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On Structural Transformations in a Material under Nonstationary Actions

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Abstract—A model of material of complex crystalline structure consisting of two lattices coupled by nonlinear interaction forces that ensure several stable equilibrium configurations is considered. The continuum model is compared with the discrete model whose analysis reveals the effect, which has been observed in high-speed deformation experiments, of decrease in the initial pulse under nonstationary actions.

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1. INTRODUCTION. STATEMENT OF THE PROBLEM

In numerous studies of shock wave loading [1, 2], it was discovered that, in a certain velocity range, a sufficiently significant part of the energy is consumed by structural transformations of the material. At the microlevel, the loss of energy is manifested in a decrease in the maximum value of the velocity on its time profile, which is the main characteristic of the dynamic response of the material to the impulse action [3]. The goal of the present paper is to develop a model whose permits demonstrating how the internal structure can affect the system dynamics. To this end, we consider a one-dimensional two-component medium [4, 5] consisting of two crystal lattices close in their physical properties and coupled by a nonlinear interaction force. It is natural to assume that the analytic expression for the force of interaction between the components contains two terms the first of which is determined by the nonlinearly elastic constraint between the components and the second is the dissipative component,

$$R = R_1(u_1 - u_2) + R_2(\dot{u}_1 - \dot{u}_2), \tag{1.1}$$

where u_i (i = 1, 2) is the displacement of each of the components. When choosing R_1 and R_2 , it is required to take into account the possibility of material transition between states. This means that the nonlinearly elastic relation must have a nontrivial stable equilibrium. Moreover, the interaction force must reflect the periodicity of the complex lattice whose structure does not vary in the case of mutual displacements of the components by a value multiple of the period *d*. It follows that one of the simplest versions of setting the force is the expression

$$R = K\sin(\lambda z) + \nu \dot{z},\tag{1.2}$$

where the parameter *K* determines the maximum value of the interaction force and the coefficient ν characterizes the dissipation. The role of the internal degree of freedom to which the energy can be transferred in a certain range of actions is played by the relative displacement of the lattices $z = u_1 - u_2$, while the measured microparameter is the displacement $U = (\rho_{10}u_1 + \rho_{20}u_2)/(\rho_{10} + \rho_{20})$ of the center

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of mass [6]. We assume that the Hooke law $sigma_i = E_i \partial u_i / \partial x$ (i = 1, 2), where σ_i is the stress and E_i is the Young modulus, is satisfied for each of the components. Then, after introducing the dimensionless variables

$$\tilde{x} = \frac{x\omega}{c_1}, \quad \tilde{t} = \omega t, \quad \tilde{U} = U\lambda, \quad \tilde{z} = z\lambda, \quad \tilde{\sigma} = \frac{c_1\lambda\sigma}{\omega^*(E_1 + E_2)}, \quad \tilde{\nu} = \frac{\nu\omega^*}{K\lambda},$$

where $\omega^* = c_1 \sqrt{(1 - \chi \delta) K \lambda / (1 - \chi \delta) E_1}$ and $\sigma = \sigma_1 + \sigma_2$, the equations of the medium become

$$\frac{\partial^2 U}{\partial \tilde{x}^2} - \frac{1}{c_u^2} \frac{\partial^2 U}{\partial \tilde{t}^2} = \alpha \frac{\partial^2 \tilde{z}}{\partial \tilde{x}^2},$$

$$\frac{\partial^2 \tilde{z}}{\partial \tilde{x}^2} - \frac{1}{c_z^2} \frac{\partial^2 \tilde{z}}{\partial \tilde{t}^2} = \sin \tilde{z} + \tilde{\nu} \dot{\tilde{z}} + \delta \frac{\partial^2 \tilde{U}}{\partial \tilde{t}^2}.$$
(1.3)

Here we have used the notation

$$A_u^2 = \frac{(1-\chi\delta)}{1-\delta}, \quad A_z^2 = \frac{1}{1-\chi\delta}, \quad \alpha = \frac{(1-\chi)\chi\delta}{1-\chi\delta}$$

By $c_1 = \sqrt{E_1/\rho_1}$ we denote the speed of sound in the first lattice, and by $c_2 = \sqrt{E_2/\rho_2}$ we denote the speed of sound in the second lattice. The coefficient $\chi = \rho_1/(\rho_1 + \rho_2)$ is the mass fraction of the first component, and the small parameter $\delta = 1 - c_1^2/c_2^2$ characterizes the weak distinction between the physical properties of the lattices. For $\delta = 0$, they coincide completely. In what follows, we assume that $\chi = 1/2$ and $\delta = 0.1$. Equations (1.3) with zero initial conditions are considered in the semi-infinite domain $0 \leq \tilde{x} < \infty$, on whose boundary the stress is given as a rectangle pulse $\sigma_{\rm imp}(t) = \sigma_0[H(t) - H(t - t_0)]$ of duration t_0 . Here H(t) is the Heaviside function. Under the assumption that the stresses on the boundary are distributed proportionally to the component densities, the boundary conditions for x = 0 have the form

$$\frac{\partial \tilde{U}}{\partial \xi}\Big|_{\xi=0} = \tilde{\sigma}_{\rm imp}(\tilde{t}) \left[1 + \frac{\chi(1-\chi)\delta^2}{1-\delta} \right], \quad \frac{\partial \tilde{z}}{\partial \xi}\Big|_{\xi=0} = \frac{\tilde{\sigma}_{\rm imp}(\tilde{t})\delta}{1-\delta}.$$
(1.4)

At infinity, we pose the standard conditions $\tilde{U}|_{\xi\to\infty}$ and $\tilde{z}|_{\xi\to\infty} = 0$. Obviously, an analytic solution of system (1.3) can hardly be constructed because of the nonlinear term. In this case, numerical procedures are used as a rule, but their use is rather complicated, because it is required to determine the parameters and the time at which the system comes to the desired state. In this connection, it is necessary to have approximates analytic formulas to be able to predict, at least qualitatively, the dynamics of the model and separate the physics of the process from the effects due to the numerical approximation.

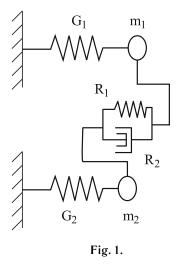
2. DISCRETE MODEL

The structural reconfiguration dynamics can be described by the variable interval method [7]. In this method, just as in the Galerkin method, the solution of the differential equation is sought as an expansion in forms, but, in contrast to the classical solution, the length of the interval is an unknown function of time. In the case of hyperbolic equations, the interval is usually the domain where the material is under perturbations. This approach turns out to be fruitful for constructing approximate analytic solutions of nonstationary problems. As a result, the continual problem reduces to solving dynamic equations for an element of the continuum in discrete representation. In the case of one-component medium, such an element is the spring pendulum, but in the case under study, it is a system of two coupled oscillators (shown in Fig. 1) with nearly the same natural frequencies. If the masses m_1 and m_2 coincide, then their behavior is described by the system of equations

$$\ddot{x} + x = \frac{\delta z}{4},$$

$$\ddot{z} + n\dot{z} + z + \kappa \sin z = \delta x.$$
(2.1)

The quantities $x = (x_1 + x_2)/2$ and $z = x_1 - x_2$ were introduce by analogy with Eqs. (2.1). The differentiation in (2.1) is carried out with respect to the dimensionless time $\tau = \omega_1 t$, where $\omega_1 = \sqrt{G_1/m_1}$



is one of the partial frequencies. The small parameter $\delta = (\omega_2^2 - \omega_1^2)/\omega_1^2$ is their relative difference. The coefficient κ of the nonlinear term is proportional to the ratio of the spring rigidity characterized by the modulus E_1 to the rigidity of the constraint between the components. In what follows, we assume that it is equal to the minimum value ($\kappa = 1$), which ensures that the energy is nonconvex in the displacement. To push the system away from the equilibrium, we assume that the initial velocity of the center of mass V_0 is different from zero. For small velocities, there is no interaction between x and z, but starting from some critical value of V_0 , the qualitative picture becomes different. The development of vibrations of x in the time, which is obtained by numerical integration of system (2.1) for n = 0.022, is shown in Fig. 2 (for $V_0 = 10$ and $\delta = 0.1$) by the dashed line. For a sufficiently large value of V_0 , a typical characteristic of the dynamic process is the existence of a time τ_* separating the two vibration modes. At the first stage, the element behaves as a linear oscillator with nearly the same frequencies. After the transient process is finished, its dynamics is also slightly different from the dynamics of a linear system with the frequency mismatch. This means that the nonlinear system is significant only on a narrow time interval. We assume that the work of this force is done directly at the point τ_* . Then the nonlinear term becomes $\kappa_0 \sin z \delta_0(\tau - \tau_*)$, where $\delta_0(\tau)$ is the delta function. The parameter κ_0 is chosen so as to change the beating of the center of mass into vibrations with a single frequency. On the one hand, this approach preserves the basic laws of the initial problem, and on the other hand, it allows one to obtain an analytic expression for the displacement of the center of mass, which will be used to analyze the continual model. This problem can be treated as a search for a control that permits changing the system response to the pulse by a timely action. The parameters κ_0 and τ_* can be determined by using the Laplace transform $f^L = \int_{-\infty}^{\infty} f(\tau) e^{-p\tau} d\tau$. Under the above assumptions with neglect of the viscous friction, the solution of

system (2.1) in the space of transforms has the form

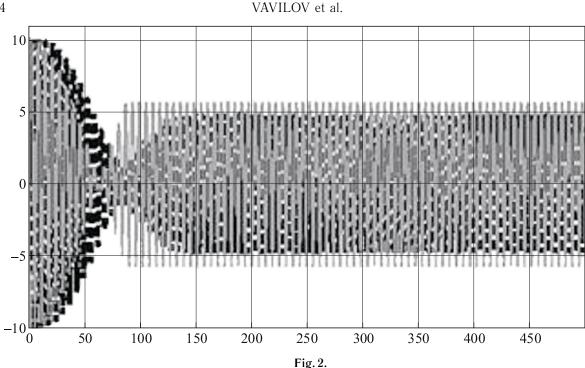
$$x^{L}(p) = \frac{(p^{2}+1)V_{0} - \delta/4\kappa_{0}\sin z(\tau_{*})e^{-p\tau_{*}}}{(p^{2}+1)^{2} - \delta^{2}/4},$$

$$z^{L}(p) = \frac{V_{0}\delta - (p^{2}+1)\kappa_{0}\sin z(\tau_{*})e^{-p\tau_{*}}}{(p^{2}+1)^{2} - \delta^{2}/4}.$$
(2.2)

To switch the center of mass from beating to a harmonic process, it is necessary to preserve only one natural frequency in the system. This can be done by assuming that one of the poles in the expression for $x^{L}(p)$ is a root of the numerator. As a result, this condition implies the following expressions for the desired parameters:

$$\tau_* = \frac{\pi k}{1 - \varepsilon/4},\tag{2.3}$$

$$\kappa_0 \sin z(\tau_*) = (-1)^{k+1} 2V_0, \tag{2.4}$$



where k denotes an unknown positive integer, which can be determined from the energy balance. For the chosen parameter values, one has k = 27. The analytic solution obtained by determining the inverse Laplace transform from $x^{L}(p)$ is depicted in Fig. 2 by the solid line. One can see that it agrees well with the results of numerical calculations.

3. CONTINUAL MODEL

After the process of energy transfer from the center of mass to the relative displacement was illustrated by an example of oscillator, it is logical to expect that a similar effect also takes place in the continual model. But there arise several additional questions as we pass to the continuum. First, it is necessary to determine the distance at which the structural changes start. To estimate this parameter is an important problem for both the experiment and the numerical simulation. To solve this problem, we apply the variable interval method to Eqs. (1.3) and seek their solution in the form

$$\tilde{U} = \sum_{n=1}^{N} Q_n(\tilde{t}) \cos \frac{\pi (2n+1)\xi}{2l} H(l-\xi), \quad \tilde{z} = \sum_{n=1}^{N} q_n(\tilde{t}) \cos \frac{\pi (2n+1)\xi}{2l} H(l-\xi).$$

Multiplying by the form and integrating from 0 to l = t, where t is the interval length, we obtain the following system of equations for the functions Q(t) and q(t):

$$\ddot{Q} + \Omega^2 Q = \frac{\Omega^2 \delta q}{4} - \frac{2\sigma_{\rm imp}(t)}{lm^2},$$

$$\ddot{q} + \nu \dot{q} + \Omega^2 q + 2J_1(q) = -\delta \ddot{Q} - \frac{2\sigma_{\rm imp}\delta}{l},$$
(3.1)

where $\Omega = \pi (2n+1)/(2l)$ is the frequency corresponding to its own form. By $J_1(q)$ we denote the Bessel function of the first kind. After eliminating the term \ddot{Q} from the second equation and introducing a new variable $\tau = \Omega t$, system (3.1) becomes

$$\ddot{Q} + Q = \frac{\delta q}{4} - \frac{2\sigma_{\rm imp}(\tau/\Omega)}{\Omega^2 lm^2},$$

$$\ddot{q} + \frac{\nu}{\Omega} \dot{q} + q + \frac{2}{\Omega^2} J_1(q) = \delta Q.$$
(3.2)

These equations do not practically differ from the equations of the discrete model, and hence all the above arguments, which permit obtaining an analytic formula showing the decrease in the oscillation amplitude of the center of mass due to the dynamics of internal displacements, can be applied to them. By analogy with coupled oscillators, we can conclude that, for a weak pulse lower than the critical value and associated with small relative displacements, there is no energy transfer from the center of mass to another degree of freedom and the waves move in the material without noticing its internal structure. In the discrete model, the time τ_* of switching from the beating regime to vibrations with a single frequency was determined after replacing the initial problem by the linear one, where the interaction force acts not during a small time interval but directly at the point τ_* . In this case, we neglect the viscous friction force and prescribe the initial velocity instead of the impulse action on the center of mass. Let us make the same transformations with Eqs. (3.2). If we have the delta function $\delta_0(ax) = \delta_0(x)/a$ for the change of variables, they can be reduced to the form

$$\ddot{Q} + Q = \frac{\delta q}{4} - \frac{2\sigma_0\delta_0(\tau)}{\Omega lm^2},$$

$$\ddot{q} + q + \frac{2}{\Omega^2}J_1(q)\delta_0(\tau - \tau_*) = \delta Q.$$
(3.3)

The parameter τ_* was determined in the discrete model from condition (2.3) saying that one of the natural frequencies is damped. This condition is here preserved, while the analog of relation (2.4) becomes

$$-\frac{2\sigma_0}{l} = \frac{(-1)^k J_1(q_z^*)}{\Omega}, \quad k = 1, 2, \dots,$$
(3.4)

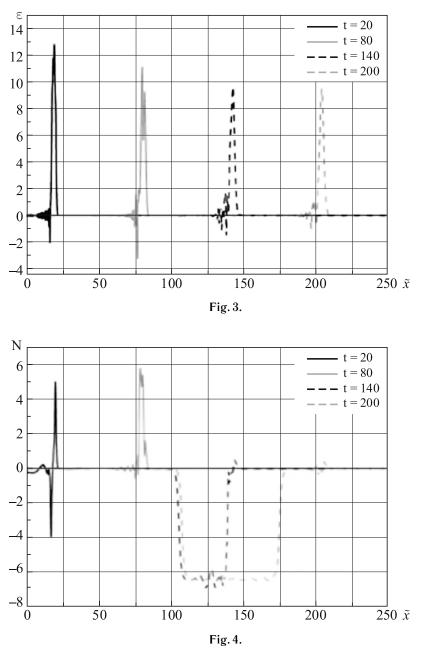
where $q_z^* = q_z(\tau_*)$. In this relation, the role of the parameter κ_0 , which determines the pulse value required to transfer the two-degree oscillator dynamics from one mode into another, is played by the distance l_* at which the motion of the center of mass starts to change due to the influence of the relative displacement. To estimate this distance, we multiply the last relation by $1/t_*$ under the assumption that the discrete model has a parameter similar to τ_* . With regard to the new variable $\tau = \Omega t$ and the interval l = tfor $\sigma_0 < \tau_*$, relation (3.4) implies

$$t_* = \tau_* \sqrt{-\frac{(-1)^k}{\sin(\frac{1}{4}\delta\tau_*)\cos\tau_*}}.$$
(3.5)

By substituting the numerical values $\delta = 0.1$ and k = 27 from the discrete model into (3.5), we determine $t_* \approx 137$. This result is confirmed by numerical integration of system (1.3) by the finite difference method for $\nu = 0.022$. Figure 3 (for $\sigma_0 = 11$ and $\tilde{t}_0 = 3$) shows the strain distribution $\varepsilon = \partial \tilde{U} / \partial x$ over the length, which demonstrates the decrease in the amplitude of input signal due to the structural transformations in the material, which, in this model, is associated with the transition of the relative displacement to a new equilibrium (Fig. 4).

4. CONCLUSION

The main result in this paper is the development of a mechanical model describing the reconfiguration of the material crystal structure due to dynamic actions. At the macrolevel, this process is manifested as the energy transfer from the system center of mass to an internal degree of freedom whose role is played by the relative displacement of the components. In the framework of this model, we considered the nonstationary problem of a rectangular pulse propagation in a complex structure consisting of two crystal lattices close in their physical properties and coupled by a nonlinear interaction force. It was analyzed by comparing the equations of motion of the continuum with the dynamics of their discrete analog, thus estimating the duration of structural transformations, which is very important for the numerical calculation. The latter was carried out on the basis of the finite difference method, which allowed revealing the transition of the system to a new equilibrium, which does not disappear after the termination of the external action.



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