5. Inequalities for an Equation of State of the Form E(v, D, Δ, S)

It is of interest to reformulate the inequalities (1.7)-(1.9) for an equation of state $E = E(v, D, \Delta, S)$, which is frequently used in applications $[\Delta = {}^1/_3\,(d_1^3 + d_2^3 + d_3^3)]$. However, the relaxation of tangential stresses as a result of plastic deformations, characterized by a relaxation time τ, occurs more rapidly the larger the value of the tangential stresses, i.e., the larger the values of D and Δ. As a result of the essentially nonlinear character of the dependence of τ on the tangential stresses [1], in actual processes

$$|d_1| + |d_2| + |d_3| \ll 1,\ D \ll 1,\ |\Delta| \ll 1.$$

Under these conditions by neglecting the terms containing d_i as factors, inequalities (1.7)-(1.9) can be written in the form

$$\left.\begin{aligned} &r = E_D > 0,\ c^2 = v^2E_{vv} + (2/3)\,E_D > 0,\\ &l = vE_{vS} < 0,\ T = E_S > 0,\ g = -E_D < 0,\\ &q = -2E_D + 2vE_{vD} + v^2E_{vvv} + (4/3)\,E_\Delta < 0,\ a^2 = v^2E_{vv} > 0. \end{aligned}\right\} \tag{5.1}$$

The inequalities

$$E_D > 0,\ E_{vv} > 0,\ E_{vS} < 0,\ E_{vD} < 0,\ E_{vvv} < 0,\ E_\Delta < 0,$$

which are satisfied for interpolation formulas of the equations of state E(v, D, S) given in [3], are sufficient to ensure that (5.1) are satisfied.

The author thanks S. K. Godunov and E. I. Romenskii for their interest in the work.

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SHOCK ADIABATS OF ALKALI HALIDE CRYSTALS

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UDC 539.21

Nonparametric calculation of shock adiabats makes it possible to relate shock-compression parameters of a material directly determinable in experiment with parameters characterizing the material on an atomic level. Establishment of such a relationship is a necessary step in preliminary calculation of shock-compression parameters, which are of great significance in planning experiments and in problems involving construction with materials having given optimum properties.

Nonparametric calculation of shock adiabats of alkali halide crystals is of interest because these crystals have been studied experimentally in great detail, allowing experimental verification of calculations. At the same time, if we consider that many inorganic materials, including sitalls, glasses, ceramics, and some explosives, have ionic or predominantly ionic bonds, study of alkali halide crystals is necessary to be able to consider the behavior of these materials under shock-compression conditions.

The shock adiabat $P_\Gamma(V)$ can be calculated with the formula [1]

$$P_\Gamma(V) = \frac{P_x(V) + \gamma(V)\,[E_0 - U(V)]/V}{1 + \gamma(V)\,[1 - V_0/V]/2}, \tag{1}$$

Tomsk. Translated from Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, No. 5, pp. 123-128, September-October, 1976. Original article submitted September 18, 1975.

TABLE 1

Chemical compound	Phase B1				Phase B2			
	$\frac{V_0}{V}$	E, kcal/mole	P_x, kbar	P_r, kbar	$\frac{V_0}{V}$	E, kcal/mole	P_x, kbar	P_r, kbar
LiBr	1.12	1.1	40	47	1.37	7.8	86	90
	1.20	2.8	75	85	1.46	10	137	158
	1.28	5.4	119	136	1.55	14	204	256
	1.36	9.2	177	205	1.66	19	288	396
	1.56	22	346	434	1.77	26	395	602
	1.80	42	618	896	1.89	35	532	918
NaBr	1.13	1.3	29	33	1.39	6.3	57	64
	1.26	5.2	78	87	1.47	8.8	90	110
	1.42	13	157	184	1.64	16	180	260
	1.50	19	212	259	1.74	22	246	392
	1.60	26	282	365	1.84	30	326	587
	1.69	36	369	514	1.95	39	425	896
KBr	1.12	1.1	21	26	1.31	3.8	22	24
	1.17	2.5	38	44	1.37	5.1	41	51
	1.23	4.6	60	69	1.45	7.3	67	89
					1.52	10	98	142
					1.60	14	138	219
					1.69	19	187	333
					1.79	25	248	511
RbF	1.06	0.4	15	21	1.30	4.4	36	39
	1.12	1.6	43	50	1.37	6.3	76	92
	1.19	3.6	79	90	1.46	9.2	128	171
	1.27	6.8	126	145	1.55	13	194	288
					1.64	19	281	469
					1.75	26	386	752
RbCl	1.14	1.4	26	30	1.33	4.2	28	31
	1.19	3.0	44	49	1.40	5.6	48	59
	1.26	5.4	66	75	1.47	8.1	75	98
					1.55	11	107	153
					1.63	15	149	232
					1.72	21	200	348
					1.82	28	265	530
RbBr	1.12	1.1	18	22	1.31	3.2	17	20
	1.16	2.5	33	37	1.37	4.6	35	44
	1.22	4.6	52	58	1.44	6.6	56	76
					1.51	9.4	83	122
					1.59	13	117	189
					1.67	18	158	287
					1.75	24	210	442

TABLE 2

Chemical compound	V_0, cm³/g		V_{0C}, cm³/g	$\gamma(V_0)$	
	calculation	experimental data [5]	calculation	calculation	experimental data [7-9]
LiBr	0.255	0.289	0.250	1.38	1.94
NaBr	0.325	0.312	0.319	1.58	1.65
KBr	0.342	0.363	0.335	1.75	1.50
RbF	0.254	0.259	0.249	1.71	1.40
RbCl	0.343	0.355	0.336	1.73	1.39
RbBr	0.284	0.298	0.278	1.86	1.42

where U(V) is the binding energy of the deformed lattice; $P_X(V)$ is the pressure at zero isotherm; $\gamma(V)$ is the Grüneisen coefficient; and V_0 and E_0 are the volume and internal energy of free crystal with lattice B1 at room temperature. A statistical approximation of the quantum theory of solids makes it possible to calculate the functions U(V) and $P_X(V)$ without use of experimental data [2]. In this approximation, which is a quasiclassical form of the Hartree–Fock method, the crystalline lattice binding energy function is expressed in terms of the electron distribution density function in the crystal and structural elements. For ionic crystals, we choose as the structural elements free ions, assuming that the electron distribution density in ions does not change upon their unification into a lattice, which, as calculations for alkali halide crystals reveal, is a good approximation. We obtain the binding energy function in the form [3]

$$U=\frac{e^2}{2}\sum_{ab}{}'\frac{Z_aZ_b}{|\mathbf{R}_a-\mathbf{R}_b|}-e^2\sum_{ab}{}'\int\frac{Z_a\rho_b(\mathbf{r})}{|\mathbf{r}-\mathbf{R}_a|}d\mathbf{r}+\frac{e^2}{2}\sum_{ab}{}'\int\int\frac{\rho_a(\mathbf{r})\rho_b(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}d\mathbf{r}'+\frac{1}{2}\sum_{ab}{}'\int\{\hat{R}[\rho_a+\rho_b]-\hat{R}[\rho_a]-\hat{R}[\rho_b]\}\,d\mathbf{r},$$

TABLE 3

Chemical compound	Parameters, a, km/sec	Calc.	Exptl. data [14]	Calc.
LiBr	a	2,58	2,6	1,89*
	b	1,40	1,4	1,51*
NaBr	a	2,59	2,6	1,93*
	b	1,43	1,3	1,53*
KBr	a	2,34	—	1,69*
	b	1,53	—	1,62*
RbF	a	2,62	—	2,12*
	b	1,53	—	1,62*
RbCl	a	2,47	1,5*	1,74*
	b	1,50	1,6*	1,61*
RbBr	a	2,09	1,4*	1,44*
	b	1,60	1,6*	1,67*

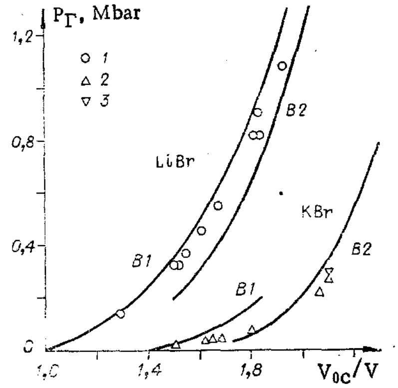

Fig. 1

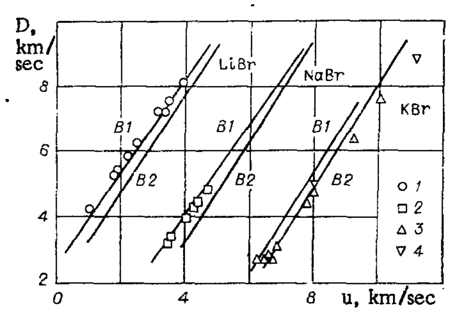

Fig. 2

where Z_a and R_a are the charge and radius-vector of the a-th nucleus; $\rho_a(\mathbf{r})$ is the electron distribution density function in the a-th ion; the nonlinear operator $\hat{R}$ is defined by the equation

$$\hat{R}[f] = \varkappa_k f^{5/3} + \varkappa_e f^{4/3},$$
$$\varkappa_k = 3^{5/3}\pi^{4/3}\hbar^2/10m, \quad \varkappa_e = -3^{4/3}e^2/4\pi^{1/3}.$$

The electron densities $\rho_a(\mathbf{r})$ are constructed from wave functions, found by solution of the Hartree–Fock equation for isolated ions. On the basis of the binding energy function obtained in the statistical approximation [4] we constructed shock adiabats of NaCl, which proved to be in good agreement with experiment, confirming the validity of the model and approximations upon which the nonparametric calculation is based.

In the present study we will perform analogous calculations for LiBr, NaBr, KBr, RbF, RbCl, and RbBr crystals. Nonparametric equations of state were obtained for these crystals in phases B1 (NaCl lattice) and B2 (CsCl lattice), which were proved valid by comparison with experiment in the static pressure region. Shock adiabats of the B1 lattice were calculated with Eq. (1) using calculated values of V_0 and E_0; calculations for the B2 lattice were performed with Eq. (1) with the same initial state parameters and values of U(V), $P_x(V)$, and $\gamma(V)$, referring to phase B2.

The shock-compression pressures $P_\Gamma(V)$ obtained are presented in Table 1, which also shows pressures P_x and energies E_x of the zero isotherms as functions of relative compression V_0/V. Table 2 presents calculated values of specific volume V_0 which are close to the experimental data of [5]. The Grüneisen coefficients $\gamma(V)$ were calculated with the formula of Zubarev and Vashchenko [6]. Values of $\gamma(V_0)$ for free lattices shown in Table 2 agree well with experimental values from [7-9].

The data of Tables 1 and 2 may be used to obtain scalar equations of state for alkali halide crystals corresponding to hydrostatic compression. To compare the results of calculation with static measurements performed at room temperature, it is necessary to take the pressure P_x as a function of relative compression V_{0c}/V, where V_{0c} is the calculated volume of a free crystal with lattice B1 at temperature 0°K.

Figure 1 shows calculated shock adiabats for crystals LiBr and KBr (experimental data: 1 – [10]; 2 – [11]; 3 – [12]). For LiBr the experimental points from [10] correlate well with the curve of phase B1; the transition to the dense phase was not achieved experimentally. In the case of KBr the phase transition occurs in the low-pressure region. In the transition region the location of the experimental points from [11] agrees well with the calculated curves for phases B1 and B2. At higher pressure the experimental data [11, 12] are close to the calculated curve for phase B2. At pressures above ~400 kbar the experimental points deviate sharply from the calculated B2-phase curve, which is evidently caused by the fusion occurring in this region [13]. Experimental data on $P_\Gamma(V)$, for other crystals presented in Table 1 were not available.

The shock adiabats obtained for LiBr, NaBr, KBr, RbF, RbCl, and RbBr crystals allow calculation of the relationship between shock-wave velocity D and mass velocity u, which can be verified experimentally. The following relationships based on conservation laws were used for calculation:

$$D(V) = \sqrt{P_\Gamma(V_0 - V)}, \quad u(V) = V_0\sqrt{P_\Gamma/(V_0 - V)},$$

in which P_Γ and V_0 were taken for our calculations. The relationship between D and u obtained with tabular values of $P_\Gamma(V)$, can be approximated well over a wide interval by a function of the form

$$D = a + bu. \tag{2}$$

Table 3 shows the parameters a and b, determined from calculated velocities D and u by the method of least squares for phases B1 and B2 (values with asterisks refer to B2 phase) for the crystals considered. As is evident from Table 3, the transition from the B1 phase to the B2 phase is related to an increase in the slope of Eq. (2) and to reduction in parameter a. Results of calculating parameters a and b agree well with experimental values from [14] for both phases. Figure 2 shows the location of experimental points referred to the lines calculated from Eq. (2) for LiBr, NaBr, and KBr crystals: 1) [10]; 2) [15]; 3) [11]; 4) [12]. For LiBr and KBr the location agrees completely with Fig. 1; for NaBr the experimental points taken with graphic accuracy from [15] fit the calculated line corresponding to the B1 phase with satisfactory accuracy.

The shock-adiabat calculation for the RbF crystal, for which experimental values are unknown, is an example of beforehand calculation of shock-compression parameters. The results obtained may be considered as a model which should be considered in interpreting experimental data.

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SHOCK WAVES AND PHASE TRANSITIONS IN IRON

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UDC 539.89

INTRODUCTION

The process of shock compression in certain solids (iron, carbon, KCl, KBr, quartz, many minerals) is accompanied at increased pressure p_S by phase transitions, i.e., formation of new crystalline phases [1]. Changes in the wave configurations which then develop [2-4] permit determination of the characteristic times of these transitions, which usually comprise 0.2-0.4 μsec. In [5-7] a single-velocity single-temperature model of a two-phase viscoplastic medium was developed, which was used for study of nonstationary shock waves in Armco iron with phase transitions, and on the basis of the relationship between phase transitions and hardening, the kinetics of the phase transition $\alpha \rightleftharpoons \varepsilon$ in iron were determined. In the present study an investigation of shock-wave propagation in Armco iron will be performed with consideration of new experiments [3, 4] in which the multiwave structure of shock waves of various intensities were fixed directly by manganin sensors and a light interferometer. Under these experimental conditions, calculations were performed for motion of shock waves on the front of which phase transitions occur. The kinetics of phase transition will be studied and presented in greater detail than in [6, 7].

§1. The basic equations in Lagrangian coordinates (r, t) for the case of one-dimensional motion with uniaxial deformation have the form

$$
\begin{gathered}
(\rho_0/\rho)\,\partial\rho_1/\partial t + \rho_1\partial v/\partial r + (\rho_0/\rho)I_{12} = 0,\\
(\rho_0/\rho)\,\partial\rho_2/\partial t + \rho_2\partial v/\partial r - (\rho_0/\rho)I_{12} = 0\\
(\rho_i = \rho_i^0\alpha_i,\ \alpha_1 + \alpha_2 = 1,\ \rho = \rho_1 + \rho_2,\ i = 1, 2),\\
\rho_0\partial v/\partial t = \partial\sigma^{11}/\partial r,\\
\rho_0/\rho\,[\rho_1\partial e_1/\partial t + \rho_2\partial e_2/\partial t + (e_2 - e_1)\,I_{12}] = \sigma^{11}\partial v/\partial r,\\
\sigma^{11} = -p + \tau^{11},\ p = p_1(\rho_1^0, T) = p_2(\rho_2^0, T),\\
d\tau^{11}/dt = (4/3)\,\mu\,(\rho_0/\rho)\,dv/\partial r,\quad \tau^{11} \leqslant \tau^*,
\end{gathered}
\tag{1.1}
$$

where ρ_i, ρ_i^0, α_i, e_i are the mean density, true density, volume content, and specific internal energy of the i-th phase; ρ, v, T are the density, velocity, and temperature; σ^{11}, τ^{11}, p are the stress tensor, stress deviator, and hydrostatic pressure in the medium; μ, τ^* are the shear modulus and elastic limit, for the description of which Mises creep conditions will be used; I_{12} is the velocity of phase transitions for which the following relationships are fulfilled: $I_{12} = j_{12} - j_{21}$; for the 2 → 1 transition $j_{12} = 0$, $j_{21} > 0$; for the 1 → 2 transition $j_{12} > 0$, $j_{21} = 0$; if there are no phase transitions $j_{12} = 0$, $j_{21} = 0$.

The intensity of the phase transitions considered is greater, the more the pressure p exceeds the phase-transition pressure $p_S(T)$, i.e., the greater the nonequilibrium. Kinetics leading to retardation of phase transition and achievement of metastable states occur in the case of the transition $Fe^{\alpha} \rightleftharpoons Fe^{\varepsilon}$. We will assume [5-7] that the phase-transition velocity depends on the difference of the phase thermodynamic potentials (for identical pressures and temperatures) and on the volume content of the original phase. Moreover, we allow saturation of phase-transition velocity for sufficiently great deviations from the equilibrium line. Then at

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Ufa. Moscow. Translated from Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, No. 5, pp. 128-135, September-October, 1976. Original article submitted October 12, 1975.