Multi-dimensional effects on the propagation of strain solitons in solids

T Kawasaki¹, S Tamura¹ and H J Maris²

¹ Department of Applied Physics, Hokkaido University, Sapporo 060-8628, Japan
² Department of Physics, Brown University, Providence, RI 02912, USA

E-mail: s-tamura@eng.hokudai.ac.jp

Abstract. Numerical simulations on the generation and the propagation of phonon solitons in crystalline solids have so far been made extensively with KdV equation in one dimension. We extend these analyses to two and three dimensions by treating the effect of the transverse directions as a small perturbation. Explicitly, we first derive the two-dimensional KP equation and also its three-dimensional version for the strain field. Then, time evolutions of the initial strain distributed with a Gaussian profile normal to the main propagation direction are studied.

1. Introduction

Recent experiments with picosecond ultrasonics have shown that the acoustic strain in crystalline solids (e.g., silicon and MgO) induced by ultrashort time-scale pulses of a high power level evolves into solitons [1, 2] and their characteristics are well explained by simulations with the Korteweg-de Vries (KdV) equation in one dimension (1D). [3] Similar experiments on the formation and propagation of strain solitons in sapphire and ruby have also been made by another group, [4] with a different experimental technique. [5]

For finite amplitude acoustic waves of wavelength much longer than the lattice spacing the motion of the lattice displacement or elastic strain is governed by non-linear elasticity theory including the lowest order dispersive effect. This continuum model for the longitudinal strain leads to the KdV equation with soliton solutions if the motion of the strain is restricted to 1D. Thus the theoretical analysis on the strain solitons has so far been made with the KdV equation that neglects the variation of the initial strain amplitude with the lateral direction in the area excited by the pump pulse. However, if we suppose that the pump beam has a Gaussian profile with a radius \( r_0 \), the initial strain amplitude at a distance \( r_0 \), for instance, from the center will be appreciably smaller than that at the center. [2] This variation means that the soliton generated at the center will travel faster than a soliton generated away from the center and as a result the experimentally measured solitons should be somewhat broader than are calculated in the 1D simulations. These effects may be observed if the probe beam is not centered on the pump beam but shifted laterally. In order to analyze these points we derive a relevant nonlinear dispersive equation beyond 1D and make numerical simulations for the evolution of elastic strain.

2. Formulation

The equation of motion for the lattice displacement \( u(r,t) \) allowing for anharmonicity up to third order in the elastic strain is
\[
\rho \ddot{u}_i = \left( c_{ijkl} + d_{ijklmn} \frac{\partial u_m}{\partial x_n} \right) \frac{\partial^2 u_k}{\partial x_j \partial x_l},
\]

where \( \rho \) is the mass density and \( d_{ijklmn} = c_{ijklmn} + c_{ijkm} \delta_{ln} + c_{iklm} \delta_{jn} + c_{ikmn} \delta_{jl} \), with \( c_{ijkl} \) and \( c_{ijklmn} \) the second- and third-order elastic stiffness tensors. We apply Eq. (1) to the case where longitudinal waves are excited predominantly and launched in the [100] axis of a cubic crystal \((x = x_1)\). Thus, \( u_1 \) should be much larger than the transverse components \( u_2 \) and \( u_3 \). We assume that the transverse dimension in the sample where the strain pulse is probed by light is of the same order of magnitude as the spot size \( r_0 \) of the pump pulse. Assuming further that the sample thickness (several \( \text{nm} \)) is much larger than \( r_0 \) (about 10 \( \text{\mu m} \), for instance), we neglect the effects of the lattice nonlinearity and dispersion normal to the \( x \) direction. Under these conditions, Eq. (1) becomes

\[
\rho \ddot{u}_1 = C_{111} \frac{\partial^2 u_1}{\partial x_1^2} + C_{44} (\partial_2^2 + \partial_3^2) u_1 + (C_{12} + C_{44}) \partial_1 (\partial_2 u_2 + \partial_3 u_3) + (C_{111} + 3C_{11}) (\partial_1^2 u_1^2 + 2(\rho C_{11})^{1/2} \gamma \partial_1^2 u_1),
\]

\[
\rho \ddot{u}_2 = C_{111} \frac{\partial^2 u_2}{\partial x_2^2} + C_{44} (\partial_1^2 + \partial_3^2) u_2 + (C_{12} + C_{44}) \partial_2 (\partial_1 u_1 + \partial_3 u_3),
\]

\[
\rho \ddot{u}_3 = C_{111} \frac{\partial^2 u_3}{\partial x_3^2} + C_{44} (\partial_1^2 + \partial_2^2) u_3 + (C_{12} + C_{44}) \partial_3 (\partial_1 u_1 + \partial_2 u_2),
\]

where we have added a dispersive term for the motion of \( u_1 \), which leads to the dispersion relation \( \omega = \nu_L k - \gamma k^3 \) in the harmonic approximation with \( \nu_L = (C_{11}/\rho)^{1/2} \) the longitudinal sound velocity. [Isotropic approximation will be also assumed.]

In order to derive a soliton equation, we may use the reductive perturbation method [6] by taking account of the relations that the quantities \( \varepsilon^{1/2}(x - \nu_L t)/a, \varepsilon^{3/2} \nu_L t/a, \varepsilon y/a, \varepsilon z/a, \varepsilon^{-1/2} u_1/a, \varepsilon^{-1} u_2/a, \varepsilon^{-1} u_3/a \) are all \( O(1) \), where \( \varepsilon \) is a small parameter and \( a \) is a normalization length. The exponents of \( \varepsilon \) have been chosen from the consideration of the balance between the nonlinearity and dispersion. Thus, for the longitudinal strain \( \varepsilon = \partial u_1 / \partial x = O(\varepsilon) \) and with \( x' \equiv x - \nu_L t \) (the longitudinal coordinate in the reference frame moving with \( \nu_L \)), we have

\[
\frac{\partial}{\partial x'} \left[ \frac{\partial \eta}{\partial t} - \beta \eta \frac{\partial \eta}{\partial x'} + \gamma \frac{\partial^3 \eta}{\partial x'^3} \right] + \frac{\nu_L}{2} \left( \frac{\partial^2 \eta}{\partial y^2} + \frac{\partial^2 \eta}{\partial z^2} \right) = 0,
\]

where \( \beta = |C_3|/2\rho \nu_L \) with \( C_3 \equiv C_{111} + 3C_{11} < 0 \). The transverse components \( u_2 \) and \( u_3 \) are related to \( u_1 \) as \( \partial u_2 / \partial x' = \partial u_2 / \partial y \) and \( \partial u_3 / \partial x' = \partial u_3 / \partial z \). If the last term \( \partial^3 \eta / \partial x'^3 \) is neglected in Eq. (5), the KP equation [7] in 2D is obtained and ignoring further the last two terms, we have the KdV equation in 1D, i.e.,

\[
\frac{\partial \eta}{\partial t} - \beta \eta \frac{\partial \eta}{\partial x} + \gamma \frac{\partial^3 \eta}{\partial x'^3} = 0,
\]

Changing the variables from \((t, x, y, u_1)\) to dimensionless ones \((\tau, X, Y, W)\), [8] and introducing the strain \( \Psi \) with \( \Psi = \partial W / \partial X \), we have a standard form of the KP equation in 2D

\[
\frac{\partial}{\partial X} \left[ \frac{\partial \Psi}{\partial \tau} - 6 \Psi \frac{\partial \Psi}{\partial X} + \frac{\partial^3 \Psi}{\partial X^3} \right] + \frac{\partial^2 \Psi}{\partial Y^2} = 0.
\]

This equation has a one-soliton soliton (sometimes called a plane soliton) [9] of the form

\[
\Psi = \frac{\partial W}{\partial X} = -2K_\tau^2 \text{sech}^2 (K_x X + K_y Y - \Omega \tau),
\]

where the dispersion relation (valid for \( K_y \ll K_x \)) is \( K_x \Omega = 4K_x^4 + K_y^2 \). Putting \( K_y = 0 \), Eq. (8) reduces to the one-soliton solution of the KdV equation. [10]
3. Simulations

The numerical simulation has been done with the standard form of the KP equation Eq. (8) and the corresponding 1D (KdV equation) and 3D (axially symmetric 3D KdV equation) versions.\[11\] The sizes of the system assumed is $4\pi$ for the X direction and $2\pi$ for the lateral direction.\[12, 13\] Periodic boundary conditions have been imposed for both directions. In order to check the validity of our computer codes we first made the simulation for the propagation of the plane soliton [Eq. (8)] with the KP equation and made sure of the stability over 80,000 time steps.

![Figure 1](color online) 2D maps of strain distributions, (a) at $\tau = 0$ and (b) at $\tau = 80,000\Delta \tau = 0.08$. Dotted line shows $X = 10 - 2Y^2$.

![Figure 2](color online) Strains at $\tau = 0.08$ evolved from the one in (a) at $\tau = 0$, by the (b) 1D KdV, (c) 2D KP, and (d) 3D KdV equations.

Figure 1 shows the 2D profile of the strain at $\tau = 0.08$ evolved from the initial strain $\Psi_0 = -2K^2 \text{sech}^2(K_x X) \exp(-X^2/2)$ with $K_x = 6$, that is, the one-soliton solution of the KdV equation but its amplitude modified by the Gaussian in the transverse direction. We see that the localized strain (soliton) is developed in the $X-Y$ plane parabolically $X = -\alpha Y^2 + X_0$ [$\alpha=2$ for the dotted line in Fig. 1(b)] but the coefficient $\alpha$ becomes smaller as time increases. Next we assume the initial strain that has a square shape in the $X$ direction and a Gaussian in the $Y$ direction [Fig. 2(a)]. Explicitly, $\Psi_0 = -A \exp(-Y^2)\{\exp[-6(X^2-1)]+1\}^{-1}$ and $Y$ should be replaced by $R$ for the simulation with the 3D KdV equation. This shape corresponds to the compressive strain excited in the experiment by Singhsomroje and Maris.\[2\] The magnitude $A = 40$ chosen corresponds to the strain produced by the highest pump power of their experiment. Figures 2(b) to 2(d) compare the 2D profiles of the strain at $\tau = 80,000\Delta \tau$ evolved by the KdV, KP and 3D KdV equations. We see that four localized strain pulses travel in the positive $X$ direction.\[2\] The profiles of the strain pulses in the $X-Y$ plane developed by the KP and 3D KdV equations are again parabolas and they are clearly more expanded transversely than in the case of the KdV equation.

We see that the strains evolved by both the KP and 3D KdV equations are well fitted by the KdV solitons along the $X$ axis as shown in the insets of Figs. 3. In these figures we find the existence of oscillations with small amplitude (ripples) in the subsonic region $X < 0$. (The
oscillations in front of the solitons are the ripples that have appeared by the periodic boundary conditions assumed. Comparing these results we recognize that the solitons in 2D and 3D are spread more slowly in the lateral directions than in 1D. At the same time soliton amplitudes are decreased slightly as they propagate and their velocities along the X direction also decrease gradually. For the KP equation the existence of a similarity variable \( Z = \tau^{-1/3}(X + Y^2/4T) \) suggests the parabolic shapes of the strain distribution in the \( X - Y \) plane at a large \( \tau \) [14].

![Figure 3.](color online) The strain \( \Psi \) versus \( X \), (a) along \( Y = 0 \) of Fig. 2(c) by the KP equation, (b) along \( R = 0 \) of Fig. 2(d) by the 3D KdV equation. Insets compare the strain profile of the largest soliton with the KdV one-soliton (circles) for \( K_x \) given in each inset.

4. Discussions
By neglecting both the nonlinearities and dispersive effects in the directions normal to the principal propagation direction, we found that the motion of longitudinal strain in a solid is subject to a 3D version of the KdV equation which reduces to the KP equation if the motion is restricted to 2D. The effects obtained by the simulations should be observed experimentally, for instance, by scanning laterally the probe pulse to see the strain in the picosecond ultrasound experiments. If we assume the parameters of MgO, both the time scale and the size of the longitudinal direction that we could simulate were about 1/10 of the experiment described in ref. 2. So, we still have to extend the simulations for much larger systems and longer time scales.

Acknowledgments
This work was supported in part by the KAKENHI of Japan (Grant No.17510106).

References
This work was supported in part by the KAKENHI of Japan (Grant No.17510106).

[1] Hao H-Y and Maris H J 2001 Phys. Rev. B64 64302
[2] Singhsonroje W and Maris H J 2004 Phys. Rev. B69 174303
[3] Korteweg D J and De Vries G 1895 Phil. Mag. 39, 422
[4] Muskens O L and Dijkhuis J J 2002 Phys. Rev. Lett. 89 285504
[5] Akimov A 2007 The paper in this Proceedings.
[6] Taniguchi T and Wei C C 1968 J. Phys. Soc. Jpn. 24 941.
[7] Kadomtsev B B and Petiau V L 1970 Sov. Phys. Dokl. 15 539
[8] t = \( \alpha \tau v_L \), \( x' = \alpha X \), \( y = \alpha (\delta Y/2)/\gamma \) and \( \eta = (6v_L/\beta)\alpha\Gamma \Psi \), where \( \Gamma = (\gamma/v_L a^2)^{1/3} \).
[9] Zakharov V E and Shabat A B 1974 Punct. Anal. Appl. 8 226
[10] The KdV soliton is narrower and travels faster when its amplitude is larger.
[11] The axially symmetric 3D KdV equation is obtained from the KP equation by the replacement \( \partial^2 \Psi/\partial Y^2 \rightarrow \partial^2 \Psi/\partial R^2 + (2/R)\partial \Psi/\partial R \).
[12] The magnitudes of unit grids are chosen as \( \delta X = \delta Y = \delta R = 2\pi/2^7 \) and \( \delta \tau = 10^{-6} \), and the number of grid points are \( N_X = 2^9 \) in the \( X \) direction and \( N_Y = N_R = 2^7 \) in the lateral direction.
[13] Correspondences to the original values are \( X = 4\pi \rightarrow x' = 0.213 \mu m \), \( Y = \pi \rightarrow y = 17.8 \mu m \), \( \tau = 0.08 \rightarrow t = 24.3 \) ns, \( \Psi = -40 \rightarrow \eta = -2.16 \times 10^{-4} \).
[14] Redekopp L G 1980 Stud. Appl. Math. 63 185