NONLOCAL MODEL FOR SHOCK-INDUCED STRUCTURE UNSTABLE STATE

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- Many problems on the shock compression of solids (strength of dynamically compressed material, shock transition and phase transformations) cannot be resolved in scope of the traditional continuum mechanics. A change in the fundamental assumptions is necessary to realize predictive capabilities.

- Experiments on the shock loading of materials show that mesoscopic effects determine the medium response to high-strain-rate, while the dissipation stage is not yet reached.

- The mesoscale level plays a role of an energy buffer between micro- and macroscopic degrees of freedom. In turn, the mesoscopic effects are the result of the nonlocal collective interaction initiating the self-organization and the feed-back in a medium.

- New self-consistent nonlocal approach based on nonequilibrium statistical mechanics had been developed and applied to the shock compression of solids. The set of integro-differential balance equations unites both wave and dissipative transport properties. Boundary and integral conditions to the set determine the internal scale spectra.

- The model is completed by a feedback that introduces the structure evolution based on the new methods of cybernetic physics.

- Resonance criteria for the structure transformation in dynamically deformed material is derived.

TRANSITION PROCESSES AND MEDIUM MODELS

Elastic medium model – wave-type transport mechanism

(stress – strain) – reversible wave process

$$\Pi = G\mathbf{e}$$

– valid for small time scales $t \square t_r$

and for small strains

Newtonian medium model – diffusive transport mechanism

(stress – strain-rate) – irreversible dissipative process

$$\Pi = \mu \frac{\partial \mathbf{v}}{\partial \mathbf{r}} = \mu \dot{\mathbf{e}}$$

– valid for large time and space scales $t \square t_r$

and for small strain-rates

What model between the limits?

(stress – strain, stress-rate, + memory effects, + structure transformation)

– both wave and diffusive mechanisms
– damping wave process
– valid for intermediate scales $t \square t_r$
– multi-scale energy exchange between different degrees of freedom including vortex structures formation at meso- and nano- scales

Nonequilibrium transport process (high-rate, high-gradient) can be followed by nonmonotonous stress relaxation, internal structure evolution (over structure unstable states) and synergetic self-organization

NONLOCAL MATHEMATICAL MODEL BASED ON NONEQUILIBRIUM STATISTICAL MECHANICS

(D.N. Zubarev)

Nonlocal relationships with memory between stress tensor $\mathbf{J}$ and strain-rate tensor $\frac{\partial \mathbf{u}}{\partial \mathbf{r}} = \frac{\partial \mathbf{e}}{\partial t}$ ($\mathbf{u}$ – momentum transport velocity, $\mathbf{e}$ – strain tensor) are valid far from equilibrium

$$\mathbf{J}(\mathbf{r},t) = -\int_0^t dt' \int_V d\mathbf{r}' \Re(\mathbf{r},\mathbf{r}',t,t') \frac{\partial \mathbf{u}}{\partial \mathbf{r}'}(\mathbf{r}',t')$$

Nonequilibrium correlation function $\Re(\mathbf{r},\mathbf{r}',t,t')$ determines the collective interaction effects on the macroscopic medium response at an intensive external loading

Unlike the local (limiting) medium models the nonlocal relationships are valid over all range of the loading regimes for all time and space scales

Nonlocal model corresponds both to the elastic medium model at an initial stage of loading $t \ll t_r$ and to the Newtonian model at a last hydrodynamic stage $t \gg t_r$. includes the stress relaxation and hardening at a transitional stage $t \sim t_r$

Nonlocal model at the transition regime describes evolving structure unstable states which can result new structure formation

PARAMETERS OF THE TRANSITION REGIME

CHARACTERIZING NONSTATIONARY WAVE PROPAGATION

$$\tau = \frac{t_r}{t_R} \square 1$$

t_r – relaxation time

t_R – loading time

$$\varepsilon = \frac{Ct_R}{L} \square \; 1$$

L – target width

$V_0 \square \; C$ – the shock velocity

$C = const$ – longitudinal sound velocity

$v \square \; C$ – mass velocity

In the transition regime momentum transport is a multi-scale group of nonlinear damping waves propagating along the x axis at the sound velocity for the elastic precursor.

New wave variables are introduced

$$\zeta = t - \frac{x}{C}, \; \xi = x; \qquad \frac{\partial}{\partial \zeta} \square \; \varepsilon \frac{\partial}{\partial \xi}$$

(2 separated scales)

Nonlocal model in new wave variables takes a form

$$J_{xx}(\zeta,\xi) = -\int_0^{\omega(\zeta)} d\zeta' \int_0^{\Omega(\zeta)} d\xi' \,\Re(\zeta,\zeta';\xi,\xi') \left[-\frac{1}{\tilde{N}} \frac{\partial v}{\partial \zeta'} + \varepsilon \frac{\partial v}{\partial \xi'} \right] (\zeta';\xi'),$$

$$\omega(\zeta) = \begin{cases} \zeta, & \zeta < 1 \\ 1, & \zeta \ge 1 \end{cases} \qquad \Omega(\zeta) = \begin{cases} C\zeta, & \tilde{N}\zeta < \Gamma \\ \Gamma, & C\zeta \ge \Gamma \end{cases}$$

ζ is normalized by t_R

Nonlocal effects along the x axis can be neglected

$$\Re(\zeta,\zeta';\xi,\xi') = \Im(\zeta,\zeta')\delta(|\xi - \xi'|)$$

MODEL OF VISCOUS ELASTIC MEDIUM

DERIVED FROM THE NONLOCAL MODEL

1) constant correlation function – elastic model of solid

$$\Im(\zeta,\zeta') = \rho_0 C^2$$

2) δ-correlation function (no correlations) – Newtonian model of fluid

(μ – viscosity)

$$\Im(\zeta,\zeta') = \rho_0 C^2 t_r \delta(\zeta-\zeta') = \mu\delta(\zeta-\zeta')$$

Linear combination of 1)-2) cases results in the model of viscous elastic medium

$$J_{xx}(\zeta,\xi) = -\int_0^{\omega(\zeta)} d\zeta' \int_0^{\Omega(\zeta)} d\xi' \, \Re(\zeta,\zeta';\xi,\xi') \left[-\frac{1}{\tilde{N}}\frac{\partial v}{\partial \zeta'} + \varepsilon \frac{\partial v}{\partial \xi'} \right](\zeta';\xi') =$$

$$= -\rho_0 C^2 \int_0^{\zeta} d\zeta' \int_0^{\Omega(\zeta)} d\xi' \delta(|\xi-\xi'|) \left[-\frac{1}{C}\frac{\partial v}{\partial \zeta'}(\zeta') \right] -$$

$$-\rho_0 C\tau\varepsilon \int_{\zeta}^{1} d\zeta' \int_0^{\Omega(\zeta)} d\xi' \delta(\zeta-\zeta')\delta(|\xi-\xi'|)\frac{\partial v}{\partial \xi'} =$$

$$= \rho_0 C \int_0^{v(\zeta,0)} dv - \rho_0 C\tau\varepsilon \int_0^{\Gamma} d\xi' \delta(|\xi-\xi'|)\frac{\partial v}{\partial \xi'}(\zeta;\xi') =$$

$$= \rho_0 C v - \hat{\mu}\frac{\partial v}{\partial x}(x;t)$$

In this way one can construct any conventional medium model, but for transition regime it is not correct, as far as the two limiting cases correspond to different stages of loading

NONLOCAL THEORY OF NONEQUILIBRIUM TRANSPORT

Nonequilibrium correlation function –

– unknown functional of strain and strain-rate.

General form of correlation function is constructed in 3 statistical moments approximation (k_0, τ, θ – the model parameters that are also unknown functionals)

$$\Im(\zeta,\zeta';\xi) = \rho_0 \tilde{N}^2 k_0(\zeta,\xi) \exp\left\{-\frac{\pi\left(\zeta-\zeta'-\vartheta(\xi)\right)^2}{\tau^2(\xi)}\right\}$$

$$\Im(\zeta,\zeta';\xi) \xrightarrow[\tau\to 0,\vartheta\to 0]{} \rho_0 \tilde{N}^2 \tau \delta\left(\zeta-\zeta'\right)$$

$$\Im(\zeta,\zeta';\xi) \xrightarrow[\tau\to\infty]{} \rho_0 \tilde{N}^2$$

Stress tensor component with the model correlation function in the 1st approximation at $\varepsilon \ll 1$

$$J_{xx}(\zeta,\xi) = \rho_0 \tilde{N}^2 k_0(\zeta,\xi) \int_0^{\omega(\zeta)} d\zeta' \exp\left\{-\frac{\pi\left(\zeta-\zeta'-\vartheta(\xi)\right)^2}{\tau^2(\xi)}\right\} \frac{1}{\tilde{N}} \frac{\partial v}{\partial \zeta'} \qquad (1)$$

The constructed model changes the type of the balance equations from the hyperbolic at the initial stage up to the parabolic one at the terminal hydrodynamic stage depending on the loading regime.

The nonlocal model related to the Green function approach and can be used to generalize the approach to nonlinear problems

MODEL PARAMETERS

FOR STRUCTURE UNSTABLE STATE

3 statistical moments for the model correlation function (the model parameters) are related to evolving scales of wave-vortex internal medium structure.

Statistical moments are coefficients in the series resulted from the integral expression for the stress component above by the series

$$\frac{\partial v}{\partial \zeta'}(\zeta',\xi) = \frac{\partial v}{\partial \zeta}(\zeta,\xi) + (\zeta'-\zeta)\frac{\partial^2 v}{\partial \zeta^2}(\zeta,\xi) + \frac{1}{2}(\zeta'-\zeta)^2\frac{\partial^3 v}{\partial \zeta^3}(\zeta,\xi)...$$

substituted under the integral

$$J(\zeta,\xi) = k_0(\zeta,\xi)\frac{\partial v}{\partial \zeta}(\zeta,\xi) + k_1(\zeta,\xi)\frac{\partial^2 v}{\partial \zeta^2}(\zeta,\xi) + \frac{1}{2}k_2(\zeta,\xi)\frac{\partial^3 v}{\partial \zeta^3}(\zeta,\xi)...$$

$$k_0(\zeta,\xi) = \int_0^{\omega(\zeta)} d\zeta' \Im(\zeta,\zeta';\xi)$$

– defines a relative effective medium viscosity in structure unstable state

$$k_1(\zeta,\xi) = \int_0^{\omega(\zeta)} d\zeta' \Im(\zeta,\zeta';\xi)\left(\zeta-\zeta'\right) = \theta(\xi)$$

$$If \;\; \Im(\zeta,\zeta';\xi) \neq \delta\left(\zeta-\zeta'\right), \;\; \theta \neq 0$$

– introduces new typical time – retardation time of the wave maximum from the elastic precursor – rise-time for the plastic front. Its evolution defines the plastic front propagation velocity as a group wave velocity while the elastic precursor propagates at phase velocity of longitudinal sound.

$$k_2(\zeta,\xi) = \int_0^{\omega(\zeta)} d\zeta' \Im(\zeta,\zeta';\xi)\left(\zeta-\zeta'\right)^2 = \tau^2(\xi) - 2\zeta\theta(\xi)$$

– defines the relaxation time as a typical time of correlation.

Statistical moments are used as parameters of the integral model.

The model parameters are connected to the boundary conditions.

INTERNAL STRUCTURE EVOLUTION
AND ADAPTIVE CONTROL WITH FEEDBACK

The nonlocal model parameters evolve according to the adaptive control theory

Goal function – minimum of the integral entropy production in the wave

$$\frac{dS}{d\xi}(\xi)=\rho_0\tilde{N}\int_0^{\infty}\mathrm{d}\zeta\,\frac{\partial v}{\partial\zeta}(\zeta,\xi)\int_0^{\zeta}\mathrm{d}\zeta'\exp\left\{-\frac{\pi\left(\zeta-\zeta'-\theta(\xi)\right)^2}{\tau^2(\xi)}\right\}\frac{\partial v}{\partial\zeta'}(\zeta',\xi) \qquad (2)$$

Speed gradient algorithm determines the parameters rates on the integral entropy production surface.

$$\frac{d\tau}{d\xi}=-g\nabla_{\tau}\frac{dS}{d\xi},\qquad \frac{d\theta}{d\xi}=-g\nabla_{\theta}\frac{dS}{d\xi} \qquad (3)$$

According the evolution equation above the model parameters in structure unstable state tend to move down the surface to reach stable state along trajectories connected to the boundary conditions.

The structure evolution is connected to the nonstationary mass velocity waveforms by feedback through the model parameters and therefore results a change of dynamical properties of a medium.

1st APPROXIMATION SOLUTION FOR NONSTATIONARY WAVEFORM

Nonstationary waveform is determined by the parameters of relaxation and retardation and depends on the initial state and strain-rate history.

In a simple case of constant initial strain-rate the problem has an explicit solution for the momentum transport equation

$$v(\zeta,\xi) = \int_0^{\omega(\zeta)} \mathrm{d}\zeta' \exp\left\{-\frac{\pi\left(\zeta'-\zeta+\theta(\xi)\right)^2}{\tau^2(\xi)}\right\} \frac{\partial v}{\partial \zeta'}(\zeta',\xi_0), \quad (4)$$

$$\frac{\partial v}{\partial \zeta}(\zeta,\xi_0) = a = const$$

$$v(\zeta,\xi) = \begin{cases} \dfrac{a\tau}{2}\left(erf\,\dfrac{\sqrt{\pi}\,(\zeta-\theta)}{\tau} + erf\,\dfrac{\sqrt{\pi}\theta}{\tau}\right), & \zeta < 1 \\ \dfrac{a\tau}{2}\left(erf\,\dfrac{\sqrt{\pi}\,(\zeta-\theta)}{\tau} + erf\,\dfrac{\sqrt{\pi}\,(1-\zeta+\theta)}{\tau}\right), & \zeta \ge 1 \end{cases} \quad (5)$$

Internal energy transport equation for structure unstable states in transition regime includes velocities at different states

$$\frac{\partial \mathrm{E}}{\partial \zeta} - \int_0^{\omega(\zeta)} \mathrm{d}\zeta' \exp\left\{-\frac{\pi\left(\zeta'-\zeta+\theta(\xi)\right)^2}{\tau^2(\xi)}\right\} \frac{\partial v}{\partial \zeta'}(\zeta',\xi_0)\frac{\partial v}{\partial \zeta}(\zeta,\xi_0) = 0$$

In the elastic limit $\tau \to \infty$ the potential elastic energy loss is due to kinetic energy growth and no dissipation is implied.

$$\frac{\partial \mathrm{E}^e}{\partial \zeta} = \int_0^{\zeta} \mathrm{d}\zeta' \frac{\partial v}{\partial \zeta'}(\zeta',\xi_0)\frac{\partial v}{\partial \zeta}(\zeta,\xi_0) = \frac{\partial (v^2/2)}{\partial \zeta}(\zeta,\xi_0)$$

In the limit $\tau \to 0$ heat energy grows due to dissipation $\dfrac{\partial \mathrm{E}^h}{\partial \zeta} = \left(\dfrac{\partial v}{\partial \zeta}(\zeta,\xi_0)\right)^2$

STRESS–STRAIN RELATION FOR LOADING

As far as strain $e\tilde{N} = a\zeta$, Eq. (4) for $\zeta < 1$ results stress–strain dependence presented on Fig. 1. Linear elastic dependences reach for large ζ (strain) constant values $a\tau$ (~ strain-rate) corresponding to hydrodynamic regime or ideal plasticity. For changing strain-rates during the loading curves can become nonmonotonuous.

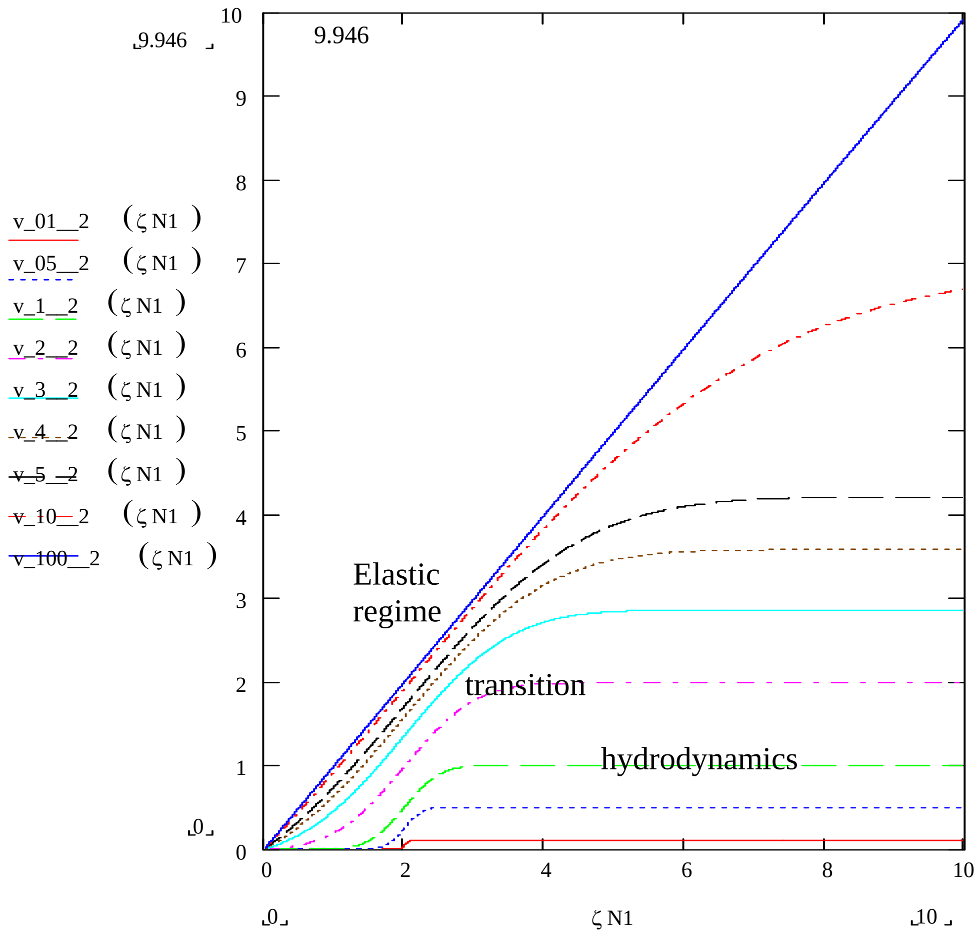


Fig. 1.

Stress – strain dependence

in the transition regime

STRESS RELAXATION

For the finite-time loading Eq. (5) for $\zeta > 1$ results stress relaxation taking into account memory effects (hardening at large τ) presented on Fig.2. Stress reach maximum for the retardation time ϑ (Fig. 3) while the rise-time and elastic precursor amplitude are damping with the relaxation time τ

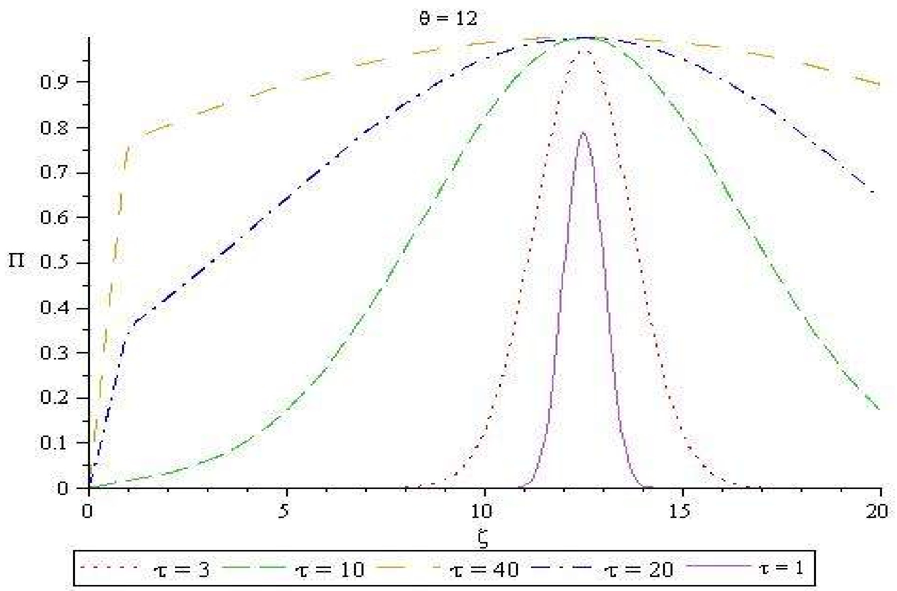


Fig. 2
Stress relaxation with damping relaxation parameter τ
at fixed retardation parameter ϑ in the transition regime

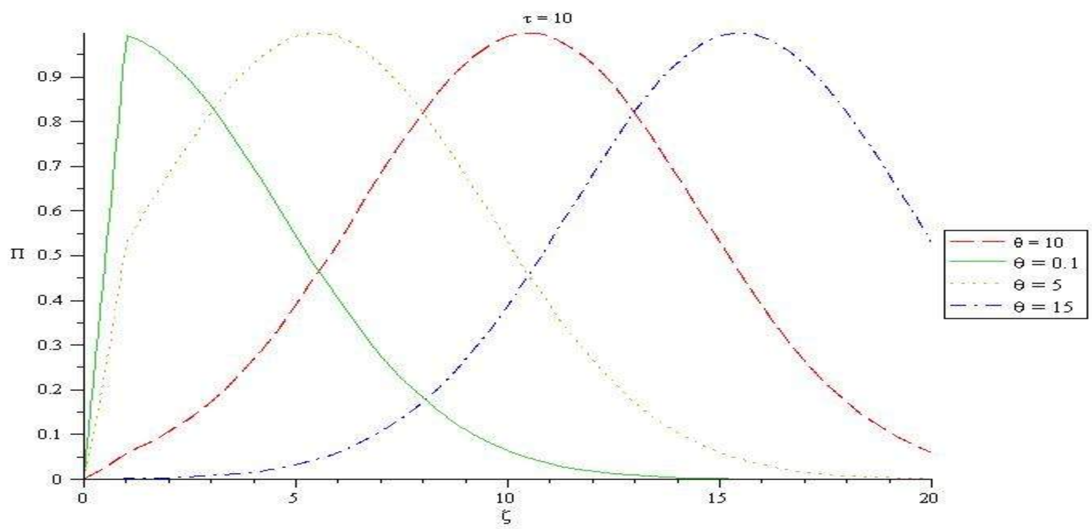


Fig. 3
Retardation of the plastic front from the elastic precursor
with growing parameter ϑ at fixed τ

ELASTIC PRECURSOR RELAXATION

Elastic precursor relaxes with growing retardation ϑ which is in turn growing as far as the pulse propagates inside a target. The alternative behavior is observed with growing relaxation parameter (Fig. 5). So, the formation of the plastic front and elastic precursor (two-wave front) is an attribute of the transition regime.

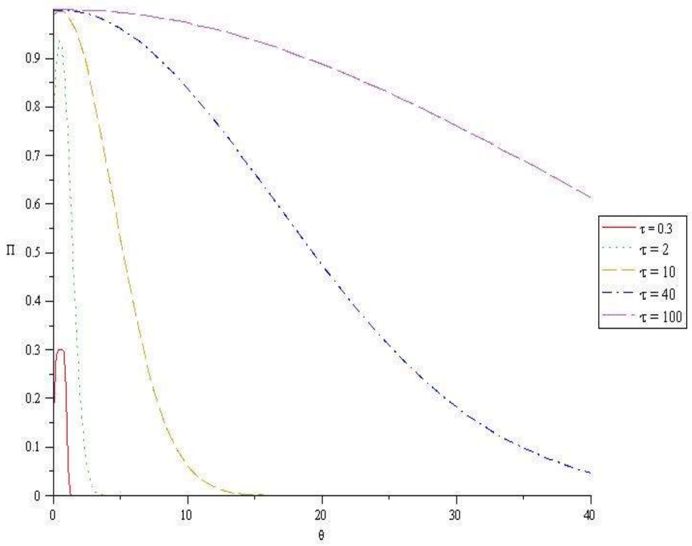


Fig. 4

Elastic precursor relaxation with the growing retardation parameter ϑ

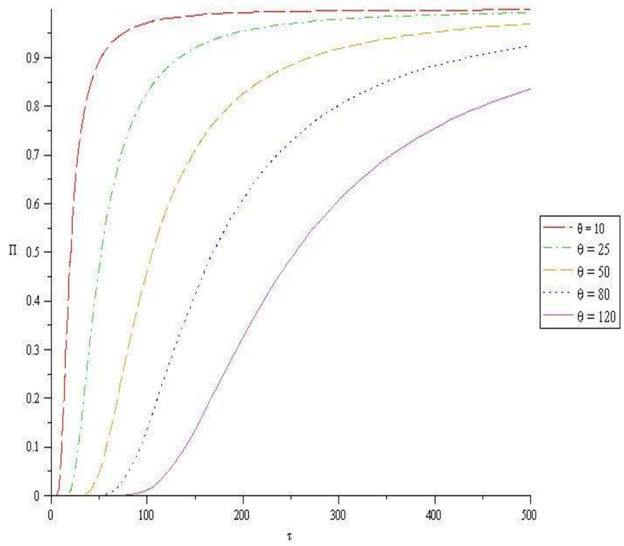
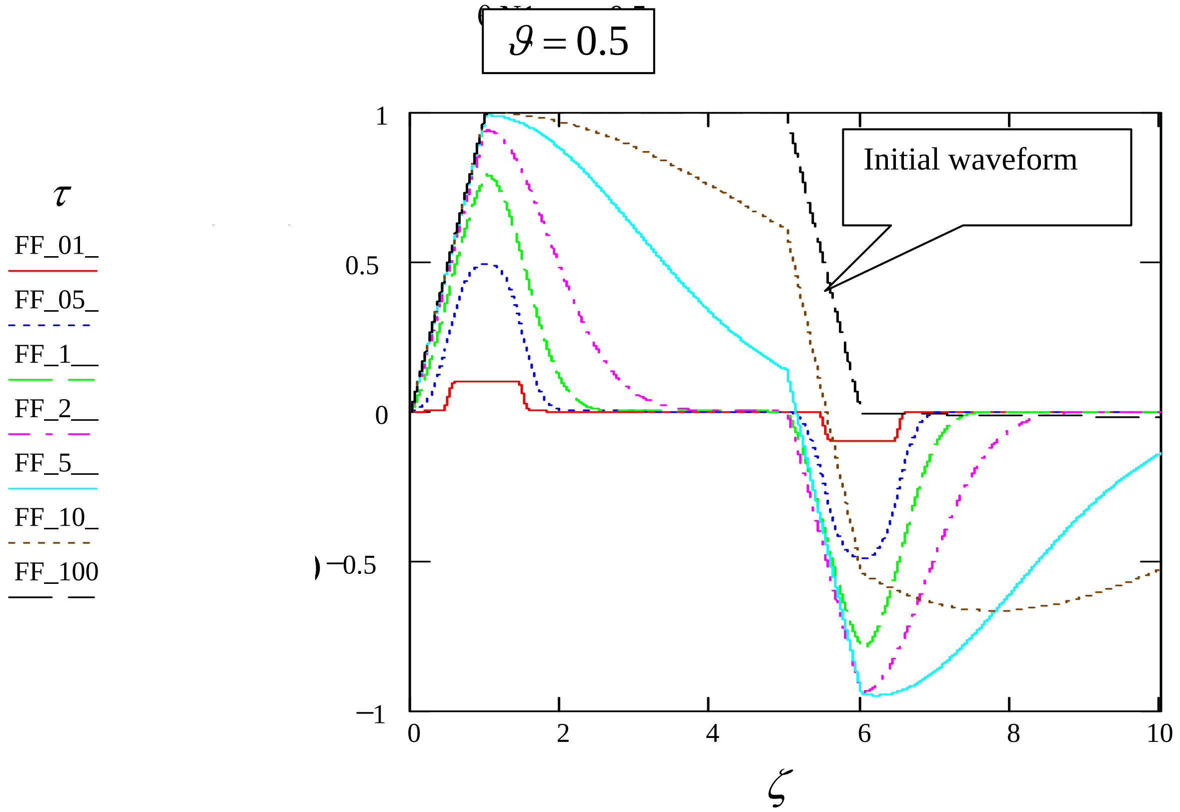


Fig. 5

Elastic precursor amplitude with the growing relaxation parameter τ

WAVEFORM RELAXATION IN THE TRANSITION REGIME



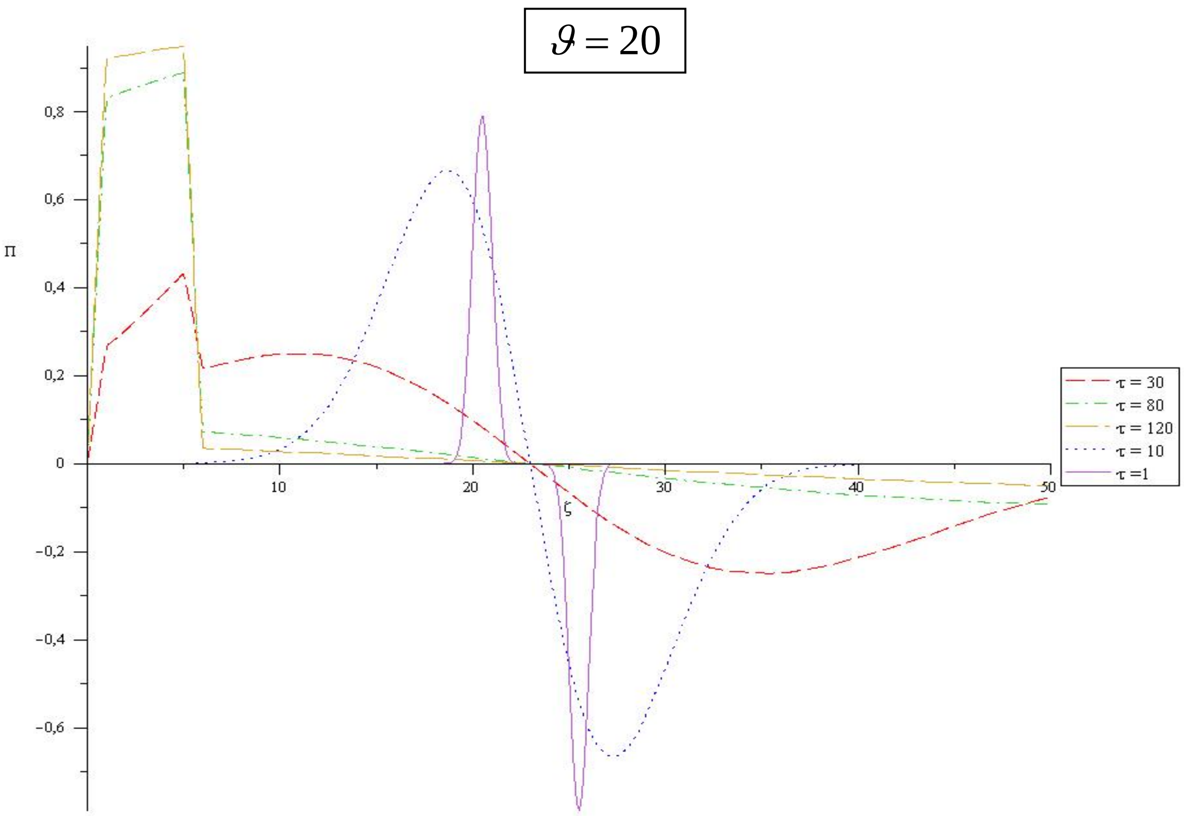


Fig. 6 a,b

MASS VELOCITY DISPERSION

The difference $\mathrm{E}^e - \mathrm{E} = \mathrm{E}^d$ – pulsation energy

$$\frac{\partial \mathrm{E}^d}{\partial \zeta} - \left[v(\zeta,\xi_0) - v(\zeta,\xi) \right] \frac{\partial v}{\partial \zeta}(\zeta,\xi_0) = 0$$

Near stable state small velocity pulsations result in dissipation

$$v(\zeta,\xi_0) - v(\zeta,\xi) \approx v(\zeta,\xi_0) - v(\zeta-\theta,\xi_0) \approx \theta \frac{\partial v}{\partial \zeta}(\zeta,\xi_0)$$

$$\frac{\partial \mathrm{E}^d}{\partial \zeta} = \theta \left[\frac{\partial v}{\partial \zeta}(\zeta,\xi_0) \right]^2$$

Far from equilibrium, in structure unstable state, instead of the heat energy a velocity dispersion is introduced

$$\mathrm{E}^d = D^2/2 = \langle v^2 \rangle - \langle v \rangle^2$$

$$\frac{\partial D^2/2}{\partial \zeta} = \left[v(\zeta,\xi_0) - v(\zeta,\xi) \right] \frac{\partial v}{\partial \zeta}(\zeta,\xi_0)$$

Integration over the rise-time results the relationship on the pulse plateau

$$D^2 \Big|_{pl} = 1 - 2 \int_0^{\zeta_{pl}} d\zeta\, v(\zeta,\xi) \frac{\partial v}{\partial \zeta}(\zeta,\xi_0)$$

The velocity dispersion on the pulse plateau determines the experimentally measured wave amplitude loss in structure unstable state while in stable state no loss is observed

$$D^2 \Big|_{pl} = 1 - 2 \int_0^{\zeta_{pl}} d\zeta\, v(\zeta,\xi_0) \frac{\partial v}{\partial \zeta}(\zeta,\xi_0) = 1 - 1 = 0$$

Near stable state for stationary waveform $D_{\max} \sim \frac{\partial v}{\partial \zeta}\Big|_{\max}$

STRUCTURE FORMATION AND STORIED ENERGY

According to the 1st law of thermodynamics the integral over the whole waveform determines the relation between the integral entropy production and potential energy after the wave propagation

$$T\Delta S - \Delta E = \int_0^\infty d\zeta \int_0^{\omega(\zeta)} d\zeta' \exp\left\{-\frac{\pi\left(\zeta'-\zeta+\theta(\xi)\right)^2}{\tau^2(\xi)}\right\} \frac{\partial v}{\partial \zeta'}(\zeta',\xi_0)\frac{\partial v}{\partial \zeta}(\zeta,\xi_0)$$

If potential energy after the wave $\Delta E = 0$, the integral entropy production $T\Delta S > 0$ defines a surface above the model parameters plane $\Psi(\tau,\theta,\Delta S)=0$, which looks like a mountain with a top in structure unstable state. $T\Delta S \xrightarrow[\tau\to 0]{} \tau\int_0^\infty d\zeta\left[\frac{\partial v}{\partial \zeta}(\zeta,\xi_0)\right]^2 \to 0$

According to speed-gradient algorithm phase trajectories tend down surface both to the hydrodynamic limit and back to the solid state depending on initial state.

If no dissipation takes place $T\Delta S = 0$ and the full energy is conserved the the elastic wave is not damping.

$$\int_0^\infty d\zeta \int_0^{\omega(\zeta)} d\zeta' \exp\left\{-\frac{\pi\left(\zeta'-\zeta+\theta(\xi)\right)^2}{\tau^2(\xi)}\right\} \frac{\partial v}{\partial \zeta'}(\zeta',\xi_0)\frac{\partial v}{\partial \zeta}(\zeta,\xi_0) \xrightarrow[\tau\to\infty]{}$$

$$\to \int_0^\infty d\zeta\, v(\zeta',\xi_0)\frac{\partial v}{\partial \zeta}(\zeta,\xi_0) = 0$$

However, in a resonance case when impactor's length coincides with $l \approx \theta\tilde{N}$

$$-\Delta E = \int_0^\infty d\zeta \int_0^{\omega(\zeta)} d\zeta' \exp\left\{-\frac{\pi\left(\zeta'-\zeta+\theta(\xi)\right)^2}{\tau^2(\xi)}\right\} \frac{\partial v}{\partial \zeta'}(\zeta',\xi_0)\frac{\partial v}{\partial \zeta}(\zeta,\xi_0) < 0$$

potential energy stays frozen after the wave propagation as storied energy $\Delta E > 0$ or $T\Delta S < 0$ in new shear-vortex structures due to self-organization.

ENTROPY PRODUCTION SURFACE

Integral entropy production surface for the initial pulse presented on Fig. 6 has a form in the phase space of the parameters (τ, ϑ) as on Fig. 7.

For a long pulse (~100) it has a form presented on Fig. 8.

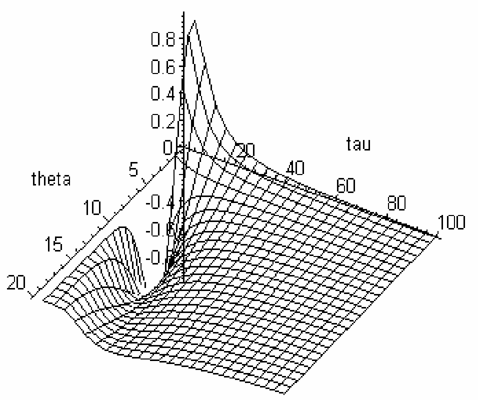


Fig. 6.

Duration ~ 5

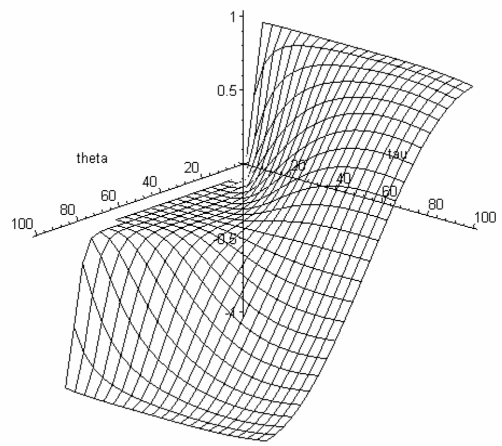


Fig. 7.

Duration ~ 100

According the Speed-gradient Eq. (3) the phase points (τ, ϑ) can move down the surface. The surface has a hole with negative entropy production values which arise in a resonance case when the pulse duration coincides to the retardation time. The resonance results new structure self-organization at mesoscale inside the front that can stay frozen in the medium after the front. The wave-vortex mesoscale structures are observed in experiments.

EXPERIMENTAL CONFIRMATION

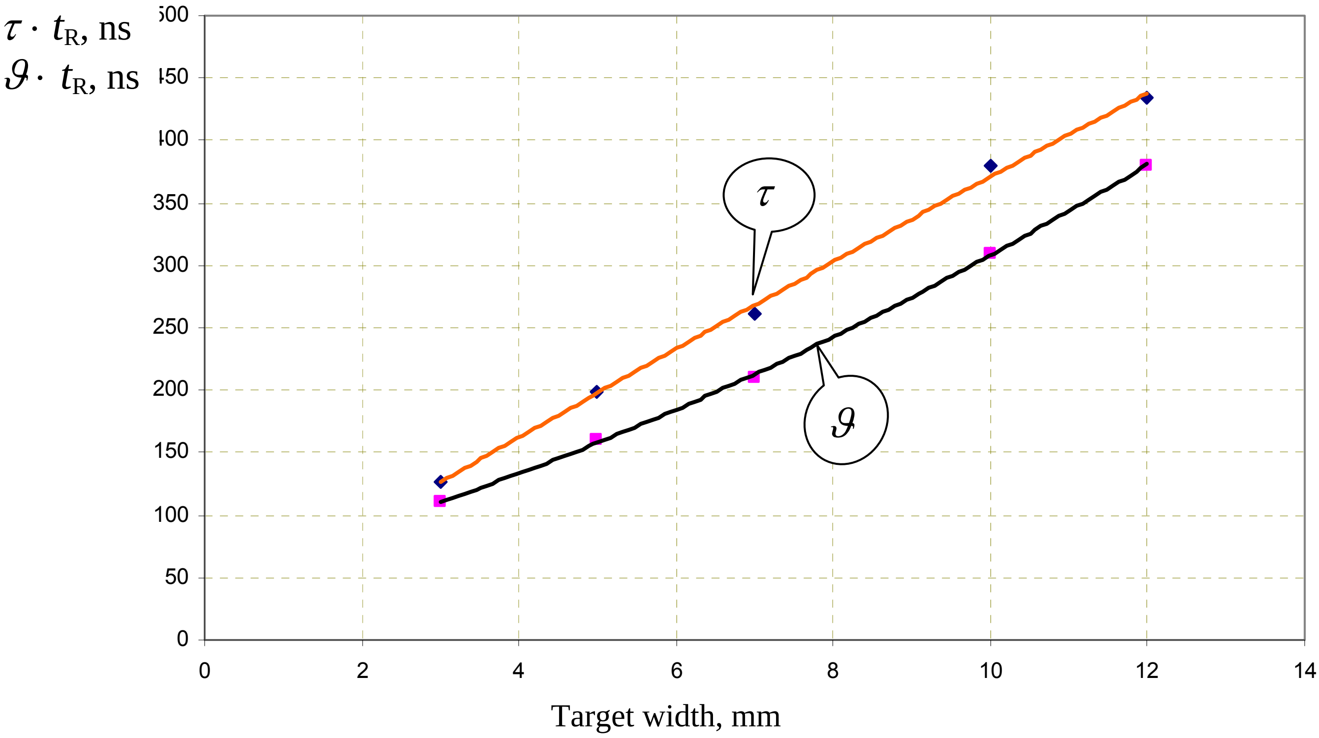


Fig. 9. Experimental data on the phase evolution during wave propagation

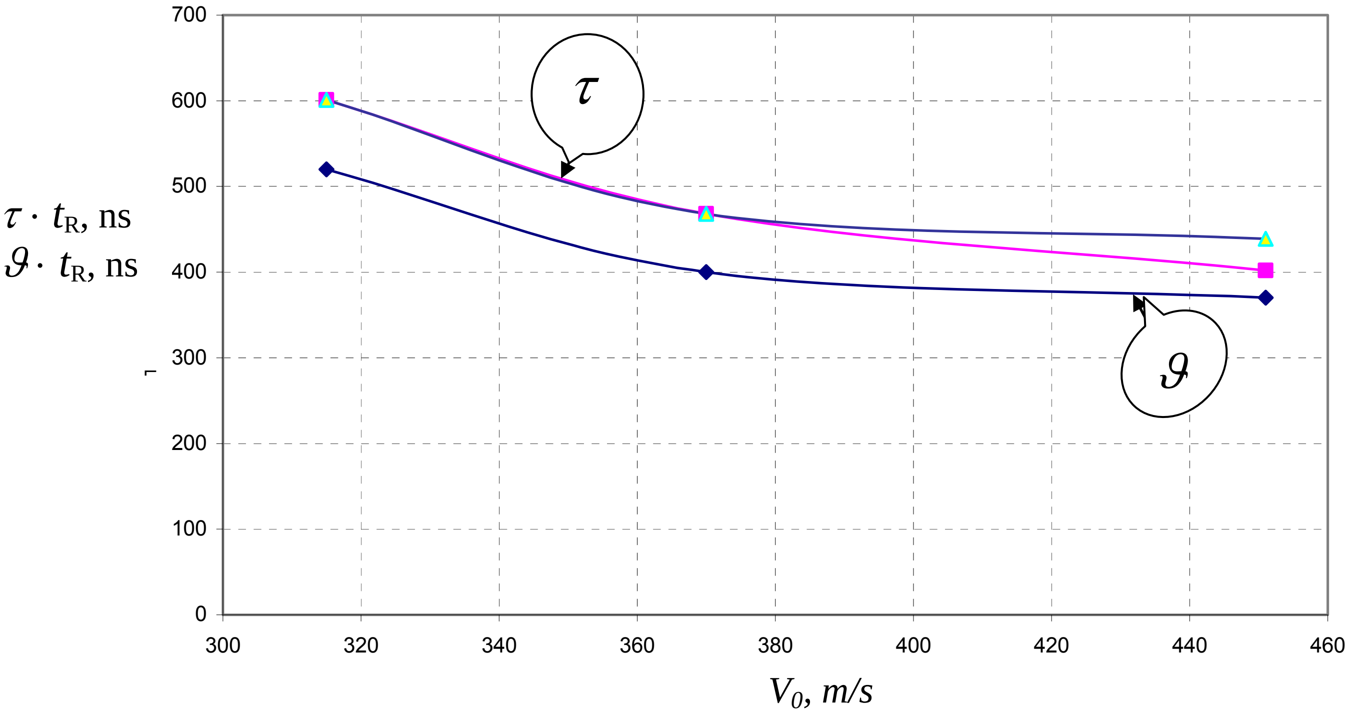


Fig. 10. Experimental data on the phase state depending on the shock velocity V_0

CONCLUSIONS

- Nonstationary wave description requires correlation dynamics involved.

- Nonlocal model allows constitutive relationships between macroscopic medium reaction to loading and its internal medium structure evolution in the transition regimes.

- Internal control at mesoscale structure is an especial feature of dynamic processes.

- The internal control goal and evolution direction is minimum of the integral entropy production in the wave.

- Synergetic shear-vortical formation at mesoscale after the wave front is originated by the resonance conditions between the loading pulse waveform and retardating medium reaction.

- External control via medium loading on the base of nonlocal theory can be used for developping new technologies to obtain nanostructures in volume.