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ABOUT FOCUSING IN NANOELASTODYNAMICS

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The paper is concerned with the focusing of ultrasonic waves in nanostructured media at the femtosecond temporal and nanometer spatial scale. Focusing and self-focusing are properties of waves experimentally observed, and their balance depends on the nanoscale properties of the medium. These properties are investigated by using the couple stresses theory and the double couple radiation pattern.

Key words: focusing, self-focusing, nanostructured materials, ultrasonic waves.

1. INTRODUCTION

Classical elasto-dynamics is based on the idea that material bodies posses continuous mass densities and laws of motion and axioms of constitution are valid for every part of the body no matter how small they may be. The classical continuum theory is believed to be inadequate for the treatment of propagation of waves in materials with nanostructure the characteristic length scale of which is in the order of a few nanometers. They include the nanocrystalline materials such as ceramic, carbon nanotubes, nanofibers and wires, etc. These materials, be metal, ceramic or polymers, are nanometer size particles, and can be engineered by controlling the sizes of the building blocks in the 1-100nm size range and their assembly. The microstructure refers to the arrangement of the atoms and the size of a solid in 1D, 2D and 3D. Effects controlling the properties of nanostructured materials include size effects, where critical length scales of physical phenomena become comparable with the characteristic size of the building blocks of the microstructure (Drexler [1–4]).

In the last decades a class of materials with a nanometer-sized microstructure have been synthesized and studied. These materials are nanocomposites that improve the macroscopic properties of products. Typically, nanocomposites are clay, polymer or carbon, or a combination of these materials with nanoparticle building blocks (Drexler, Peterson, and Pergamit [5]). By integrating nanotubes into traditional materials (epoxy matrices) it is possible to improve their strength and damping properties. Nanocomposites have a reduced weight and volume, in comparison to polymeric damping materials, and have a high damping capabilities. Since their discovery in 1991, the carbon nanotubes offer an interesting combination of light and stiff, of high strength and damping. Since the carbon nanotubes are so thin, they possess a big amount of surface area for the volume they occupy ($10^3 m^2/gm$), giving them a great capacity to dissipate energy (Ko *et al*.[6]). Carbon nanotubes are up to 100 times stronger than steel at only a sixth the weight, and have attracted much research as potential to improve the strength of composite materials. The effect of structure in nanocomposites becomes important in transmitting waves of small wavelength and high frequency. When the wavelength is comparable with the average grain size, the motion of the grains must be taken into account (Chiroiu *et al*. [7]). Models of media with couple stresses (Eringen [8], Eringen and Jafadar [9], Erofeev and Potapov [10], Potapov [11], Bagdoev and Shekoyan [12], Parfitt and Eringen [13]) and the double couple radiation pattern (Chiroiu and Nicolae [14], Chiroiu, Nicolae and Munteanu [15] can be used to describe this category of materials with extra independent internal degrees of freedom for the local

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rotations. The radiation force acts upon the body likewise a friction force. The rate of work of this force is equals to the radiation of energy that leaves acoustically the body per unit time.

The constituents like grains and molecules are allowed to rotate independently without stretch. The behavior of waves in such media exhibits new features as dispersion, concentration and focusing (Chiroiu and Munteanu [16], Munteanu [17]).

The waves interact with matter inducing a wide range of nonlinear effects, experimentally observed such as generation of high energy local fields by focusing and self-focusing phenomena (Stockman [18]).

The paper is concerned with the focusing of ultrasonic waves in nanostructured media at the femtosecond (10^{-15}s) temporal and nanometer spatial scale (10^{-9}m). The media considered are dissipative. The focusing phenomenon consists in a nano narrow beam of nonlinear ultrasonic wave, which can focus. The self-focusing consists in a generation of new waves, which is appearing at some distances, due to interaction between stable and unstable waves. Self-focusing could be observed in nano-piezo-semiconductors (Stockman [18]). These properties are investigated in this work by using the couple stresses theory and the double couple radiation pattern.

2. GENERAL THEORY

Since size is important in nanoelastodynamics, the ratio of surface area to volume is large for small systems, that means $(V^{2/3}/V)=1/V^{1/3}$ becomes smaller and smaller as V grows. The surface effects dominate in the nanostructures in contrast to the macroscopic state. In cristalography for example, the transition to the nanoscale appears for $V/V_c<10^6$, where V is the volume of crystallites in the solid and V_c is the unit cell volume. This volume ratio can be converted in to a ratio for the number of particles by substituting the number of atoms per unit cell. In Bravais lattices, this number rarely exceeds four. It leads to the ratio of $N/N_c<10^4$, which seems to be obeyed by Bose-Einstein condensates that occur only when $N\geq 10^4$. The transition to bulk behavior can be taken for $N/N_c>10^5$ (Ghanashyam Krishna and Srinivasan [19]).

To model the behavior of a nanocrystalline medium, we start with considering that the micromedium is composed from microvolumes V_m enclosed within its surface in the medium, and each microvolume contains discrete nanovolumes V_n, with $V_m/V_n<10^6$. The nanovolumes are similar to what is observed experimentally, i.e. 8–64 grains in a $10.6\,\text{nm}^3$ of material, with a grain modeled as a sphere with diameter of 3.3–6.6 nm. Consider that the medium has the initial volume V_0 and surface S_0 in its undeformed and unstressed state, and the properties of V_m are averaged discrete microvolumes properties. If the physical phenomenon under study has a certain characteristic length such as wavelength, comparable with the size of V_n in the body, then the nanostructure of the material must be taken into consideration. The state of deformation of such a body in the rectangular frame of reference x_k, $k=1,2,3$ is described by two tensors

$$e_{kl}=\frac{1}{2}(u_{k,l}+u_{l,k}+u_{i,k}u_{i,l}), \tag{2.1}$$

$$\Gamma_{klm}=-u_{l,km}, \quad i,k,l,m=1,2,3, \tag{2.2}$$

where e_{kl} are components of the Green's strain tensor which characterizes relative displacements of centers of mass of microvolumes V_m, Γ_{klm} components of the nanodeformation gradient which characterizes relative displacements of nanovolumes of the same microvolume, and $u_k(x_k,t')$ components of the displacement vector, in Lagrangian variables. A subscript after a comma means differentiation with respect to the indicated coordinate.

To derive basic equations of nanoelastodynamics we define the action functional

$$I = \int_{t_1'}^{t_2'} \mathrm{d}t \int_{V_0} \mathrm{L}\,\mathrm{d}V_0 \,, \tag{2.3}$$

where the Lagrangian L of the medium is given by

$$\mathrm{L} = K - \rho_0 U \,, \tag{2.4}$$

with the kinetic energy K and the potential energy $\rho_0 U$ expressed as

$$K = \frac{1}{2}\rho_0 \dot{u}_i^2 \,, \tag{2.5}$$

$$\rho_0 U = \frac{\lambda}{2} e_{kk}^2 + \mu e_{ik}^2 + 2\mu M^2 (\Gamma_{klm}^2 + \nu \Gamma_{kim}\Gamma_{ikm}) + \frac{A}{3} e_{ik}e_{il}e_{kl} + B e_{ik}^2 e_{ll} + \frac{C}{3} e_{kk}^3 \,, \tag{2.6a}$$

with $i,k,l,m = 1,2,3$, and ρ_0 the density of the body in the initial state. Here λ, μ are Lame second-order elastic constants, A, B, C third-order Landau constants, and M, ν nanostructure constants (characterize the rotation and the gradient of rotation of internal degree of freedom), which can be positive or negative. Determination of elastic constants can be performed directly, from their definition as second and third order derivatives of the total energy per unit cell or nanovolume with respect to strain. The calculations are based on the Berruti and Delsanto approach (Berruti, Delsanto *et al* .[20]). The pseudopotential energy consists in writing the total crystal energy as a sum of several contributions (Delsanto, Provenzano and Uberal [21])

$$E = \rho_0 U = E_{es} + E_{fe} + E_{be} + E_r \,, \tag{2.6b}$$

where E_{es} represents the electrostatic Coulomb energy of positive point charges in the uniform negative charge background (the Madelung energy), E_{fe} is the free electron energy, which depends on the crystal volume, E_{be} is the band structure energy and E_r the ion-core (Born-Mayer) repulsive energy. From calculations, it was conclude that E_r (expressed as $E_r = 0.5\alpha \sum_n \exp(-\beta R^{(n)})$, where α is the repulsive energy parameter and β is the repulsive range parameter) is the predominant term for calculations of the material constants (Jankowski and Tsakalakos [22]. The sum is extended to all the nearest neighbors, which are located ar distances $R^{(n)}$.

We assume that nanostrain effects are weak and only squared terms in Γ_{klm} are included in (2.6). The balance of momentum, the balance of moment of momentum and the conservation of energy are obtained from extremum conditions of the functional (2.3). The equation of motion including the mechanical radiation has the form

$$\rho_0(\ddot{u}_i + \tau \dddot{u}_i) = \frac{\partial}{\partial x_k}\left[\frac{\partial \rho_0 U}{\partial u_{i,k}} - \frac{\partial}{\partial x_m}\left(\frac{\partial \rho_0 U}{\partial u_{i,km}}\right)\right], \tag{2.7}$$

where τ is the radiation time $0 \le \tau \le 1$. The state of stresses of the medium is given by

$$\sigma_{kl} = \frac{\partial \rho_0 U}{\partial u_{l,k}}, \quad \sigma_{kl} = \frac{\partial \rho_0 U}{\partial \Gamma_{klm}} \quad , \quad k,l,m = 1,2,3 \,, \tag{2.8}$$

where σ_{kl} is the microstress tensor and σ_{klm} the nanostress tensor. The antisymmetric part of σ_{klm} is the tensor of couple stresses. The energy transport equation is

$$\dot{W} + \operatorname{div} S = 0 \,, \; W = \frac{1}{2}\rho_0 \dot{u}_i^2 - \rho_0 U \,, \tag{2.9}$$

where W is the internal energy density, and

$$S_j = \frac{\partial \rho_0 U}{\partial u_{i,j}} \dot{u}_i - \frac{\partial \rho_0 U}{\partial u_{i,kj}} \dot{u}_{i,k} + \frac{\partial}{\partial x_k}\left[\frac{\partial \rho_0 U}{\partial u_{i,kj}}\right]\dot{u}_i , \tag{2.10}$$

are components of the energy flux density or Poynting vector. The momentum transport equation is given by

$$\dot{G} + \operatorname{div} T = 0 \ , \quad G_m = -\dot{u}_i u_{i,m} , \tag{2.11}$$

where G_m are components of the wave momentum vector, and

$$T_{mj} = \delta_{mj}\left(\frac{1}{2}\dot{u}_i^2 - \rho_0 U\right) + \frac{\partial \rho_0 U}{\partial u_{i,j}} u_{i,m} + \frac{\partial \rho_0 U}{\partial u_{i,lj}} u_{i,lm} - \frac{\partial}{\partial x_k}\left[\frac{\partial \rho_0 U}{\partial u_{i,lj}}\right] u_{i,m} , \tag{2.12}$$

are components of the momentum flux density tensor or the radiation stress tensor. Equations (2.9) and (2.11) are important dynamic characteristics of waves. Summation is made over repeated subscripts and δ_{nj} is the Kronecker delta symbol.

As an example, if consider the plane longitudinal elastic waves in the x_1 direction with vanishing body loads, described by (2.7) with $u = [u(x,\tau),0,0]$. By substituting (2.1), (2.2), (2.6) into (2.7) we obtain the motion equation in displacements

$$\ddot{u} + \tau \ddot{u}_{xx} - u_{xx} + \beta u_{xxxx} = \alpha u_x u_{xx} \tag{2.13}$$

where

$$u = \frac{u_1}{\varepsilon_0 \Lambda d} \ , \ x = \frac{x_1}{\Lambda d} \ , \ t = \frac{c_1 t'}{\Lambda d} \tag{2.14}$$

are dimensionless variables. Here $\varepsilon_0 \in [10^{-7}, 10^{-6}]$ is a characteristic value of the elastic strains, $c_1^2 = \dfrac{\lambda + 2\mu}{\rho_0}$ the characteristic longitudinal wave velocity in the material, $\Lambda = \dfrac{L}{d}$ the dimensionless wave scale, d the grain diameter, and L the wavelength. Parameters β and α characterize the dispersion and nonlinearity of the medium and are given by

$$\beta = 4\mu M^3 \frac{1+\nu}{(\lambda + 2\mu)\Lambda^2 d^2} \ , \ \alpha = \varepsilon_0 \frac{3 + 2(A + 3B + C)}{\lambda + 2\mu} . \tag{2.15}$$

We anticipate that for (2.13) the dispersive effects are given by terms $\tau \ddot{u}$ and βu_{xxxx}, and concentrating effects by $\alpha u_x u_{xx}$. We shall examine the balance between these effects.

For $\alpha = 0$ and $\tau = 0$ any solution of (2.13) can be represented as a superposition of Fourier components. Using the method of normal modes with harmonic independent components $u = u_0 \exp \mathrm{i}(\omega t - kx)$, with k the wave-number, ω the angular frequency and $\alpha = 0$ in (2.13) we obtain the dispersion relation which gives the frequency ω as a function of the wave-number k

$$\omega^2 - k^2 - \beta k^4 = 0 . \tag{2.16}$$

From it we deduce the phase velocity ω / k

$$\omega^2 / k^2 = 1 + \beta k^2 . \tag{2.17}$$

The dispersion of longitudinal waves can be either positive for $\beta > 0$ or negative for $\beta < 0$. This depends on the nanostructure constant i.e. $\nu > -1$ for the first case and $\nu < -1$ for the second. In negative-dispersion media the phase velocity ω / k decreases with increasing wave number and in positive-dispersion media the phase velocity increases with increasing the wave number. The presence of nonlinear term in

(2.13) and the nonvanishing parameter τ change the aspect of the waves. In contrast to dispersion, nonlinearity leads to the concentration of the wave energy. For $\tau = 0$ and a strong dispersion $\beta k^4 >> 1$, $\Lambda << 1$ we are seeking for (2.13) waves of permanent shape and size by trying solutions such that

$$u(x,t) = u(\psi)\ ,\ \psi = x - ct\ , \tag{2.18}$$

with constant wave velocity c. Solutions of (2.13) are given by

$$u(x,t) = a + \frac{3(c^2-1)}{\alpha}\tanh\left[\frac{c^2-1}{-4\beta}\right]^{1/2}(x-ct)\ , \tag{2.19}$$

where a and $c > 1$ are arbitrary constants that can be determined from the initial or/and boundary conditions attached to (2.13). For a negative-dispersion media equation (2.19) is equivalent to the solution used by Taylor to describe the structure of a weak shock wave in a real fluid. This solution is a kink because its derivative with respect to the variable ψ is the known Boussinesq soliton expresssed as a *sech*-squared solution (Munteanu and Donescu [23]). The solution (2.19) is a localized entity, which may keep its entity in the field of propagation. The concentration of wave energy is described by the nonlinear term of (2.13). The balance or non-balance between the dispersion and the concentration effects depend on the mechanical property of the medium.

3. STATEMENT OF THE FOCUSING

We assume the longitudinal wave propagation in nanostructured medium so that in the $x_3 = 0$ plane the displacements $u_1 = u_2 = 0$ and $u_3 \neq 0$ within a limited domain. Also we assume that in the medium we have $|u_{1,2}| << |u_3|$. For simplicity, we investigate the wave propagation in the half-space $x_3 > 0$ medium with randomly distributed spherical grains. When the waves are propagating inside the half-space along the x_3-axis, the dissipation and dispersion effects with the presence of grains modeled as spherules, do not give a high order contribution to the equations for u_1 and u_2, so we will consider only the equation for the longitudinal displacement u_3 (Bagdoev and Sheroyan [12]).

Let assume here that the general solution of (2.7) is a superposition of solitons

$$u_i = \sum_{n=1} U_n(x_1, x_2, x_3)\,\mathrm{sech}^2 n(\omega t - k\,x_3 + \gamma_n)\ ,\ i = 1,2,3\ , \tag{3.1}$$

where amplitudes U_n are functions of coordinates, ω the cyclic frequency and k the wave number. For studying the focusing we consider the first-order approximations as

$$U_1 = U(x_1, x_2, x_3)\exp\left[kV(x_1, x_2, x_3)\right] \tag{3.2}$$

It is convenient to work in cylindrical coordinates r, θ, z (suppose all functions are uniform with respect to θ). Substituting (3.1) for $n = 1$ with (3.2) into (2.7) and neglecting the high order differentiation of U and V, we obtain

$$2k^2 V_{,z} U + \bar{\alpha} V_{,r}^2 U - \bar{\alpha}(U_{,rr} + r^{-1}U_{,r}) = -\bar{\beta}U^3\ , \tag{3.3a}$$

$$2kUU_{,z} + 2\bar{\alpha}V_{,r}UU_{,r} + U^2\bar{\alpha}(V_{,rr} + r^{-1}V_{,r}) = \bar{\beta}U^4\ , \tag{3.3b}$$

where $\bar{\alpha}$, $\bar{\beta}$ are given by

$$\bar{\alpha} = \frac{\alpha}{k^2\omega^2(1+\tau)}\ ,\ \bar{\beta} = \frac{\beta}{k^2\omega^2(1+\tau)}\ . \tag{3.4}$$

For $\tau = 0$, equations (3.3) have the same form with similar equations found by Bagdoev and Shekoyan [12]. The solutions of (3.3) are sought in the form

$$V = 0.5 r^2 \hat{R}(z), \quad U^2 = \frac{U_0^2}{L^2} \exp \frac{-r^2}{L_0^2 L^2}, \tag{3.5}$$

where $L(z)$ is the dimensionless width of the wave, $L_0 = L(0)$ the dimensionless initial width of the wave, $\hat{R}^{-1}(z)$ the variable radius of curvature of the wave front, and U_0 the amplitude $z = 0$ $(x_3 \equiv z)$. Boundary conditions are

$$\hat{R}(0) = R^{-1}, \quad L(0) = 1. \tag{3.6}$$

Substituting (3.5) into (3.3) we obtain

$$L_{,zz} L^3 = \gamma, \tag{3.7a}$$

$$L_{,z} = \hat{R}\bar{\alpha} L + \frac{\bar{\beta} U_0^2}{2kL}, \tag{3.7b}$$

$$\gamma = \frac{16\bar{\alpha}^2}{k^2 L_0^4} - \frac{4k^2 L_0^2}{U_0^2 L_0^2 - 4\bar{\alpha}}, \quad 2\bar{\alpha} + \bar{\beta} U_0^2 = 0. \tag{3.7c}$$

From (3.6) and (3.7a) we obtain

$$L_{,z}(0) = \frac{\bar{\alpha}}{R} - \frac{\bar{\beta} U_0^2}{2k}, \tag{3.8}$$

$$L_{,z} = -\left[L_{,z}^2(0) + \gamma(1 - L^{-2}) \right]^{1/2}. \tag{3.9}$$

The focusing is observed only for negative values of $L_{,z}$. If $\gamma < 0$ and $\bar{\beta} < 0$ the function L does not have an extremum. The function of wavelengh L continuously decreases with z until it vanishes at a distance z_f called the focal point given by

$$z_f^{-1} = \sqrt{-\gamma} - L_{,z}(0). \tag{3.10a}$$

If $\gamma > 0$ and $\bar{\beta} < 0$ the function L has a minimum. Therefore, the width of the wave is minimal at the focal point given by

$$z_f = -\frac{L_{,z}(0)}{\gamma + L_{,z}^2(0)}. \tag{3.10b}$$

The width of the wave is

$$L_f^2 = \frac{\gamma}{\gamma + L_{,z}^2(0)}. \tag{3.11}$$

When $R \to \infty$, we see from (3.8) that $L_{,z} < 0$ if $\bar{\beta} > 0$, so the self-focusing takes place. In conclusion, the solution u_3 is obtained from (3.1)

$$u_3(r,z,t) = U \exp(kV)\,\mathrm{sech}^2(\omega t - k z + \gamma_0) = \\ = \left(\frac{U_0^2}{L^2} \exp \frac{-r^2}{L_0^2 L^2} \right)^{1/2} \exp[0.5 k r^2 \hat{R}]\,\mathrm{sech}^2(\omega t - k z + \gamma_0), \tag{3.12}$$

where $L(z)$ and $\hat{R}(z)$ verify (3.7a) and (3.7b).

4. SUMMARY

In this paper the effect of nanostructure in the ultrasonic wave propagation field is investigated using the couple stress theory, which incorporates the local deformations and rotations of internal grains, and the double couple radiation pattern, which introduce the radiation force which acts upon the body likewise a friction force. The rate of work of this force is equals to the radiation of energy that leaves acoustically the body per unit time.

In a natural way this theory gives rise the desired effects missing in the classical theory i.e. concentration of energy by focusing and self-focusing waves phenomena. It is found that the focusing depends directly on the sign of parameters describing dispersion and nonlinearity. In negative-dispersion media waves are stable, while in positive-dispersion media they are unstable.

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