Models for essentially nonlinear strain waves in complex materials

Alexey V. Porubov

Institute of Problems in Mechanical Engineering
of the Russian Academy of Sciences,
Bolshoy av. 61, V.O., Saint-Petersburg 199178, Russia

porubov.math@mail.ioffe.ru

October 6, 2009

Outline of the talk

- Structural essentially nonlinear models for complex materials
  - Governing equations
  - Solitary wave solutions
  - Nonlinear and dispersive features
  - Deviations in the internal structure
- Phenomenological essentially nonlinear models
  - Model based on a single governing equation
  - Coupled equations: choice of nonlinearity
  - Nonlinearity at the macro-level
  - Nonlinearity at the micro-level
- Conclusions

Structural essentially nonlinear model after G. Pouget, G.A. Maugin and M.K. Sayadi (1984-1991)

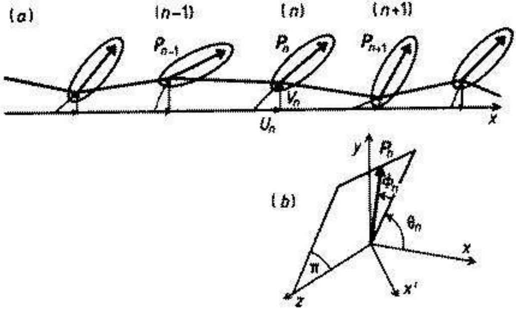


Figure 1. Lattice model: (*a*) one-dimensional atomic chain equipped with rotatory molecular groups (microstructures), (*b*) angles of rotations for the dipoles or molecular groups. θ_n, rotation about the z axis; φ_n, rotation about the x' axis.

Structural essentially nonlinear model after G. Pouget, G.A. Maugin and M.K. Sayadi (1984-1991)

Governing equations in the 1D case are

$$\rho U_{TT} - c_L^2 \; U_{XX} \;=\; \alpha_L (1 + \cos(\phi))_X \,,$$

$$\phi_{TT} - \phi_{XX} \;=\; (\alpha_L U_X + \chi) \sin(\phi),$$

where $U(X, T)$ is longitudinal displacement, $\phi(X, T)$ - rotation in the plane perpendicular to the direction of the longitudinal wave propagation.

Structural essentially nonlinear model after E.L. Aero (2002-2007)

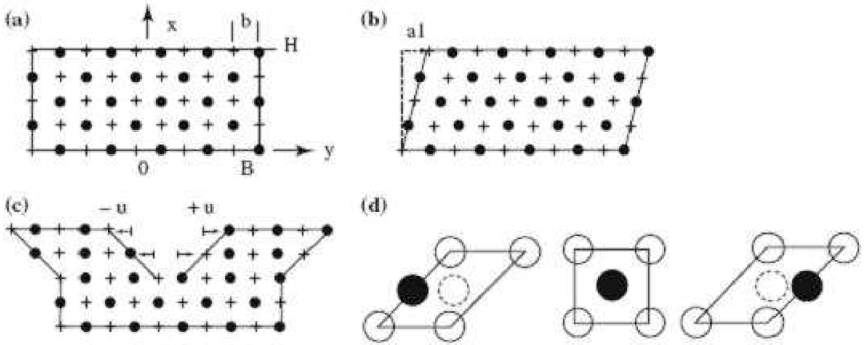


Figure 1. (a) The complex crystalline lattice consisting of two sublattices. (b) Macroscopic deformation without a relative shear of sublattices. (c) Microdeformations at twinning. (d) Bifurcation of the structure of an elementary cell during microdefomation.

Structural essentially nonlinear model after E.L. Aero (2002-2007)

Governing equations in the 1D case are

$$\rho U_{tt} - E\ U_{xx} = S(\cos(u) - 1)_x,$$

$$\mu u_{tt} - \kappa u_{xx} = (SU_x - p)\sin(u).$$

where

$$U = \frac{m_1 U_1 + m_2 U_2}{m_1 + m_2},\ u = \frac{U_1 - U_2}{a}$$

a is a period of sub-lattice, U is a macro-displacement and u is a relative micro-displacement for the pair of atoms with masses m_1, m_2.

Travelling strain wave solutions

$$\cos(u) = 1 - ((E - \rho V^2)v - \sigma)/S,$$

σ is a constant of integration, $v = U_\theta$, $\theta = x - V\,t$.

$$v_\theta^2 = a_0 + a_1\,v + a_2\,v^2 + a_3\,v^3 + a_4\,v^4$$

ODE of the Gardner equation also arising for large amplitude internal waves in fluids.

Important feature:

$$a_i = a_i(V).$$

Expression for a_i see in Porubov, Aero, Maugin (2009).

Solitary wave solutions

$$v_1 = \frac{A}{Q\ \cosh(k\ \theta) + 1},\ v_2 = -\frac{A}{Q\ \cosh(k\ \theta) - 1}.$$

For $\sigma = 0$

$$A = \frac{4\ S}{\rho(c_0^2 + c_L^2 - V^2)}, Q_\pm = \pm\frac{c_L^2 - V^2 - c_0^2}{c_L^2 - V^2 + c_0^2}, k = 2\sqrt{\frac{p}{\mu(c_l^2 - V^2)}}$$

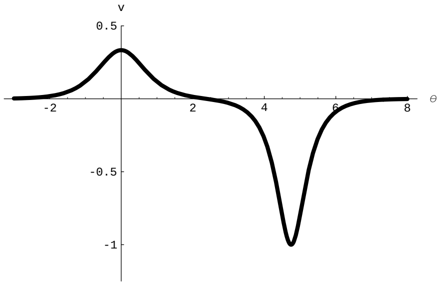
and for $\sigma = -2S$

$$A = \frac{4\ S}{\rho(c_0^2 + V^2 - c_L^2)}, Q_\pm = \pm\frac{V^2 - c_L^2 - c_0^2}{V^2 - c_L^2 + c_0^2}, k = 2\sqrt{\frac{p}{\mu\ (V^2 - c_l^2)}}$$

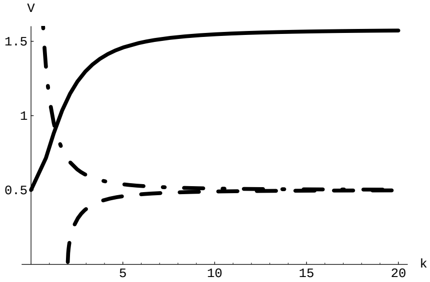
where $c_L^2 = E/\rho$, $c_l^2 = \kappa/\mu$, $c_0^2 = S^2/(p\ \rho)$.

- No simultaneous existence of the compression and tensile macro-strain waves
- Mode with cut-off or optical mode, no acoustical one

Nonlinear and dispersive features



Simultaneous existence of tensile and compression waves.



Acoustical mode (solid line) optical mode (dotted line), and mode with cut-off wave number (dashed line).

Deviations in internal structure

Expression for u is obtained depending whether the first derivative u_θ exists or not at $\theta = 0$

bell-shaped wave

$$u = \pm \arccos\left(\frac{(\rho V^2 - E)v}{S} + 1\right) \text{ for } -\infty < \theta < \infty,$$

or kink

$$u = \pm \arccos\left(\frac{(\rho V^2 - E)v}{S} + 1\right) \text{ for } \theta \leq 0,$$

$$u = \pm 2\pi \mp \arccos\left(\frac{(\rho V^2 - E)v}{S} + 1\right) \text{ for } \theta > 0,$$

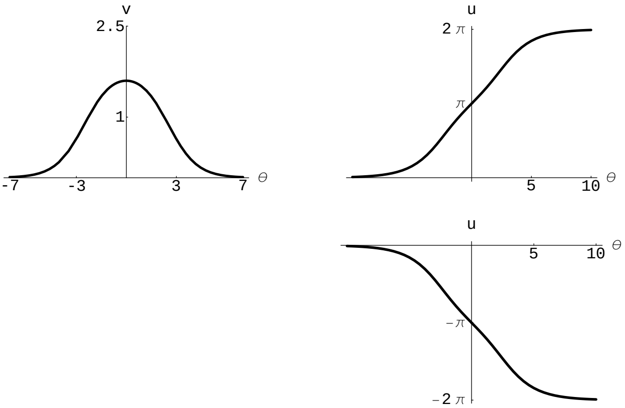
Symmetric profiles of u for any v!

Deviations in internal structure

Table: Wave shapes for $\sigma = 0$

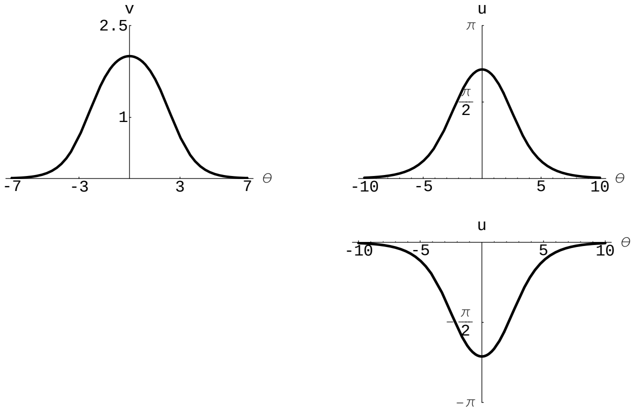
V^2	$(0; c_L^2 - c_0^2)$	$(c_L^2 - c_0^2; c_L^2)$	$(c_L^2; c_L^2 + c_0^2)$	$> c_L^2 + c_0^2$
Shape of v	Tensile v_1	Tensile v_1	Compression v_2	Compression v_1
Shape of u	Kink	Bell-shaped	Kink	Kink
Choice of $Q_\pm$	Q_+	Q_-	Q_+	Q_+

Deviations in internal structure



Similar macro-strains v give rise to different kink-shaped variations u of the internal structure

Deviations in internal structure



Similar macro-strains v give rise to different bell-shaped variations u of the internal structure

Solitary waves on a pedestal

$$v_3 \;=\; \frac{A}{Q\ \cosh(k\ \theta)+1}+F,\;\; v_4 \;=\; -\frac{A}{Q\ \cosh(k\ \theta)-1}+F.$$

The first solution arises for

$$F \;=\; \frac{\sigma}{\rho(c_L^2-V^2)}$$

with parameters given by

$$A \;=\; \frac{4\ S(V^2-c_L^2+c_1^2)}{\rho(V^2-c_L^2)(c_0^2+c_L^2-c_1^2-\ V^2)}, Q_{\pm} \;=\; \pm\frac{c_L^2-\ V^2-c_0^2-c_1^2}{c_L^2-\ V^2+c_0^2-c_1^2},$$

$$k \;=\; 2\sqrt{\frac{p(c_1^2-c_L^2+\ V^2)}{\mu(c_l^2-\ V^2)(V^2-c_L^2)}}$$

where $c_1^2 \;=\; \sigma S/(p\rho)$.

Dispersive features

$$\mu\ k^2V^4 + (4p - \mu k^2(c_l^2 + c_L^2))V^2 + 4p\ c_1^2 + c_L^2(\mu k^2 c_l^2 - 4p)\ =\ 0$$

The first root of the equation, V_1 belongs to the acoustical mode. It tends to

$$V_1^2 = c_L^2 - c_1^2$$

as $k \to 0$. The second root, V_2 belongs to the mode with cut-off, it tends to

$$V_2^2\ =\ c_l^2 + c_1^2\ - \frac{4p}{\mu\ k^2}$$

as $k \to 0$.

The second solution arises for

$$F\ =\ \frac{\sigma + 2S}{\rho(c_L^2 - V^2)}$$

Need in phenomenological models

- Parameters of the structural models are unknown as a rule
- How to apply these models to the real media?
- Is it possible to develop another modelling that describes nonlinear and dispersive features like structural models but admits estimation of the parameters?

Phenomenological model based on a single governing equation

The Murnghan model for the energy

$$\Pi = \frac{\lambda + 2\mu}{2}\, I_1^2 - 2\mu\, I_2 + \frac{l + 2m}{3}\, I_1^3 - 2m\, I_1 I_2 + n\, I_3 + \nu_1\, I_1^4 + \nu_2\, I_1^2 I_2 + \nu_3\, I_1 I_3 + \nu_4\, I_2^2,$$

or the stress-strain relationship in the 1D case

$$P = E^* U_x + C_1 U_x^2 + C_2 U_x^3$$

Classic elastic materials: typical elastic strain $U_x \sim 10^{-3} - 10^{-5}$ and $C_2 U_x^3 << C_1 U_x^2 << E^* U_x \Rightarrow$ truncated expansions
Non-classic materials (rocks, soils, some crystals): typical elastic strain $U_x \sim 10^{-4} - 10^{-5}$ and $C_2 U_x^3 \sim C_1 U_x^2 \sim E^* U_x \Rightarrow$ exact representations
Internal structure is introduced via the coefficients and dispersion.

Phenomenological models: essential nonlinearity

- Tuff with grains: $C_1/E^* \sim 130$, $C_2/E^* \sim 10^4$
  Loam soil: $C_1/E^* \sim 10^3$, $C_2/E^* \sim 10^7$ (Belyaeva et al. (1993,1994))
- Medium with cracks: $C_1/E^* \sim 10^2$, $C_2/E^* \sim 10^8$ (Nazarov, Sutin (1997))
- Crystal V_3Si: $C_1/E^* \sim 86$, $C_2/E^* \sim 10^4$ (Testardi (1973), Barsch (1974))
- Crystal MgO with paramagnetic ions Fe^{2+} and Ni^{2+} in an external magnetic field: $C_1/E^* \sim 10^{-3}$, $C_2/E^* \sim 10^8$ (Bugai, Sazonov(2005))

Phenomenological models: essential nonlinearity

- There exist materials with abnormal nonlinear features, e.g., rocks, paramagnetic crystals. Hence even small amplitude waves should be considered as non-linear ones.
- There exist materials whose cubic nonlinear features are equal to the quadratic ones. Hence an improved description may be developed taking into account both nonlinearities.

Phenomenological model based on a single governing equation

Formal use of the truncated expansions of the weakly nonlinear theory yields the equation for longitudinal strains

$$v_{tt} - a\, v_{xx} - c_1\,(\,v^2)_{xx} - c_2\,(\,v^3)_{xx} + \alpha_3\, v_{xxtt} - \alpha_4\, v_{xxxx} = 0.$$

where $v = U_x$, $a = E^*/\rho$, $c_1 = 2C_1/\rho$, $c_2 = 3C_2/\rho$
The equation for travelling wave solution reads

$$v_\theta^2 = \frac{1}{6(\alpha_3 V^2 - \alpha_4)}\left(\alpha_0 + \alpha_1\; v + 6(V^2 - a)v^2 - 4c_1 v^3 - 3c_2 v^4\right).$$

where $\theta = x - V\; t$, α_0, α_1 are constants of integration.
Similar to that of the structural model!

Distinctions in the features of the solutions: solitary waves

$$v_1 = \frac{A}{Q\ \cosh(k\ \theta)+1},$$

$$v_2 = -\frac{A}{Q\ \cosh(k\ \theta)-1}.$$

with

$$A = \frac{3(V^2-a)}{c_1},\ Q = \sqrt{1+\frac{9c_2}{2c_1^2}(V^2-a)},\ k^2 = \frac{V^2-a}{\alpha_4-\alpha_3 V^2}.$$

- Simultaneous existence of the compression and tensile macro- strain waves
- Acoustical mode
- Micro-field deviations are not described

Phenomenological model based on the coupled equations

Linearized coupled governing equations for the macrodispalcement $U(x,t)$ and microstrain $\psi(x,t)$,

$$\rho\ U_{tt} - A\ U_{xx}\ =\ D\ \psi_x,$$

$$I\ \psi_{tt} - C\ \psi_{xx}\ =\ -D\ U_x - B\ \psi,$$

where I is the microinertia, possess both acoustical and optical modes, see Engelbrecht, Berezovski, Pastrone and Braun (2005).

Phenomenological model based on the coupled equations: choice of nonlinearity

Previous models: Khustnutdinova (1992), Dragunov, Pavlov, Potapov (1997), Engelbrecht & Pastrone (2003),Porubov & Pastrone(2004), Janno & Engelbrecht (2005) etc.

Nonlinearity at the macro-level

$$\rho\ U_{tt} - A\ U_{xx} \ =\ N\ U_x U_{xx} + M U_x^2 U_{xx} + D\ \psi_x,$$

$$I\ \psi_{tt} - C\ \psi_{xx} \ =\ -D\ U_x - B\ \psi,$$

The ODE equation for travelling macro-strain solitary waves $v = U_\theta$ is

$$v_\theta^2 \ =\ a_0 + a_1\ v + a_2\ v^2 + a_3\ v^3 + a_4\ v^4,$$

$a_i = a_i(V)$, again similar to that of the structural model!

Phenomenological model based on the coupled equations: nonlinearity at the macro-level

$$\psi = -\frac{N}{2}v^2 - \frac{M}{3}v^3 + \frac{\rho V^2 - A}{D}\; v_\theta + G$$

$$v_1 = \frac{A}{Q\ \cosh(k\ \theta) + 1} + F,\ \ v_2 = -\frac{A}{Q\ \cosh(k\ \theta) - 1} + F.$$

Features of the solitary wave solution:

- Both acoustical and optical modes are possible but independent of F!
- Simultaneous existence of compression and tensile waves
- No symmetric profiles for ψ for any v
- Only bell-shaped profiles of ψ are described

Phenomenological model based on the coupled equations: choice of nonlinearity

Nonlinearity at the micro-level

Using the power series truncation for trigonometric functions in the structural model

$$\rho U_{tt} - E\ U_{xx} \ = \ S(\cos(u) - 1)_x,$$

$$\mu u_{tt} - \kappa u_{xx} \ = \ (SU_x - p)\sin(u).$$

one can suggest the phenomenological model

$$\rho\ U_{tt} - A\ U_{xx} \ = \ D\ \psi\psi_x,$$

$$I\ \psi_{tt} - C\ \psi_{xx} \ = \ -(D\ U_x + B)\ (\psi - \psi^3/6),$$

Phenomenological model based on the coupled equations: nonlinearity at the micro-level

Travelling wave solution for $v = U_\theta$, ψ

$$\psi^2 = (2\rho/S)((c_L^2 - V^2)v - \sigma_1/\rho)$$

$$v_\theta^2 = a_0 + a_1\ v + a_2\ v^2 + a_3\ v^3 + a_4\ v^4$$

Solitary wave solution exists when $a_0 = 0$, $a_1 = 0$:

$$v_1 = \frac{A}{Q\ \cosh(k\ \theta) + 1},\ v_2 = -\frac{A}{Q\ \cosh(k\ \theta) - 1}.$$

$$A = -\frac{6D}{\rho(3c_0^2 - c_L^2 - V^2)}, k^2 = \frac{2B}{I(c_I^2 - V^2)},$$

$$Q = \pm\frac{\sqrt{(c_L^2 - V^2 - c_0^2)^2 + 8c_0^4}}{3c_0^2 + c_L^2 - V^2}$$

where $c_L^2 = A/\rho$, $c_I^2 = C/I$, $c_0^2 = -\sigma_1 D/(\rho B)$.

Close to the solution of the structural model

- mode with cut-off
- no simultaneous existence of compression and tensile waves
- two symmetric profiles of micro-strain waves correspond to the same macro-strain wave

Far from the solution of the structural model

- only bell-shaped micro-strains are described, not kinks

Conclusions

- Internal structure provides abnormal or essential nonlinearity and equal contributions of the quadratic and cubic nonlinearities in the governing equation for macro-strains.
- Essentially nonlinear models based on phenomenological and structural approaches give rise to the same governing ODE for the macro-strain waves.
- Distinctions in the equation coefficients yield different nonlinear and dispersive features of the solutions for the structural model and phenomenological model based on a single equation.
- Phenomenological model based on coupled equations allows us to describe most of nonlinear and dispersion features of the solution more or less close to the structural model with the exception of various kinds of micro-strains (kink or bell-shaped) corresponding to the similar bell-shaped macro-strains.

Open question

What kind of modelling, structural or phenomenological, is more suitable for a description of internal structural deviations in complex materials?