnitude with the number of load cycles until failure in single and polycrystalline metals and alloys [3, 4]. Thus, nonlinear ultrasonics has the potential to monitor the entire fatigue life. Unfortunately, the underlying mechanisms giving rise to the increase in β are not well understood. The anharmonicity of the crystal itself leads to nonlinearities, but for the range of deformations considered its contribution to β essentially remains constant [5]. Prior to cracking, there are significant microstructural changes in the material associated with the growth and patterning of dislocations. The interaction of the ultrasonic waves with the dislocations is thought to be the cause of the variation in β . Proposed analytical models include a dislocation segment bowing between pinning points in its glide plane and the oscillation of two dislocations in a dipole [3, 6]. These two dislocation effects have served as the foundation of more advanced models [7, 8, 9]. However, the relative weights of these effects have not been conclusively determined. There has yet to be any direct comparison of β calculated using these models to experiments, because of the complexity of real dislocation structures. Not understanding the mechanisms makes it impossible to quantitatively predict β or how a given value of β relates to the damage in the material. Dislocation dynamics (DD) simulations have the potential to model realistic dislocation microstructures in monotonic and fatigue loading conditions, but have yet to be applied to the acoustic nonlinearity. Thus, the goal of this paper is to use DD simulations to examine the analytical models and establish DD as a method to predict

the contribution of dislocations to β .

2. Simulation design

The DD simulations were performed using a quasi-static loading assumption, as opposed to modeling the dynamic wave propagation. A series of simulations were performed for a given dislocation structure over a range of static external stresses. The structure was allowed to reach equilibrium and the plastic strain due to dislocation motion was calculated. A relationship between stress and plastic strain was then derived. The deviation of this relationship from linearity is measured by β , as explained later in this paper. The quasi-static loading assumption has been used in previous analytical models and greatly reduces the complexity of the simulations [6]. It is valid because inertial forces on dislocations can be ignored for the loading frequency applied by ultrasonic transducers (0.1-100 MHz) and the small stresses applied by the transducer essentially result in a perturbation about a given stress on the quasi-static stress-strain relationship.

To be consistent with the notation used by DeWit and Koehler [10], all the simulations performed in

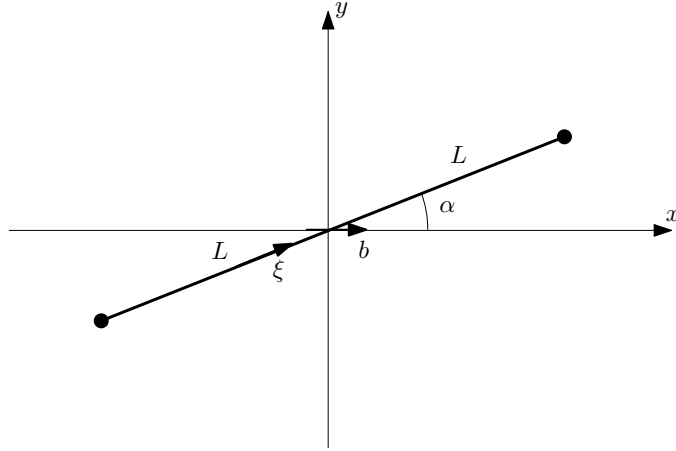


Figure 1: Schematic of model design. Initially-straight dislocation segment of length $2L$ in the x - y plane with a Burgers vector b along the x -axis. The dislocation is oriented along the line direction ξ at an angle α relative to the x -axis

this paper are of a single straight dislocation in the x - y plane with initial length $2L$. Its Burgers vector b is along the x -axis and its line direction ξ is oriented at an angle θ relative to b , as shown Fig. 1. An application of a resolved shear stress results in a local radius of curvature r .

The simulations were performed using the ParaDiS code [11]. These simulations are limited to the bulk of an FCC single crystal oriented for single slip and the dislocations are initialized as perfect dislocations. The model assumes that cross-slip and thermally-activated climb do not occur, because of the small

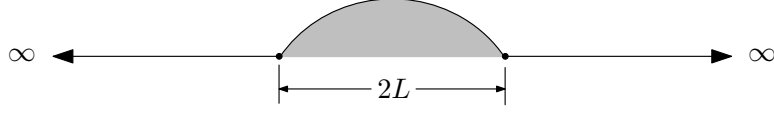


Figure 2: Infinitely-long, straight dislocation pinned along majority of its length modeled by the elastic interaction DD simulations

stresses applied by the ultrasound transducers and short time scales present in physical experiments. The dislocation interactions will be modeled throughout this paper using either a line-tension model or using elastic interactions [11, 12]. For the case of the elastic interactions, the dislocation will be treated as a long, straight dislocation pinned along the majority of its length, as shown in Fig. 2, to avoid terminating the dislocation inside the crystal and to include the interaction forces of remote segments. Additional simulation parameters are provided in subsequent sections for individual cases.

3. Constant line tension model of Hikata et al.

3.1. Model Construction

The model developed by Hikata et al. was the first to employ the quasi-static loading assumption for the bowing dislocation line [6]. For the past four decades, it has been the widely accepted model for the acoustic nonlinearity arising from the self-interaction of a single dislocation. Only a brief description of this model is given here; the reader is referred to the detailed derivation given by Cantrell [13]. However, a trivial deviation from previous derivations has been made here to consider a shear wave passing through the material as opposed to a longitudinal wave; this only simplifies the notation.

A line tension approximation is used to represent the shape of the dislocation bowing between pinning points under an applied stress σ . The line tension T is assumed to be constant regardless of orientation, $T = \mu b^2/2$. Therefore, screw and edge dislocations possess the same line energy, and the equilibrium shape is that of a circular arc with a constant constant radius of curvature. The area swept by the dislocation can be expanded in a series approximation to yield an expression for plastic strain in terms of a powers of applied stress σ :

$$\epsilon^{dis} = \frac{2}{3} \frac{\Omega \Lambda^{dis} L^2 R^3}{\mu} \sigma + \frac{4}{5} \frac{\Omega \Lambda^{dis} L^4 R^3}{\mu^3 b^2} \sigma^3, \quad (3)$$

where Λ^{dis} is the dislocation density, μ is the shear modulus, R is an orientation factor between the applied stress and the resolved shear stress, and Ω is conversion factor between shear strain in the slip direction and

measured strain.

The elastic strains of the lattice can also be expressed as a series in terms of σ :

$$\epsilon^{lat} = \frac{\partial u_1}{\partial x_2} = \frac{1}{A_{66}}\sigma - \frac{1}{2} \frac{A_{666}}{A_{66}^3}\sigma^2, \quad (4)$$

where A_{66} and A_{666} are the second and third-order elastic stiffnesses in Voigt notation, respectively. The total strain¹ ϵ is thus the summation of the elastic lattice strain and the plastic strain of the dislocation:

$$\epsilon = \epsilon^{lat} + \epsilon^{dis} = \left(\frac{1}{A_{66}} + \frac{2}{3} \frac{\Omega \Lambda^{dis} L^2 R^3}{\mu} \right) \sigma - \frac{1}{2} \frac{A_{666}}{A_{66}^3} \sigma^2 + \frac{4}{5} \frac{\Omega \Lambda^{dis} L^4 R^3}{\mu^3 b^2} \sigma^3. \quad (5)$$

The ultrasonic wave creates a small oscillatory stress of amplitude $\Delta\sigma$ in addition to the static stress σ , which in turn causes an additional strain $\Delta\epsilon$. This can be represented as:

$$\Delta\sigma = \frac{\partial\sigma}{\partial\epsilon} \Delta\epsilon + \frac{1}{2} \frac{\partial^2\sigma}{\partial\epsilon^2} (\Delta\epsilon)^2 + \dots = \left(\frac{\partial\epsilon}{\partial\sigma} \right)^{-1} \Delta\epsilon - \frac{1}{2} \frac{\partial^2\epsilon}{\partial\sigma^2} \left(\frac{\partial\epsilon}{\partial\sigma} \right)^{-3} (\Delta\epsilon)^2 + \dots \quad (6)$$

where the derivatives of ϵ can be derived from Eq. (5). It can be shown from Eq. (6) that the total acoustic nonlinearity parameter β^{total} is:

$$\beta^{total} = \frac{\partial^2\epsilon}{\partial\sigma^2} \left(\frac{\partial\epsilon}{\partial\sigma} \right)^{-2} = \left(-\frac{A_{666}}{A_{66}^3} + \frac{24}{5} \frac{\Omega \Lambda^{dis} L^4 R^3}{\mu^3 b^2} \sigma \right) \left(\frac{1}{A_{66}} + \frac{2}{3} \frac{\Omega \Lambda^{dis} L^2 R^3}{\mu} \right)^{-2}. \quad (7)$$

In most cases

$$\frac{2}{3} \frac{\Omega \Lambda^{dis} L^2 R^3}{\mu} \ll \frac{1}{A_{66}}. \quad (8)$$

β^{total} can then be simplified to

$$\beta^{total} = -\frac{A_{666}}{A_{66}} + \frac{24}{5} \frac{\Omega \Lambda^{dis} L^4 R^3 A_{66}^2}{\mu^3 b^2} \sigma, \quad (9)$$

where A_{666}/A_{66} is the lattice contribution, which is essentially invariant over the range of interest and will henceforth be omitted.

3.2. Comparison with elastic-interaction DD Simulations

In an isotropic elastic medium, A_{66} is simply the shear modulus μ . In addition, if the applied stress is chosen to act directly on the slip system of the dislocation and the strain is measured relative to the slip direction, Ω and R will both be unity. The contribution of dislocation monopoles to the acoustic nonlinearity for this special case can then be found from Eq. (9):

$$\beta^{dis} = \frac{24}{5} \frac{\Lambda^{dis} L^4}{\mu b^2} \sigma. \quad (10)$$

¹The strains here are a result of the applied stress and should not be confused with the arbitrarily small displacements from the acoustic wave.

The analytical model can now be compared with an elastic interaction DD simulation of a pinned dislocation of length $2 \mu\text{m}$ ($L = 1 \mu\text{m}$) between pinning points and Burgers vector b of 1 nm . The shear modulus μ of the material is taken to be 27 GPa with a dislocation density Λ^{dis} of $2 \times 10^6 \text{ m}^{-2}$ and a Poisson's ratio ν of 0.40 . The dislocation density is very small because there is only one dislocation in the entire simulation cell.

The first equality in Eq. (7) shows that β^{dis} can be calculated from DD by taking the first and second derivatives of the dislocation plastic strain with respect to stress about the equilibrium stress σ :

$$\beta^{dis} = \frac{\partial^2 \epsilon^{dis}}{\partial \sigma^2} \left(\frac{\partial \epsilon}{\partial \sigma} \right)^{-2} = \frac{\partial^2 \epsilon^{dis}}{\partial \sigma^2} \left(\frac{1}{A_{66}} + \frac{\partial \epsilon^{dis}}{\partial \sigma} \right)^{-2} \approx \mu^2 \frac{\partial^2 \epsilon^{dis}}{\partial \sigma^2} \quad (11)$$

where again, the plastic contribution $\partial \epsilon^{dis} / \partial \sigma$ to $\partial \epsilon / \partial \sigma$ is minuscule.² Therefore, a series of constant-stress simulations were performed to determine the equilibrium plastic strain ϵ^{dis} . $\partial^2 \epsilon^{dis} / \partial \sigma^2$ was then found using a central difference scheme.

The results in Fig. 3(a) highlight the disagreement between the Hikata et al. model and the DD

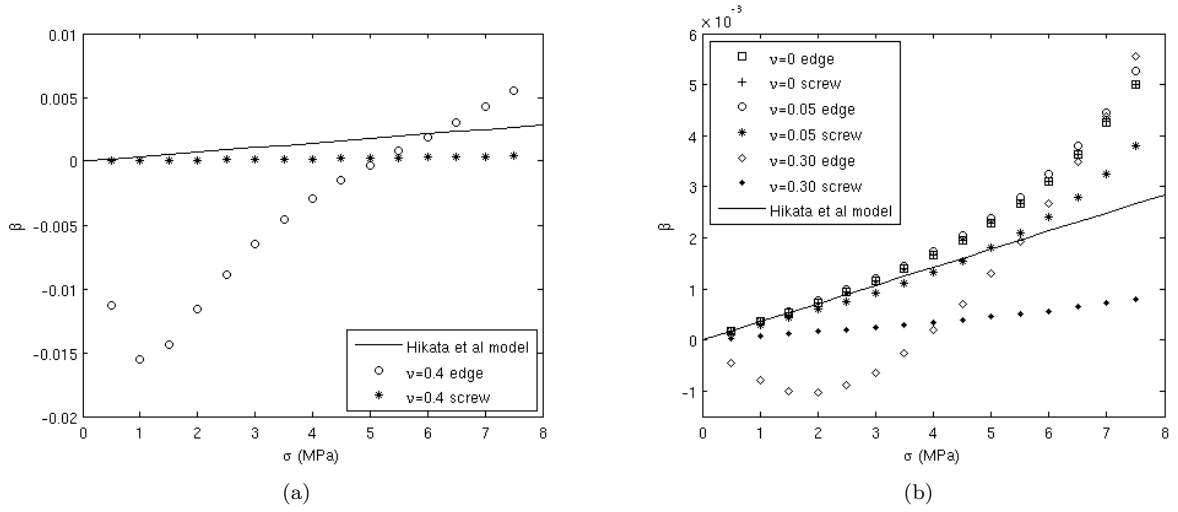


Figure 3: Comparison of DD simulations with the model of Hikata et al.

simulations. The deviation from the linear relationship of β^{dis} and σ predicted by the model is most dramatic for the edge dislocation with a negative β^{dis} at small stresses.

3.3. Comparison with line-energy DD Simulations

In order to simplify the DD simulations and better evaluate the analytical model, a series of simulations using an orientation-dependent line-energy model were performed [12]. A comparison of these simulations

²This assumption has been numerically verified, but the discussion is omitted here.

and the analytical results are shown in Fig. 3(b) for pure edge and screw monopoles over a range of Poisson's ratios ν and σ .³ When σ is small, the results agree well for both screw and edge if ν is close to zero. This is because the line tension of an edge dislocation is $1/(1 - \nu)$ times that of a screw. Thus, when the Poisson's ratio is zero, there is constant line tension – the assumption used by Hikata et al.

When ν is increased the line-energy DD predictions deviate from the Hikata model, with that of the edge taking on a wildly different shape for ν greater than approximately 0.2. Unfortunately, most engineering metals and alloys commonly used in fatigue susceptible applications possess Poisson's ratios in the range of 0.2-0.4. These results clearly illustrate the importance of the orientation dependence of the line energy and the initial edge character of the straight dislocation. It is thus desired to develop an analytical model that can explain the trends seen in the simulations.

4. Variable line-energy model

The previous section has illustrated that a major shortcoming of the Hikata et al. model is the oversimplification of the dislocation line energy. The major difficulty that arises when moving to a variable line tension is that the shape of the bowed dislocation can no longer be described by a simple circular arc with constant radius of curvature. The equilibrium shape of a bowing monopole under an arbitrary load was solved by DeWit and Koehler by balancing the work done by the external stress and the change in the self-energy of the dislocation[10]. The equilibrium shape of a dislocation loop under an external stress τ with Burgers vector b along the x -axis can be parameterized in terms of θ :

$$x = \frac{1}{\tau b} \left[\sin \theta E(\theta) + \cos \theta \frac{dE}{d\theta} \right] \quad (12)$$

$$y = \frac{1}{\tau b} \left[\cos \theta E(\theta) - \sin \theta \frac{dE}{d\theta} \right] \quad \theta \in [0, 2\pi]. \quad (13)$$

The orientation-dependent line energy $E(\theta)$ is commonly expressed as

$$E(\theta) = \frac{\mu b^2}{4\pi(1 - \nu)} (1 - \nu \cos^2 \theta) \ln \left(\frac{r_o}{r_i} \right) \quad (14)$$

in an isotropic elastic medium, where r_o and r_i are the outer and inner cut-off radii, respectively [14]. A numerical implementation of this model is employed in the aforementioned line-energy DD simulations [12].

³It should be noted that by varying ν while holding μ constant in an elastically isotropic medium will cause the Young's modulus E of the material to change. This obviously can't be accomplished in a physical experiment, but is done here to illustrate the problem.

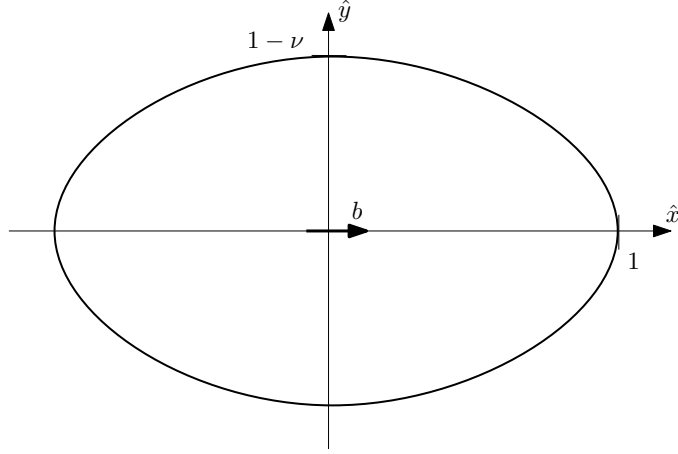


Figure 4: Equilibrium shape of dislocation loop for $\nu = 0.33$ in scaled coordinates

By approximating $\ln(r_o/r_i)$ as 2π we can define

$$M = \frac{\mu b^2 \ln\left(\frac{r_o}{r_i}\right)}{4\pi(1-\nu)} = \frac{\mu b^2}{2(1-\nu)} \quad (15)$$

and rewrite Eq. (14) as

$$E(\theta) = M(1 - \nu \cos^2 \theta). \quad (16)$$

In the case of $\nu = 0$, Eq. (16) simplifies to the constant line energy, $\mu b^2/2$, as used in the Hikata et al. model.

Evaluating Eq. (12) and Eq. (13) with the line energy defined in Eq. (15) and Eq. (16) yields

$$\hat{x} = \frac{\tau b x}{M} = \left(1 + \frac{\nu}{4}\right) \sin \theta + \frac{\nu}{4} \sin 3\theta \quad (17)$$

$$\hat{y} = \frac{\tau b y}{M} = \left(1 - \frac{5\nu}{4}\right) \cos \theta + \frac{\nu}{4} \cos 3\theta, \quad (18)$$

which defines the parameterized curve for the generalized equilibrium shape of the dislocation loop, as shown in Fig. 4 for $\nu = 0.33$. Although the curve may appear nearly elliptical, any such approximation should be avoided because the errors in the shape of the curve will be amplified in the derivatives of Eq. (7) to find β^{total} . The deviation from ellipticity becomes apparent at Poisson's ratios approaching 0.5. In the case of $\nu = 0$, the dislocation loop simplifies to a unit circle in the $\hat{x}, \hat{y}$ coordinate system. To simplify the notation, Eq. (17) and Eq. (18) are rewritten as

$$\hat{x} = C \sin \theta + D \sin 3\theta \quad (19)$$

$$\hat{y} = U \cos \theta + V \cos 3\theta, \quad (20)$$

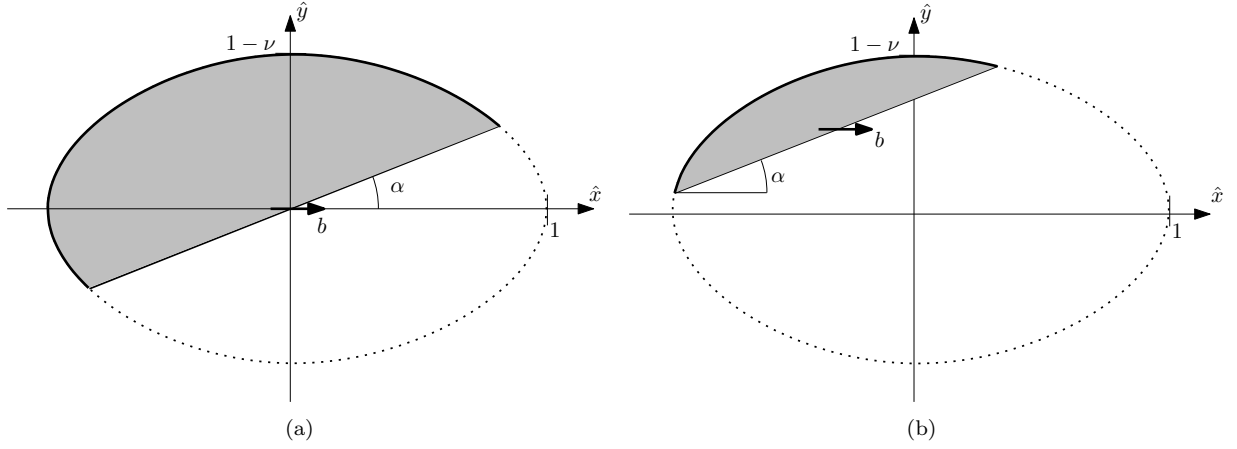


Figure 5: Curve of an arbitrary pinned dislocation under a resolved shear stress from the equilibrium shape of a dislocation loop using a variable line energy

where

$$C = 1 + \frac{\nu}{4}; \quad D = \frac{\nu}{4}; \quad U = 1 - \frac{5\nu}{4}; \quad V = \frac{\nu}{4}. \quad (21)$$

The unstable equilibrium shape of any dislocation at activation can be found by passing a line through the origin at an angle α , as shown in Fig. 5(a), where α is the angle between the Burgers vector and the initial line direction. The shape of the deformed dislocation prior to activation can be found from the generalized curve by shifting the line along its normal, as shown in Fig. 5(b).

The strain caused by dislocation motion can again be related to the area swept out by the dislocation. The area can be found for an arbitrary dislocation using Eq. (17) and Eq. (18), but for simplicity only initially-pure edge and screw dislocations will be considered here. In these special cases, the bowed out shape of the dislocation is symmetric with respect to a plane normal to the initial line direction of the dislocation and passing through its midpoint.

In the case of a screw dislocation, the x -axis is parallel to its initial line direction and the y -axis is along the glide direction. The area swept out by the screw dislocation can be expressed as:

$$A = \int_{-L}^L y(x)dx - y(x=L) \cdot 2L = 2 \int_0^L y(x)dx - y(x=L) \cdot 2L \quad (22)$$

where y is now a function of x . Evaluating this expression is not a trivial matter; two different approaches will be taken in the following two sections. The edge dislocation's initial line direction is along the y -direction and the dislocation bows out in the x -direction. To simplify derivations later in this paper, a coordinate transformation is performed so that the edge is initially along the x -direction and glides in the y -direction,

as shown in Fig. 6(b). The equation of the dislocation loop in this coordinate system is

$$\hat{x} = \frac{\tau b x}{M} = U \sin \theta - V \sin 3\theta \quad (23)$$

$$\hat{y} = \frac{\tau b y}{M} = C \cos \theta - D \cos 3\theta. \quad (24)$$

Eq. (22) can then be used to find the area swept by the edge dislocation.

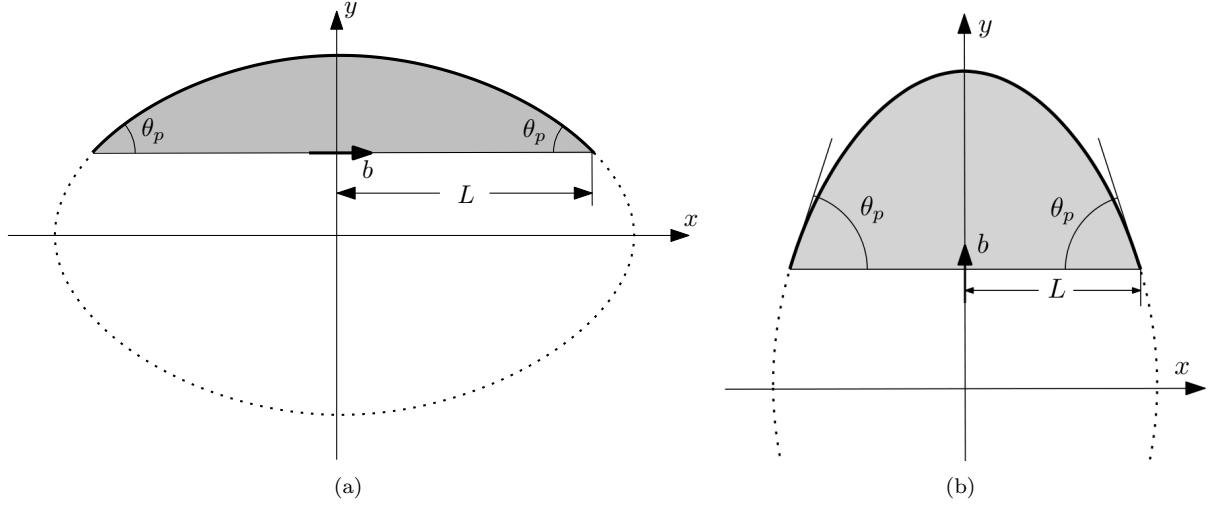


Figure 6: Shape of pinned dislocations subjected to a resolved shear below the activation stress

5. Power series solution

5.1. Model Construction

In this section, the technique used by Hikata et al. to express the strains in terms of a power series of stress is applied to the cases of initially edge and screw dislocations with variable line energy defined in the previous section.

The dislocation curve described in Eq. (19) and Eq. (20) is shifted so that the peak of the curve coincides with the origin. $\hat{y}$ can be approximated as a power series of $\hat{x}$:

$$\hat{y}(\hat{x}) = \frac{\zeta}{2} \hat{x}^2 + \frac{\eta}{4!} \hat{x}^4 + \frac{\kappa}{6!} \hat{x}^6, \quad (25)$$

where the odd powers of $\hat{x}$ are obviously zero by symmetry and higher order terms are ignored. Expanding Eq. (17) and Eq. (18) for an initially-screw dislocation yields:

$$\zeta = -\frac{1}{1+\nu} \quad (26)$$

$$\eta = -\frac{3(1+3\nu)}{(1+\nu)^4} \quad (27)$$

$$\kappa = -\frac{45(1+6\nu+13\nu^2)}{(1+\nu)^7}. \quad (28)$$

The area in Eq. (22) can be expressed in scaled coordinates as

$$\hat{A} = 2 \int_0^{\hat{L}} \hat{y}(\hat{x}) d\hat{x} - \hat{y}(\hat{L}) \cdot 2\hat{L} = -\frac{2}{3}\zeta\hat{L}^3 - \frac{1}{15}\eta\hat{L}^5 - \frac{1}{420}\kappa\hat{L}^7. \quad (29)$$

To solve for the real area,

$$\hat{L} = \frac{\tau b}{M} L \quad (30)$$

$$\hat{A} = \left(\frac{\tau b}{M}\right)^2 A \quad (31)$$

are substituted into Eq. (29) to yield

$$A = -\frac{2}{3} \frac{bL^3\zeta}{M} \tau - \frac{1}{15} \frac{b^3L^5\eta}{M^3} \tau^3 - \frac{1}{420} \frac{b^5L^7\kappa}{M^5} \tau^5. \quad (32)$$

The area swept by the dislocation is directly proportional to the plastic strain of the dislocation,

$$\epsilon^{dis} = \frac{b\Omega\Lambda^{dis}}{2L} A = -\frac{1}{3} \frac{b^2L^2\Omega\Lambda^{dis}\zeta}{M} \tau - \frac{1}{30} \frac{b^4L^4\Omega\Lambda^{dis}\eta}{M^3} \tau^3 - \frac{1}{840} \frac{b^6L^6\Omega\Lambda^{dis}\kappa}{M^5} \tau^5, \quad (33)$$

where again Λ^{dis} is the dislocation density. Substituting the values of ζ , η , κ and M into Eq. (33) and taking $\tau = R\sigma$ as before:

$$\begin{aligned} \epsilon^{dis} = \frac{2}{3} \frac{(1-\nu)\Omega\Lambda^{dis}L^2R}{(1+\nu)\mu} \sigma + \frac{4}{5} \frac{(1+3\nu)(1-\nu)^3\Omega\Lambda^{dis}L^4R^3}{(1+\nu)^4\mu^3b^2} \sigma^3 \\ + \frac{12}{7} \frac{(1+6\nu+13\nu^2)(1-\nu)^5\Omega\Lambda^{dis}L^6R^5}{(1+\nu)^7\mu^5b^4} \sigma^5. \end{aligned} \quad (34)$$

Using derivations similar to that of Hikata et al. in Section 3.1, the initially-screw dislocation contribution to the acoustic nonlinearity can then be expressed as

$$\beta_s^{dis} = \frac{24}{5} \frac{(1+3\nu)(1-\nu)^3\Omega\Lambda^{dis}L^4R^3}{(1+\nu)^4\mu b^2} \sigma + \frac{240}{7} \frac{(1+6\nu+13\nu^2)(1-\nu)^5\Omega\Lambda^{dis}L^6R^5}{(1+\nu)^7\mu^3b^4} \sigma^3. \quad (35)$$

In the case of $\nu = 0$ and the orientation factors R and Ω are unity, β_s^{dis} reduces to

$$\beta_s^{dis}|_{\nu=0} = \frac{24}{5} \frac{\Lambda^{dis}L^4}{\mu b^2} \sigma + \frac{240}{7} \frac{L^6\Lambda^{dis}}{\mu^3b^4} \sigma^3. \quad (36)$$

The first-order term is identical to the β^{dis} derived by Hikata et al. in Eq. (11). Similar analysis for an initially-edge dislocation described by Eq. (23) and Eq. (24) reveals

$$\beta_e^{dis} = \frac{24}{5} \frac{(1-4\nu)(1-\nu)^3 \Omega \Lambda^{dis} L^4 R^3}{(1-2\nu)^4 \mu b^2} \sigma + \frac{240}{7} \frac{(1-8\nu+20\nu^2)(1-2\nu)^7 \Omega \Lambda^{dis} L^6 R^5}{(1+\nu)^7 \mu^3 b^4} \sigma^3 \quad (37)$$

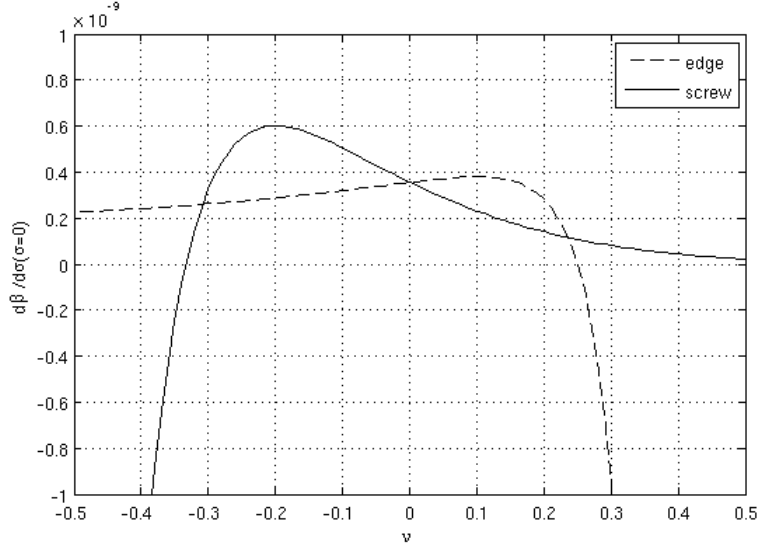


Figure 7: $\partial\beta/\partial\sigma$ at $\sigma = 0$ over a range of Poisson's ratio.

Fig. 7 plots the initial slope of the $\beta(\sigma)$ curve as a function of ν and illustrates the importance of the variable line energy. The differences between edge and screw dislocations is readily apparent for nonzero Poisson's ratios. Edge dislocations are seen to have initially negative values of β^{dis} for ν greater than 0.25, and tends toward negative infinity as ν approaches one-half. In screw dislocations the slope is negative for ν less than negative one-third. However, in subsequent analyses only positive Poisson's ratios will be considered.

5.2. Comparison with line-tension DD Simulations

The newly derived analytical expression for β^{dis} was compared with the aforementioned line-energy DD simulations, as shown for screw dislocations in Fig. 8(a) and for edge dislocations in Fig. 8(b). It is apparent that the power-series solution agrees with the DD simulations significantly better than the Hikata et al. model and is able to capture the initially negative β^{dis} exhibited by edge dislocations in materials with large Poisson's ratios. The power-series model agrees well for screw dislocations for any ν and for edge dislocations with $\nu < 0.25$. However, for the case of edge dislocations in materials with large ν , the model is only able to roughly predict the general trend at small stresses. This is a consequence of using a truncated

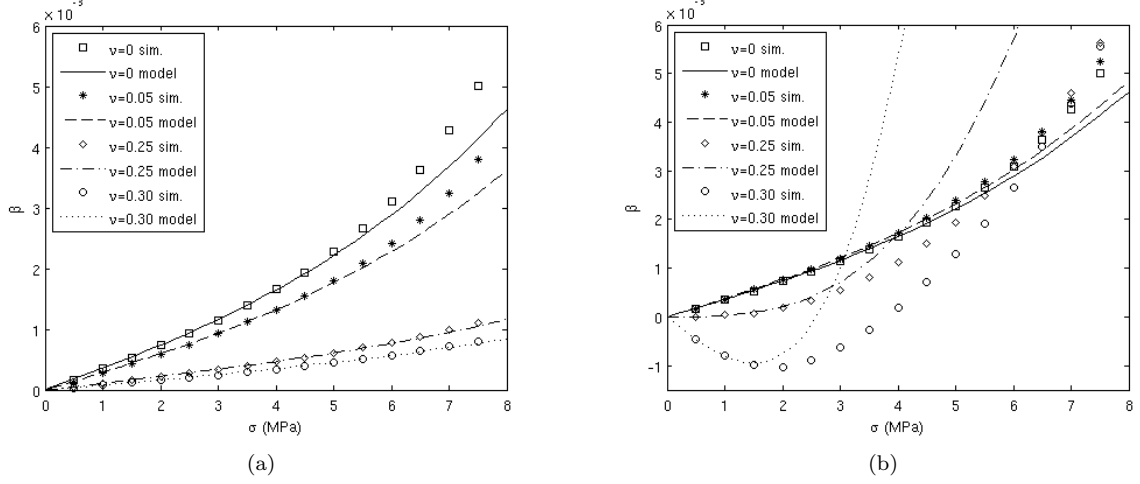


Figure 8: Comparison of orientation-dependent, line-energy DD simulations with the power-series model

power series expanded about zero stress.

6. Implicit solution

6.1. Model Construction

In order to avoid the shortcomings of the power-series model at high stress values, the area of the bowed out dislocation in Eq. (22) must not be approximated. However, this integral cannot immediately be evaluated because x and y are expressed in terms of the parameter θ . Therefore, the area for initially edge or screw dislocations is now expressed in terms of θ as

$$A(\tau, \theta_p) = 2 \int_0^{\theta_p} y(\theta) \frac{dx}{d\theta} d\theta - y(\theta = \theta_p) \cdot 2L, \quad (38)$$

where θ_p is the angle at the pinning point, as shown in Fig. 6(a). This equation is only valid for initially-pure edge and screw dislocations, because of their aforementioned symmetry. In addition, it holds true only if $E(\theta) + d^2 E(\theta)/d\theta^2 > 0$ [10], because the angle θ must increase monotonically from the midpoint to the pinning point.⁴

Eq. (38) expresses A as a function of the applied stress τ and θ_p . But, τ can be expressed as a function of θ_p by evaluating Eq. (19) at $x = L$ and $\theta = \theta_p$ and solving for τ . After substituting $\sigma = R\tau$ the resolved shear stress σ can be expressed as

$$\sigma_s(\theta_p) = \frac{1}{2} \frac{(1 + \nu \cos^2 \theta_p) \sin \theta_p R b \mu}{L(1 - \nu)} \quad (39)$$

⁴This model could be used for an arbitrary dislocation, but calculating A will be more difficult.

for an initially-screw dislocation. In the case of an initially-edge dislocation, the same steps can be performed to Eq. (23) to yield

$$\sigma_e(\theta_p) = \frac{1}{2} \frac{(1 - \nu - \nu \cos^2 \theta_p) \sin \theta_p R b \mu}{L(1 - \nu)}. \quad (40)$$

Substituting the results of Eq. (19), Eq. (20), and Eq. (39) into Eq. (38) gives an expression for A as a function of θ_p for an initially-screw dislocation:

$$A_s(\theta_p) = \frac{-L^2 \left\{ \frac{1}{2} \sin 2\theta_p [8\nu^2 \cos^4 \theta_p - (10\nu^2 - 16\nu) \cos^2 \theta_p + (\nu^2 - 24\nu + 8)] + \theta_p (\nu^2 + 8\nu - 8) \right\}}{8R^2 \sin^2 \theta_p (\nu \cos^2 \theta_p + 1)^2}. \quad (41)$$

For an initially-edge dislocation, Eq. (23), Eq. (24), and Eq. (40) can be substituted into Eq. (38) to yield

$$A_e(\theta_p) = \frac{-L^2 \left\{ \sin \theta_p [8\nu^2 \cos^5 \theta_p + \nu(6\nu - 16) \cos^3 \theta_p - (15\nu^2 - 8\nu - 8) \cos \theta_p] + \theta_p (\nu^2 + 8\nu - 8) \right\}}{8R^2 \sin^2 \theta_p [\nu^2 \cos^4 \theta_p + 2\nu(\nu - 1) \cos^2 \theta_p + \nu^2 - 2\nu + 1]}. \quad (42)$$

The dislocation strain ϵ^{dis} can then be expressed as⁵

$$\epsilon^{dis}(\theta_p) = \frac{b\Omega\Lambda^{dis}}{2L} A(\theta_p). \quad (43)$$

Knowing ϵ^{dis} allows β^{dis} to be expressed as

$$\beta^{dis}(\theta_p) = \frac{\partial^2 \epsilon^{dis}}{\partial \sigma^2} \left(\frac{\partial \epsilon}{\partial \sigma} \right)^{-2}, \quad (44)$$

where ϵ is the total strain. Because ϵ^{dis} is expressed as a function of θ , the derivatives in Eq. (44) must be evaluated as

$$\frac{\partial \epsilon}{\partial \sigma} = \frac{\partial \epsilon^{dis}}{\partial \sigma} + \frac{1}{A_{66}} = \frac{\partial \epsilon^{dis}}{\partial \theta_p} \left(\frac{\partial \sigma}{\partial \theta_p} \right)^{-1} + \frac{1}{A_{66}} \quad (45)$$

$$\frac{\partial^2 \epsilon^{dis}}{\partial \sigma^2} = \frac{\partial^2 \epsilon^{dis}}{\partial \theta_p^2} \left(\frac{\partial \sigma}{\partial \theta_p} \right)^{-2}. \quad (46)$$

Substituting the solutions of Eq. (45) and Eq. (46) into Eq. (44) solves for β^{dis} as a function of θ_p .

Thus, an implicit solution for β^{dis} as a function of applied stress σ can be formed by Eq. (39) or Eq. (40) and Eq. (44) in terms of the parameter θ_p for initially screw or edge dislocations, respectively.

6.2. Comparison with Simulations

As expected, the implicit solution exactly agrees with the orientation-dependent line energy DD simulations to within the error introduced by the discretization of the dislocation (not shown). However, special consideration is required to accurately compare the implicit solution with fully-elastic DD simulations. The tension factor M of the variable line energy must be scaled, because the exact value of $\ln(r_o/r_i)$ is unknown

⁵The solution to Eq. (43) and all subsequent steps of the derivation of this model are omitted to save space.

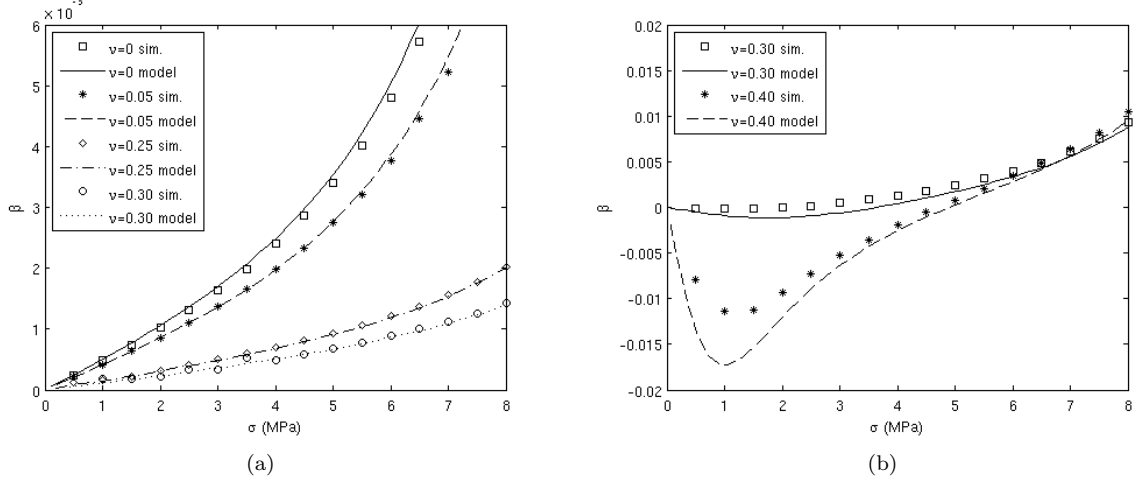


Figure 9: Comparison of elastic-interaction DD simulations with the implicit model

for an arbitrary dislocation shape. The elastic DD results can not be simply scaled to match the implicit model because the solution of Eq. (44) has a nontrivial dependence on M . Thus, Eq. (15) can be rewritten as

$$M = \frac{\mu b^2}{4\pi(1-\nu)} t \quad (47)$$

where t is scale factor that is found by fitting the activation stress of the line-tension model with that of the elastic interaction DD simulation for a single value of ν . This same value of t is then applied to the implicit model for any Poisson's ratio. The model closely agrees with the elastic DD simulations for any value of ν for initially screw dislocations, as shown in Fig. 9(a). For initially edge dislocations, the model also accurately predicts β^{dis} for $\nu < 0.25$ (not shown) and only slightly exaggerates the magnitude β^{dis} at small applied stresses for $\nu > 0.25$, as shown in Fig. 9(b). This deviation may be a result of the finite core radius or discretization of the DD simulations.

The implicit model offers a vast improvement over the Hikata et al. and the power-series model. It highlights the importance of the orientation dependence of line energy and the necessity of accurately calculating the area swept by a dislocation in calculating the ultrasonic nonlinearity parameter β . The elasticity DD simulations are sensitive to the orientation of the remote pinned segments, which cannot be captured by a line-tension model. However, initially-screw dislocations are only marginally affected. Although the implicit solution for β^{dis} is lengthy, the solution process is conceptually simple and can be easily evaluated using a computer program.

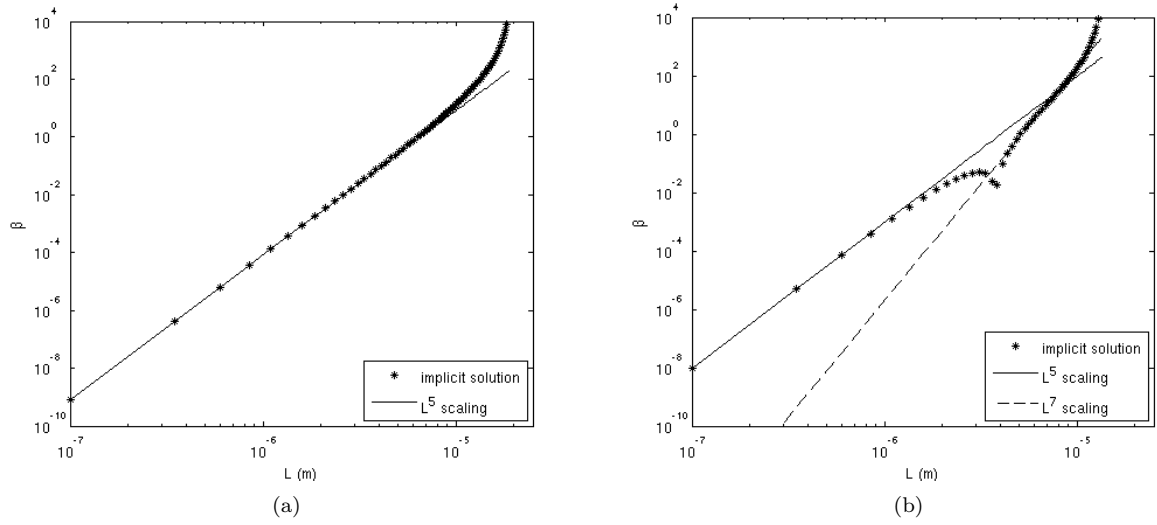


Figure 10: Dependence of β on distance between pinning points ($\nu = 0.30, \sigma = 1$ MPa)

7. Length dependence of β^{dis}

The proposed models can also be used to predict how β depends on the distance between the pinning points. The first-order and third-order terms of the power-series solution in terms of σ in Eq. (35) and Eq. (37) depend on L^4 and L^6 for a constant dislocation density, respectively. However, for DD simulations of a single dislocation in a periodic array with a fixed periodicity, the dislocation density Λ^{dis} is defined as $2L/V$, where V is the representative volume. This definition of Λ^{dis} will be used throughout this section. Thus, the first-order and third-order terms of the power-series solution depend on L^5 and L^7 in this case.

For stresses well below activation, β is predicted to depend on L^5 for screw and edge dislocations. This was verified using the implicit model for the case of ν 0.30 and an applied shear of 1 MPa. L^5 scaling is clearly exhibited by screw dislocations for lengths well below the critical value for Frank-Read source activation, as illustrated in Fig. 10(a). β tends to infinity at lengths approaching the activation length. Fig. 10(b) reveals this is also the case for edge dislocations, but the deviation from L^5 occurs at smaller lengths. The cusp in Fig. 10(b) is a result of β changing sign for edge dislocations; β is negative at lengths smaller than the cusp, but the absolute value is taken for the logarithmic plot. Thus, β scales with L^5 for lengths with negative β values. However, the scaling is L^7 for positive values of β at lengths below the activation length. It should be noted that this behavior is only observed for edge dislocations where β changes sign; For $\nu < 0.25$ the results for edge dislocations qualitatively resemble those of screw in Fig. 10(a).

8. Comparison with previous experiments

One of the main predictions of this work is that the dislocation contribution to acoustic nonlinearity, β^{dis} , can be negative. However, existing experiments only measure the amplitude of β , and provide no information on its sign. Assuming that the lattice contribution to acoustic nonlinearity, β^{lat} , is positive, a negative β^{dis} would lead to a decrease of the measured β with increasing stress. Unfortunately, there have been few experiments to measure how β depends on the applied stress, with the notable exception of the original papers by Hikata et al. [5, 6].

For an unannealed sample, Hikata et al. [6] show a linear increase of β until attenuation becomes significant. Notably different behaviors are observed in their annealed samples, some of which have undergone plastic deformation before the acoustic measurement. All of these samples show an initial decrease of β , which is inconsistent with the constant line-tension model. Hikata et al. tried to explain this discrepancy in terms of internal stresses caused by the plastic deformation. This argument would lead to the prediction that β will increase with applied stress after the magnitude of the applied stress exceeds the internal stress. However, this is inconsistent with the data for the annealed sample that had not undergone any plastic deformation, as well as samples subjected up to 200 g/mm² stressing. In these cases, β decreased over the entire range of applied stress. In contrast, these results can be naturally explained in terms of the negative dislocation contributions to β .

The drastically different behavior after annealing indicates a significant change of dislocation microstructures. It is known that annealing reduces dislocation density and promotes the formation of stable dislocation structures [15, 16]. An isolated dislocation monopole, considered by Hikata et al. and this work, is likely a better model for the microstructure after annealing. Hence, the observed decrease of β with stress in annealed FCC samples strongly supports the proposed orientation-dependent line energy model.

A dislocation monopole is only one of the proposed microstructures that contribute to acoustic nonlinearity. Another well-studied microstructure is a dislocation dipole [3, 7]. It is predicted that a dislocation dipole has a positive contribution to β at zero applied stress, while the monopole contribution is zero. Therefore, it is reasonable to expect that the magnitude of contribution from dislocation dipoles to the experimentally measured β should be significantly larger than that from dislocation monopoles in materials under no applied stress. Hence, the decrease of β by irradiation [17] can be explained by the reduction of dipole contribution to β , which is caused by the immobilization of dislocation dipoles.

Furthermore, care should be taken when comparing the predictions of monopole models with experimental measurements of fatigued samples [3, 18, 19, 20]. Many of these experiments are performed on single

crystals, whose microstructure is expected to be primarily composed of edge dislocation dipoles [1]. Therefore, dipole interactions should be the predominant dislocation mechanism that contributes to β , especially at zero applied stress.

9. Conclusions

The models developed in this paper using an orientation-dependent line energy offer a vast improvement over the current model using a constant line tension. The agreement of the analytic solution of this model with DD simulations using elastic interactions verifies its accuracy and establishes the utility of DD simulations for studying β . DD simulations will allow for studying dislocation structures beyond the scope of analytical models and capture β as the structures evolve.

Although the implicit solution is significantly more accurate in general, the power series solution has its own advantage. The simplicity of the power series solution allows one to easily predict when dislocations will have initially negative values of β , as shown in Fig. 7. Eq. (35) and Eq. (37) also reveal that β is expected to scale with L^5 for stresses well below the activation stress. This suggests that β could be possibly be used as a measure of the length distribution of dislocation segments between pinning points.

It is shown for the first time that a dislocation's contribution to β can be of opposite sign for a given stress state depending on the the character angle of the dislocation, the distance between pinning points, and the Poisson's ratio of the material. The negative values of β can be quite significant for pure-edge dislocations in materials with large Poisson's ratios. This is particularly important in FCC engineering metals, because edge dislocations are dominant in their fatigued microstructures. This allows for the cancellation of different contributions to β , such as that of the lattice or dislocation dipole motion.

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References

- [1] Suresh, S. *Fatigue of Materials* (1998). Cambridge University Press.

- [2] Chang, FK, ed. Structural Health Monitoring: Current Status and Perspectives (1997). CRC Press.
- [3] Cantrell, JH, Yost, WT. International Journal of Fatigue. 23, S487 (2001).
- [4] Frouin, J, Sathish, S, Na, JK. Proceedings of the SPIE. 3993, p60 (2000).
- [5] Hikata, A, Chick, BB, Elbaum, C. Applied Physics Letters. 3, 11 (1963).
- [6] Hikata, A, Chick, BB, Elbaum, C. Journal of Applied Physics. 36, 1 (1965).
- [7] Cantrell, JH. Proc. R. Soc. Lond. A. 460, p757 (2004).
- [8] Cantrell, JH. Journal of Applied Physics. 105, 043520 (2009).
- [9] Oruganti, RK, Sivaramanivas, R, Karthik, TN, Kommareddy V, Ramadurai, B, Ganesan, B, Nieters, EJ, Gigliotti, MF, Keller, ME, Shyamsunder, MT. International Journal of Fatigue. 29, p2032 (2007).
- [10] DeWit, G, Koehler, JS. Physical Review, 116, 5 (1959).
- [11] Arsenlis, A, Cai, W, Tang, M, Rhee, M, Oppelstrup, T, Hommes, G, Pierce, TG, Bulatov, VV. Modelling and Simulation in Materials Science and Engineering. 15, p553 (2007).
- [12] Dupuy, L, Fivel, MC. Acta Materialia. 50, p4873 (2002).
- [13] Cantrell, JH. Fundamentals and Applications of Nonlinear Ultrasonic Nondestructive Evaluation. In: Kundu, T, ed. Ultrasonic Nondestructive Evaluation (2004). CRC Press.
- [14] Foreman, AJE. Acta Metallurgica. 3, p322 (1955).
- [15] Hirsch, PB, Horne, RW, Whelan, MJ. Philosophical Magazine. 1, p677 (1956).
- [16] Keh, AS, Weissmann, S. Deformation Substructure in Body-Centered Cubic Metals. In: Thomas, G, Washburn, J, editors. Electron Microscopy and Strength of Crystals (1962). John Wiley & Sons.
- [17] Breazeale, MA, Ford, J. Journal of Applied Physics. 36, p3486 (1965).
- [18] Frouin, J, Sathish, S, Matikas, TE, Na, JK. J. Mater. Res. 14, p1295 (1999).
- [19] Kim, JY, Jacobs, LJ, Qu, J, Littles, JW. J. Acoust. Soc. Am. 120, p1266 (2006).
- [20] Cantrell, JH. Journal of Applied Physics. 100, 063508 (2006).