

NUMERICAL MODELING OF COMPRESSION
AND RAREFACTION WAVES IN METALS

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Various possibilities are considered for mathematical description of the behavior of media during dynamic deformation with both elastoplastic [1-7] and nonlinear viscoelastoplastic models considering microstructural plasticity mechanisms [8-11].

1. Basic Equations and Relationships Defining the Process. The medium through which compression and rarefaction waves propagate will be assumed isotropic. The state of this medium is characterized by a distribution of deformation tensors ϵ_i and stress tensors σ_i , a velocity vector u , and an internal energy E . Here $i = 1, 2, 3$ are the major axes of the stress and deformation tensors. We write the deformation increment tensor in the form of a sum $\dot{\epsilon}_i = \dot{\epsilon}_i^e + \dot{\epsilon}_i^p$ where ϵ_i^e , ϵ_i^p are the elastic and plastic deformation tensors, respectively. Elastic deformation is characterized by the expression $\dot{\sigma}_i = \lambda \dot{\delta} + 2\mu \dot{\epsilon}_i^e$ ($i = 1, 2, 3$), where $\dot{\delta} = \sum_{i=1}^3 \dot{\epsilon}_i$; λ and μ are Lamé parameters and the plastic components satisfy the condition $\sum_{i=1}^3 \dot{\epsilon}_i^p = 0$. The dot denotes the time derivative along the trajectory of an element of the medium.

The relationships for the increment in hydrostatic pressure, the maximum value of tangent stress, and the major value of the plastic deformation tensor have the form

$$\dot{p} = \frac{\dot{\sigma}_1 + 2\dot{\sigma}_2}{3}, \quad \dot{\tau} = \frac{\dot{\sigma}_1 - \dot{\sigma}_2}{2}, \quad \dot{\epsilon}^p = \frac{\dot{\epsilon}_1^p - \dot{\epsilon}_2^p}{2} = \frac{3}{4} \dot{\epsilon}_1^p.$$

Considering a state of uniaxial stress, where

$$\dot{\sigma}_2 = \dot{\sigma}_3 = 0, \quad \dot{\sigma}_1 \neq 0, \quad \dot{\epsilon}_1 \neq 0, \quad \dot{\epsilon}_2 = \dot{\epsilon}_3 \neq 0.$$

we find

$$\dot{\epsilon}_2^e = -\frac{\lambda}{2(\lambda + \mu)} \dot{\epsilon}_1^e, \quad \dot{\sigma}_1 = E_0 \left(\dot{\epsilon}_1 - \frac{4}{3} \dot{\epsilon}^p \right), \quad E_0 = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu},$$

$$\dot{\tau} = \dot{\sigma}_2/2, \quad P = \dot{\sigma}_1/3.$$

Similarly, for the uniaxially deformed state

$$\dot{\epsilon}_2 = \dot{\epsilon}_3 = 0, \quad \dot{\epsilon}_1 \neq 0, \quad \dot{\sigma}_1 \neq 0, \quad \dot{\sigma}_2 = \dot{\sigma}_3 \neq 0$$

we obtain

$$\dot{\sigma}_1 = (\lambda + 2\mu)\dot{\epsilon}_1 - (8/3)\mu\dot{\epsilon}^p, \quad \dot{\sigma}_2 = \lambda\dot{\epsilon}_1 - (4/3)\mu\dot{\epsilon}^p,$$

$$\dot{\tau} = \mu(\dot{\epsilon}_1 - 2\dot{\epsilon}^p), \quad \dot{p} = K\dot{\epsilon}_1, \quad K = (3\lambda + 2\mu)/3. \quad (1.1)$$

In the motion of a continuous medium the laws of conservation of mass, momentum, and energy must be fulfilled, which in Lagrangian coordinates (h) have the form

$$\partial \epsilon_1 / \partial t = -\partial u / \partial h, \quad \rho_0 \partial u / \partial t = -\partial \sigma_1 / \partial h, \quad \rho_0 \partial E / \partial t = \sigma_1 \partial \epsilon_1 / \partial t. \quad (1.2)$$

where t is time and ρ_0 is the initial density of the medium. Deformation and stress are defined as positive for the compressed state. Depending on the actual problem considered, it is necessary to choose the corresponding uniaxial state.

System (1.2), describing the processes of propagation and interaction of compression and rarefaction waves, is not complete. Since in the future we will be considering propagation of strong shock waves in metals, following [12, 13] we will write the caloric equation of state in additive form [14]

$$p = p_x + p_R + p_e, E = E_x + E_R + E_e, \quad (1.3)$$

where

$$p_x = \frac{k}{\gamma} [(\rho/\rho_0)^\gamma - 1]; E_x = \int_{\rho_0}^{\rho} p_x(\rho) d(1/\rho);$$

$$p_R = \Gamma_R E_R \rho; E_R = c_V(T - T_0) + E_0;$$

$$p_e = \Gamma_e E_e \rho; E_e = \frac{1}{2} \beta_0 (\rho_0/\rho)^{\Gamma_e} T^2.$$

Here Γ_R is the Grüneisen parameter, which in the general case may depend upon $v = 1/\rho$; Γ_e , a coefficient defining the ratio of thermal electron pressure to electron thermal energy density; c_V , specific heat; k , γ , E_0 , β_0 , constants characterizing the properties of the given medium.

To evaluate the relative effect of the components appearing in Eq. (1.3), these relationships were calculated for shock waves in aluminum, copper, iron, and lead. The initial state corresponded to $p = 0$, $T = 293^\circ\text{K}$, $\rho/\rho_0 = 0.987$. The Grüneisen coefficient in this case is calculated with the formula of [12], for $E_0 = 0.161 \text{ J/g}$, $k = 764 \text{ kbar}$, $\gamma = 4.1$, $\beta_0 = 0.5$, $\Gamma_e = 0.5$, $p = 1 \text{ atm}$, $T = 20^\circ\text{C}$.

Analysis of the calculation results permits the conclusion that at loading rates $u_0 \leq 4 \text{ km/sec}$ the contributions of the thermal components to p and E may be neglected, which is not possible at higher interaction rates.

The mathematical model of the medium is completed by the equation of plastic flow, which defines the dependence of plastic flow velocity $\dot{\epsilon}^P$ on the remaining characteristics of the medium (in particular, the shear stress τ , temperature T , etc.).

Thus, for the uniaxial deformed state the following models may be employed:

hydrodynamic ($\tau = 0$)

$$\dot{\epsilon}^P = (1/2)\dot{\epsilon}_1;$$

elastic

$$\dot{\epsilon}^P = 0;$$

elastoplastic

$$\dot{\epsilon}^P = (1/2)(\dot{\epsilon} - \dot{Y} \mu) \text{ for } \tau \geq Y,$$

$$\dot{\epsilon}^P = 0 \text{ for } \tau < Y,$$

where Y , the yield point of the medium, may be a function of ρ , p , T , $\dot{\epsilon}^P$ and the other parameters of the medium. Thus, for $Y = Y_0 = \text{const}$ we have an ideally plastic model

$$\tau = \begin{cases} \mu(\dot{\epsilon} - 2\dot{\epsilon}^P), & \tau < Y_0, \\ Y_0, & \tau \geq Y_0; \end{cases}$$

the dislocation model

$$\dot{\epsilon}^P = b N_d v_d,$$

where b is Burgers vector; $N_d = \varphi(\dot{\epsilon}^P)$, mobile dislocation density; $v_d = \Phi(\tau, p, E)$ dislocation displacement rate. The actual forms of the functions φ , Φ and Y will be established below.

2. Mathematical Formulation of the Problem of Collision of Two Plates. Method of Solution. The problem of collision of two plates is the model problem whose solution provides information on the dynamic compressibility of a material and the interaction of shock waves with unloading waves. On the other hand, the processes occurring upon collision of two plates are easily realizable in experiment.

Let a plate of thickness l collide normally at a velocity u_0 upon the surface of another plate with thickness $L \gg 1$. We choose the plate length much greater than the thickness, permitting study of the physical process in the one-dimensional approximation. In the general case the materials from which the two plates are constructed may differ.

Thus, the given problem can be formulated mathematically as follows: One must find functions $u, \sigma_1, \varepsilon_1, \varepsilon^p, \sigma_2, \tau, p, E, T \in C^1(D_Z)$, which in the region $D_Z = \{-l \leq h \leq L, 0 \leq t < \infty\}$ satisfy the system of differential equations (1.1)-(1.3) and one of the functions $\varepsilon^p(\tau, p, E)$ with initial

$$u = \begin{cases} u_0 > 0, & -l \leq h < 0, \\ 0, & 0 \leq h \leq L \end{cases}$$

and boundary conditions

$$\sigma_1(t, -l) = 0, \sigma_1(t, L) = 0, t > 0.$$

Only for very special equations of state can this problem be solved analytically, and the case of greatest practical interest was considered in [15]. A solution was obtained there with the approximation of smallness of the stress deviator components in comparison to the stress discontinuity on the shock wave front. In the general case analytic consideration of the problem is difficult. Thus, a numerical solution without limitations on the mathematical model of the medium or collision parameters is of interest. Such a numerical calculation was performed with Wilkins-type oblique counting difference scheme. The artificial viscosity was chosen in the form

$$q = \left(q_1 \rho_0 c_0 + q_2 \rho_0 \left| \frac{\partial u}{\partial h} \right| \right) \frac{\partial u}{\partial h}, \quad q_1 = q_1^0 \Delta h, \quad q_2 = \frac{q_2^0}{\alpha^2} (\Delta h)^2,$$

where Δh is the Lagrangian grid step; $q_1^0 = 0.2$; $q_2^0 = 5.0$.

The coefficients q_1^0 and q_2^0 were chosen to diffuse the shock fronts in three or four calculation cells without counting oscillations behind the wave front. Calculations revealed that the process of shock wave propagation and interaction depends not only quantitatively, but also qualitatively, on the mathematical model chosen. This is related foremost to the complex structure of the waves.

Calculations of this problem in the elastoplastic approximation by the algorithm described above for $\nu = \text{const}$ (Poisson coefficient), $K = p(\rho, T)/\varepsilon_1$, $Y = Y(p)$ and $Y = Y(\varepsilon^0)$ for aluminum show qualitative agreement in their wave patterns with the results of [6, 7, 15]. Collision velocity was varied over the range 0.1 to 5 km/sec.

3. Calculation Results. We will examine in greater detail the results obtained with the medium described by the dislocation model. Here the functions $\varphi(\varepsilon^p)$ and $\Phi(\tau, p, E)$ are taken in the form

$$\begin{aligned} \frac{dN_d}{dt} &= M |\dot{\varepsilon}^p|, \quad N_d|_{t=0} = N_0, \\ v_d &= \begin{cases} c_1 \exp\left(-\frac{\tau_1}{|\tau| - \tau^*}\right), & |\tau| > \tau^*, \\ 0, & |\tau| \leq \tau^*, \end{cases} \end{aligned} \quad (3.1)$$

where M is the dislocation multiplication coefficient (constant); c_1 , sonic shear velocity; τ_1 , creep coefficient; τ^* , threshold value of shear stress below which all dislocations in the medium are immobile. Equation (3.1) is generalized in comparison to previous expressions [8-10] in that it will be valid not only for loading, but also for unloading. It should be noted that the dislocation density will increase not only in a compression wave, but also in a rarefaction wave.

TABLE 1

Fig. No.	Striker parameters		hydrodynamic					Model elastoplastic				dislocation					
	u_0 , km/sec	l , mm	ρ_0	K	γ	E_0	c_T	F_R	ν	Y_0 , kbar	α_1	α_2	b , cm	N_0 , cm ⁻²	M , cm ⁻²	τ_1	τ^*
2	1,2	1,5	2,787	764	4,1	161	0,896	2,088	0,33	2,5	0,056	1,002	$2,86 \cdot 10^{-8}$	$3,75 \cdot 10^6$	$7,80 \cdot 10^{10}$	5,0	2,5
3	3,2	3,0															
4	5,4	2,0															

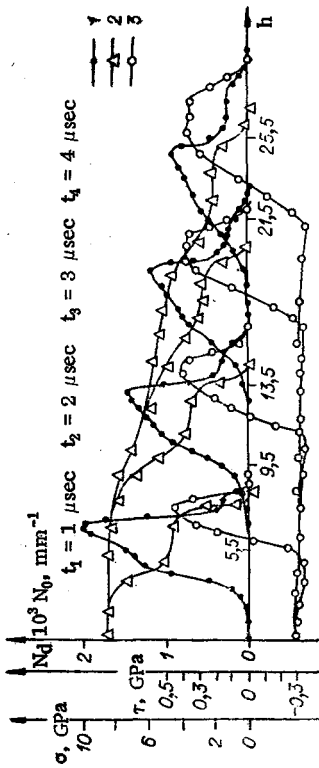


Fig. 1

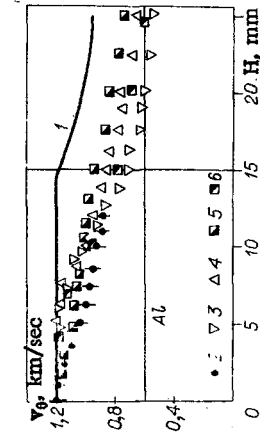


Fig. 2

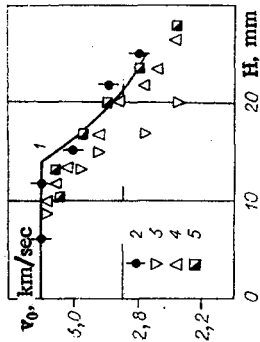


Fig. 3

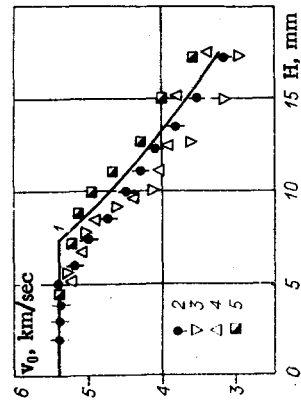


Fig. 4

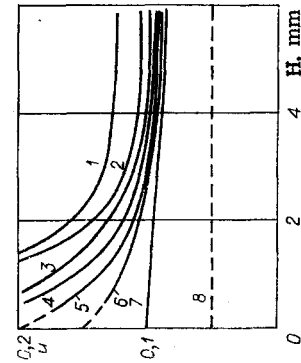


Fig. 5

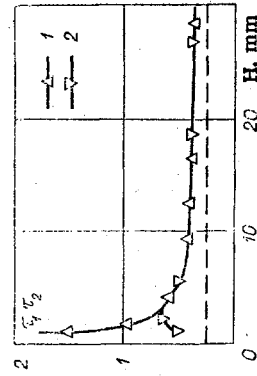


Fig. 6

Figure 1 presents profiles of the stress $\sigma_1 = \sigma_1(h)$ at various times (curve 1) for $u_0 = 1.2$ km/sec, $l = 1.5$ mm and material parameters: $b = 2.86 \cdot 10^8$ cm, $N_0 = 3.75 \cdot 10^6$ cm², $M = 7.8 \cdot 10^{10}$ cm², $c_1 = 3.2$ km/sec, $\tau^* = 2.5$ kbar, $\tau_1 = 5$ kbar, $\rho_0 = 2.787$ g/cm³. At the initial moment there propagate in different directions from the contact plane $h = 0$ shock waves of a two-wave structure, the forward fronts of which move at the rate of elastic waves, while behind these there propagate plastic compression waves which bring the medium parameters into their final state corresponding to the collision velocity. The plastic wave amplitude and velocity depend significantly on the collision velocity. Because of the plasticity delay effect, the transition to the plastic state of the medium is complicated by the fact that the stress in the elastic precursor exceeds Y_0 and varies with time.

From the free surface of the colliding plate ($h = -l$) the compression waves reflect elastic and plastic unloading waves. Since the elastic unloading wave propagates through material loaded previously, after a certain time interval it overtakes the front of the plastic compression wave. As a result of their interaction the amplitude of the plastic compression wave decreases, and the elastic loading wave is reflected from the plastic front in the form of an elastic compression wave which will move from the point of interaction in the direction of the plastic unloading wave. After this, this elastic wave interacts with the plastic unloading wave. As a result of this decay of the discontinuity, a reflected unloading wave develops, which again overtakes the plastic loading wave and decreases its intensity. At later times the entire process is repeated.

In the dislocation model of plastic deformation, due to plasticity delay the intensity of the elastic unloading wave will be higher than the intensity of that wave calculated in the elastoplastic approximation. This leads to more rapid damping of the plastic unloading wave front.

Simple experimental studies can be of great importance, since they permit not only development of a qualitative picture of the phenomenon, but also comparison with results of numerical experiments to determine the effect of the defining parameters of the mathematical model. Thus, the problem formulated above was calculated with four different mathematical models. Results showing the damping of the maximum velocity of the free surface of the plate as a function of its thickness are shown in Figs. 2-4. In all the models considered in Eq. (1.3) the contribution of electron components p_e and E_e was neglected in comparison to p_x , p_R and E_x , E_R . The plate material was assumed to be aluminum, although the same qualitative pattern obtains for copper and iron. In the ideal-plasticity model we assume $\nu = \lambda/2(\lambda + \mu) = \text{const}$, $K = (3\lambda + 2\mu)/3 = p(\rho, T)/\epsilon_1$, $Y = Y_0 = \text{const}$, while in the elastoplastic model with strengthening we take $Y = Y_0 + \alpha_1 p - \alpha_2 p^2$, where α_1 and α_2 are constants. The numerical values of the constants for the models of the striker and target plates are shown in Table 1.

In hydrodynamic theory (curve 1, Figs. 2-4) the damping process is of a monotonic character and commences later. This is because in this case the dissipative energy is less than in the other cases (points 2 are the results of experiments from [16-18]). The greatest quantitative divergence occurs in the range of relatively low collision velocities, i.e., in the loading rate range where effects due to the presence of shear stresses are most significant. Thus, even at $u_0 = 5.4$ km/sec all the mathematical models give similar results, i.e., within the limits of experimental error.

A comparison of the experimental data of [16-18] with results of calculations shows that the commencement of damping is determined significantly by the velocities of the elastic unloading and plastic loading fronts, while the amount of damping depends on the amplitude of the elastic unloading wave. Introduction of additional parameters α_1 and α_2 in the elastoplastic model with strengthening (points 3, Figs. 2-4) permits consideration of the dependence of the medium's mechanical properties upon pressure.

Thus, the pattern of shock wave damping upon interaction with the unloading wave is in better agreement with the experimental results than the hydrodynamic or ideal-plasticity models (points 4, Figs. 2-4). It is evident from the data of Figs. 2-4 that the damping process in the collision velocity range under consideration is described best by models which consider the physical theory of plasticity, i.e., dislocation models, described by Eq. (3.1) (points 5).

It should be noted that the generally accepted dislocation model is not a complete one from the physical viewpoint. Slippage of dislocations at a certain velocity v_d leads not only to plastic flow at the point under consideration, but also to displacement of the dislocation. As a result, the transition of the medium from the elastic to the plastic state can be accomplished not only by multiplication of dislocations, but also due to the presence of a flow of dislocations (diffusion of plasticity). For a mathematical description of dislocation kinetics one must consider the distribution of their slip velocities and Burgers vectors. In the simplest case the dislocation density may be represented as the sum of the densities of positive and negative dislocations,

having identical, but oppositely directed velocities, $N_d = N_+$ and N_- . We assume that multiplication of the dislocations of different signs occurs identically, and that they slip only in the plane of maximum tangential stress. This gives the following kinetic equations:

$$\begin{aligned} \frac{dN_+}{dt} + \frac{1}{\sqrt{2}} \frac{\partial}{\partial h} (N_- v_d) &= \frac{M}{2} \left| \frac{d\varepsilon^p}{dt} \right|, \\ \frac{dN_-}{dt} - \frac{1}{\sqrt{2}} \frac{\partial}{\partial h} (N_- v_d) &= \frac{M}{2} \left| \frac{d\varepsilon^p}{dt} \right|, \\ \frac{d\varepsilon^p}{dt} &= b(N_+ + N_-) v_d, \\ v_d &= \begin{cases} c_1 \exp(-\tau_1/(|\tau| - \tau^*)), & |\tau| > \tau^*, \\ 0, & |\tau| \leq \tau^*. \end{cases} \end{aligned}$$

Calculations by this model with consideration of dislocation kinetics (Fig. 2, points 6) agree well with experimental results.

A detailed picture of the behavior of the basic parameters in the dislocation model, described by Eq. (3.1) is presented in Fig. 1, where the distributions $N_d(h)$, $\tau(h)$ are shown by curves 2, 3 for four different times. It is evident that the mobile dislocation density wave front has a two-step configuration, and, as was predicted by theory, increases sharply, correlating with the loading and unloading waves. Meanwhile, the beginning of the increase in N_d coincides with the maximum in the elastic precursor.

To study the effect of collision velocity upon plasticity delay in aluminum, a numerical solution was obtained for the classical problem of propagation of a compression wave in the following formulation: Determine the functions u , σ_1 , σ_2 , ε_1 , ε^p , τ , p , E , $T \in C^1(D_Z)$, which in the region $D_Z = \{0 \leq h < \infty, 0 \leq t < \infty\}$ satisfy the system (1.1)-(1.3), (3.1) with initial $u = \sigma_1 = \sigma_2 = \varepsilon_1 = \varepsilon^p = 0 \forall h$ and boundary conditions $u = u_0 > 0$ at $h = 0$, $t \geq 0$.

The solution was found numerically, in a manner similar to the previous problems. The basic parameters of the medium used in the solution are presented in Table 1. Figure 5 shows the curves of mass velocity damping obtained behind the elastic precursor upon its propagation in aluminum for various loading rates (1, $u_0 = 2.0$; 2, 1.5; 3, 1.0; 4, 0.5; 5, 0.4; 6, 0.3; 7, 0.2 km/sec). Damping of the elastic precursor in the given model is explained by the interaction of the elastic compression wave with the unloading wave which develops immediately behind the elastic precursor due to stress relaxation. It follows as a result of this interaction that after a certain time the amplitude of the elastic precursor wave will no longer depend on the velocity u_0 , and all parameters will tend to asymptotic values corresponding to the ideal-plasticity model, i.e.,

$$\begin{aligned} u_0 &= \sqrt{\frac{\sigma}{\rho} (\rho/\rho_0 - 1)}, \quad \rho = \rho_0 \left(1 + \frac{4 \cdot 3 \cdot Y_0}{(\gamma - 1) \rho_0}\right)^{1/\gamma}, \\ \sigma &= 3 \frac{1 - \gamma}{1 + \gamma} \rho_0 [(\rho/\rho_0)^\gamma - 1], \end{aligned}$$

$$\rho_0 = 2.785 \text{ g/cm}^3, \quad p_0 = 149.8 \text{ kbar}, \quad \gamma = 5.1, \quad Y_0 = 2.5 \text{ kbar}.$$

For each point in space the function $\sigma(\varepsilon)$ may be constructed. Such a function is not unambiguous, and over the parameter range considered will have local maxima and minima, the numerical values of which depend on loading rate. The shear stresses corresponding to these points τ_1 (curve 1) and τ_2 (curve 2) as a function of distance h for $u_0 = 1$ km/sec are shown in Fig. 6. It is evident that the difference between these values decreases rapidly, after which τ_1 and τ_2 tend asymptotically to the value of the static yield point, denoted by the dashed line in Fig. 6.

Thus, the study performed permits the conclusion that the mathematical models proposed are applicable for calculation of elastoplastic processes over a wide range of deformation.

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