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14. ABSTRACT
We have established Dislocation Dynamics (DD) simulations as a practical method to compute the acoustic nonlinearlity parameter, beta, which forms the bases of the emerging metal fatigue detection technique of nonlinear ultrasonics. Our study have uncovered mistakes in two well-known theoretical models in this field and leads to a deeper understanding of the dislocation mechanism to acoustic nonlinearity. For a single dislocation bowing in its glide plane between two pinning points (i.e. the monopole model), our simulations and analytic derivations show a strong dependence of beta on the dislocation orientation, which is missed by the previous model (Hikata et al. 1965). For parallel dislocations forming a multipole configuration (as a model for the vein structure in fatigued metal), our simulations show a pronounced dependence of beta on the applied stress (with beta=0 at zero stress), which contradicts the previous model that predicts a constant beta independent of stress (Cantrell et al. 2001). Our analytic derivations have pinpointed the mistake in the previous model.

15. SUBJECT TERMS
metal fatigue, non-destructive evaluation, dislocation, ultrasound

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Annual Report:
Physical Mechanisms underlying Ultrasonic Non-Destructive Evaluation of Fatigue

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1. Single Dislocation Line Interaction with Ultrasound

We have studied the process of dislocation interaction with an oscillating stress field in great detail, both using Dislocation Dynamics (DD) simulations and analytic modcls. A classical problem is illustrated in Fig. 1, whcre the bowing out of the dislocation line (pinned at both ends) produces a strain that is non-linear with the applied stress. This gives rise to acoustic non-linearity β, which can be measured experimentally from the amplitude of second harmonics.

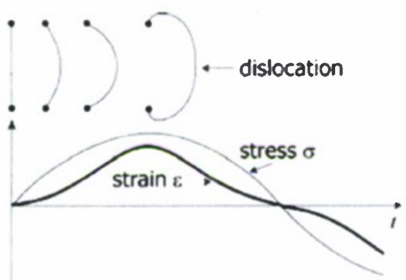
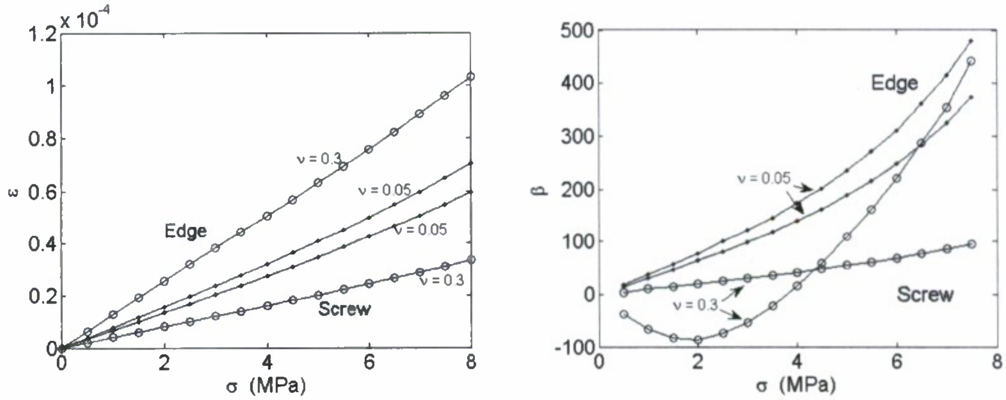


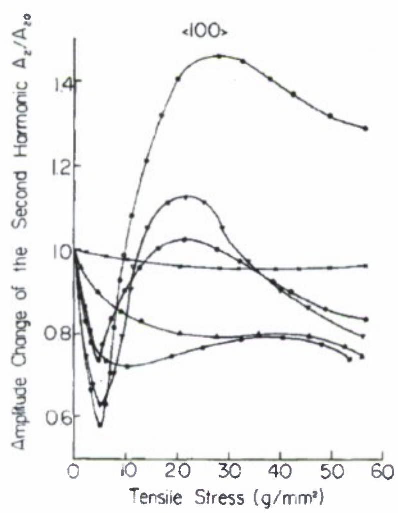
Figure 1. Schematics of a dislocation segment with ends pinned by obstacles vibrating under the stress field of an ultrasound.

Previous studies have assumed a simple model for dislocations --- the dislocation is reprcsented as a string with a constant line tension (Hikata et al. J. Appl. Phys. 36, 229, 1965). The model predicts linear dependence of beta on thc applied stress σ (for small σ) in thc casc of a singlc dislocation pinncd at two end points. Our explicit Dislocation Dynamics simulations showed that the acoustic non-linearity parameter beta depends critically on the orientation of the dislocation and material's Poisson ratio (see Fig. 2). The cdge and screw orientation bccomes equivalent only in the limit of Poisson's ratio going to 0. But for most materials, Poisson's ration is around 0.3, in which casc the behavior of edge dislocations is very different from that predictcd by the simple line tension model. At thc same time, thc microstructure of fatigued metals is dominated by edge dislocations. This means the previous understandings of dislocation microstructurc – ultrasound interaction needs to be drastically altcred.

We found that the deviation from the cxplicit DD simulations and constant linc-tcnsion model is mainly duc to thc dependence of dislocation line tension on line orientation. By allowing thc line tcnsion to depend on linc orientation, we havc obtained analytic expressions for the acoustic non-lincarity that agrees well with our DD simulations. These results are described in a manuscript currently under review in Acta Matcrialia [7]. This work corrects an important error in previous predictions of acoustic non-linearity β and this the first time β is calculated explicitly from DD simulations. For the first time, we show dislocation contribution to β can be negative. It means sometimes dislocation mechanisms can reduce the measured value of β. This naturally explains the decrease of β in some of the experimental data reported in the original paper of Hikata et al. (1965), see Fig.2(c), which was difficult to explain with the previous model that ignored orientation effects.



(a) (b)

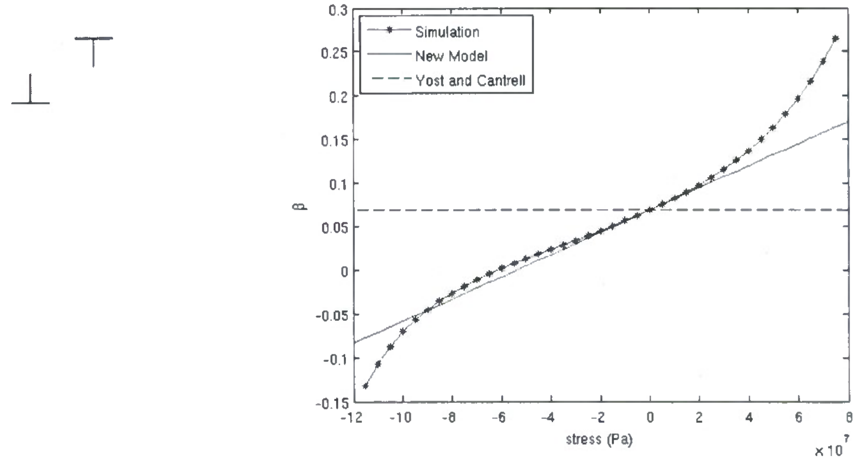


(c)

Figure 2. (a) Predicted stress-strain relationship for edge and screw dislocations in an elastic medium with different Poisson's ratio ν when orientation effects are included. (b) Predicted acoustic non-linearity parameter β based on the stress-strain relationship in (a). Notice β becomes negative in some stress regime for edge dislocations in materials with ν = 0.3. (c) Experimental data for β as a function of applied stress in the original paper by Hikata et al. (1965) for aluminum samples pre-deformed to different amount of strains. Notice the initial decrease of β.

2. Dislocation Dipole and Multipole Interaction with Ultrasound

(a)



(b)

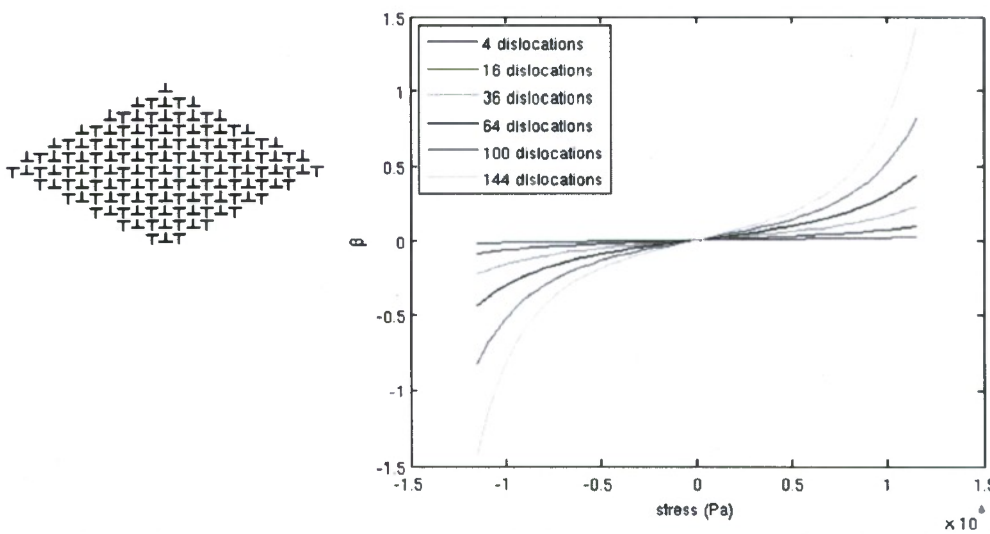


Figure 4. (a) Acoustic nonlinearity β of a dislocation dipole (left) as a function of applied stress predicted by DD simulations (stars) and our analytic solution (solid line). The prediction from the previous model (Cantrell 2001) is plotted as dashed line. (b) Acoustic nonlinearity β as a function of applied stress of a group of dislocations forming a Taylor lattice (left) by DD simulations.

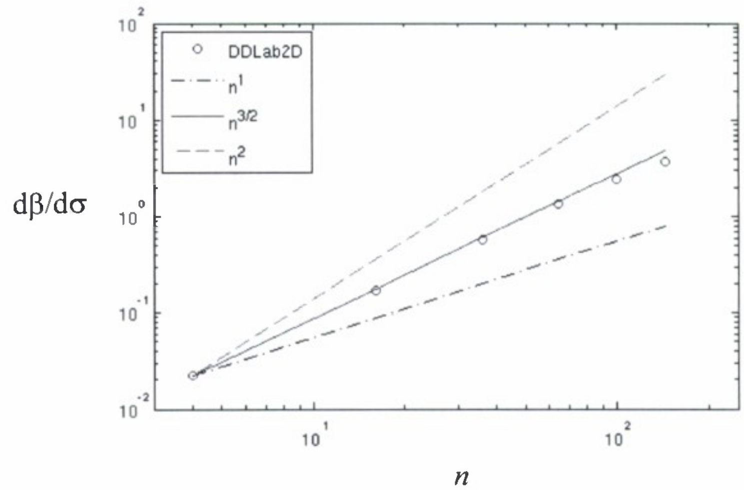


Figure 5. Slope of the curves in Fig.4 (i.e. dβ/dσ) at σ=0 as a function of the size *n* of Taylor lattice (circles). *n* is the number of dislocations in the Taylor lattice. The straight lines are drawn to indicate that dβ/dσ scales as $n^{3/2}$.

In the case of two parallel dislocations forming a dipole, an earlier model (Cantrell et al. Int. J. Fat. 23, S487, 2001) predicts that β is a (positive) constant that is independent of stress σ (see Fig.4(a), dashed line). This prediction has been used extensively in subsequent publications to estimate the value of β for configurations containing multiple dislocations. However, our DD simulations show that β has a pronounced dependence on stress. Furthermore, we have performed analytic derivations to pinpoint the mistake in the previous solution --- the series expansion has not been carried out to sufficient order.

For parallel dislocations forming a multipole configuration such as a Taylor lattice (which is a model for the vein structure in fatigued metal), the earlier model would estimate the value of β by multiplying the value of the zero-stress value of β for a dipole by the number of equivalent dislocation dipoles in the Taylor lattice. This would again predict a β value that is independent of the applied stress. However, our DD simulations show that the β value at zero stress is actually zero, and that β has a strong stress-dependence (Fig.4(b)). Our analytic derivations show that β=0 at σ=0 is a consequence of the mirror symmetry of the Taylor lattice, which is lacking in the dipole configuration. Furthermore, the slope of the β(σ) curve at σ=0 scales as $n^{3/2}$, where *n* is the number of dislocations in the Taylor lattice. This means that one cannot assume the dislocation multipole structure is a simple sum of dipoles, each making an identical contribution to β.

The finding from this analysis completely changes our understanding of the dislocation mechanism to acoustic nonlinearity in fatigued metals. We expect them to have profound impact on the development of the ultrasonic non-destructive evaluation method for metal fatigue based on the acoustic nonlinearity effect.

3. Dislocations in Anisotropic Elastic Media

Most of the engineering metals are elastically anisotropic. For simplicity, most of the dislocation dynamics simulation programs, including ParaDiS (used in this project), assume isotropic elasticity. We have designed and implemented efficient algorithms to enable dislocation dynamics simulations under anisotropic elasticity. The algorithms have been implemented and extensively tested in a Matlab code (DDLab) and has recently been implemented in ParaDiS [6]. The resulting algorithm is significantly faster than previous attempts (e.g. Rhee et al. Mater. Sci. Eng. A 309-310, 288, 2001).

4. Collaboration with AFRL scientists:

I am in contact with Satish Rao, Mike Uchic, Dennis Dimiduk, Chris Woodward in Wright-Patterson AFB, helping them with the ParaDiS program. I have visited these scientists in WPAFB in Feb. 2009 to discuss research collaborations on dislocation dynamics. I have also discussed with Satish Rao and Mike Uchic during the annual grantee's meeting in July 2009 in Fairborn, OH.

5. Publications from This Project (2008-present):

1. C. R. Weinberger and W. Cai, Surface Controlled Dislocation Multiplication in Metal Micropillars, Proceedings of the National Academy of Sciences, 105, 14304 (2008).
2. W. Cai and C. R. Weinberger, Energy of a Prismatic Dislocation Loop in an Elastic Cylinder, *Mathematics and Mechanics of Solids*, 14, 192 (2009).
3. C. R. Weinberger, S. Aubry, S.-W. Lee, W. D. Nix and W. Cai, Modelling Dislocations in Free-Standing Thin Films, *Modelling and Simulation in Materials Science and Engineering*, 15, 075007 (2009).
4. C. R. Weinberger, S. Aubry, S.-W. Lee and W. Cai, Dislocation Dynamics Simulations in a Cylinder, *IOP Conference Series: Materials Science and Engineering*, 3, 012007 (2009).
5. C. R. Weinberger and W. Cai, "Orientation dependent plasticity in metal nanowires under torsion: twist boundary formation and Eshelby twist", *Nano Letters*, 10, 130142 (2010).
6. J. Yin, D. M. Barnett and W. Cai, Efficient Computation of Forces on Dislocation Segments in Anisotropic Elasticity, *Modelling and Simulation in Materials Science and Engineering*, in press (2010).
7. W. Cash and W. Cai, Dislocation contribution to acoustic nonlinearity: The effect of orientation-dependent line energy, submitted to Acta Materialia, (2010).
8. W. Cash and W. Cai, Dislocation dipole contribution to acoustic nonlinearity, in preparation for Acta Materialia.