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CALCULATION OF SHOCK ADIABATS IN SOLIDS

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A knowledge of shock adiabats of solid is required in problems dealing with the behavior of matter under shock loading. The calculation of pressure on the shock adiabat p_H as a function of volume V is usually carried out with equations of state the parameters of which are related to experimental [1] or theoretical [2] characteristics of the highly compressed material, with model representations of the Gruneisen coefficient $\gamma(V)$ [1, 3]. At the same time, many materials of practical interest such as metal alloys, mining ores, and ceramics have been studied insufficiently at high pressures, complicating use of this traditional approach. In connection with this, it is of significant interest to determine the laws of shock loading with the aid of reliable and easily measurable characteristics of the undeformed material. In the present study shock adiabats of a wide range of materials will be calculated using as experimental parameters the adiabatic modulus of omnidirectional compression K_S and the thermochemical internal energy E_0.

To specify the pressure on the isentrope p_S semiempirical equations corresponding to the Morse formula are used:

$$p_S = \frac{2E_0\alpha}{3V_0} x^{-2/3} [\exp 2\alpha(1 - x^{1/3}) - \exp \alpha(1 - x^{1/3})] \quad (1)$$

together with a modified Lennard–Jones formula

$$p_S = \frac{E_0 n(n-1)}{V_0} [x^{-1} - 1] x^{-n}, \quad (2)$$

where $x = V/V_0$; V_0 is the specific volume of the undeformed material. The parameters α and n are expressed in terms of the modulus of omnidirectional compression K_S and energy E_0, using the formulas Equations (1), (2) reliably describe the behavior of materials over a wide range of hydrostatic deformations [4]. In considering shock loading the dependence of shock velocity D on mass velocity of the material U is approximated by a quadratic relationship

$$D = a + bU + cU^2. \quad (3)$$

To determine the parameters a, b, c, an approach based on the relationships between the first, second, and third derivatives of $p_H(V)$ and $p_S(V)$ at the point V_0 is used [5, 3]:

(4)

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TABLE 1

No.	Material	E_0, kJ/g	$K_S \cdot 10^5$ Pa	α	a, km/sec	b	c, sec/km
1	2	3	4	5	6	7	8
1	Li	23,14	120	2,09	4,74	1,022	+0,009
2	Be	36,18	1144	2,76	7,88	1,19	0,000
3	B	52,0	1810	2,52	8,56	1,13	+0,018
4	C(d)	59,5	5460	3,40	12,4	1,35	—0,020
5	Na	4,7	73,8	2,68	2,76	1,17	+0,014
6	Mg	6,02	339	3,84	4,44	1,46	—0,020
7	Al	11,91	764	3,28	5,32	1,32	+0,024
8	Si	16,21	978	3,40	6,48	1,35	—0,037
9	S(r)	8,68	191	2,32	3,22	1,08	+0,128
10	K	2,28	34,9	2,84	2,01	1,21	+0,013
11	Ca *	4,34	172	3,40	3,36	1,35	—0,041
12	Sc *	8,40	578	3,24	4,40	1,31	—0,017
13	Ti	9,80	1061	3,28	4,85	1,32	—0,013
14	V	10,1	1543	3,36	5,06	1,34	—0,010
15	Cr	7,64	1924	3,96	5,17	1,49	—0,027
16	Mn	5,15	610	2,68	2,87	1,17	—0,032
17	Fe	7,43	1731	3,64	4,69	1,41	—0,006
18	Co	7,26	1904	3,64	4,64	1,41	+0,008
19	Ni	7,32	1875	3,60	4,59	1,40	+0,002
20	Cu	5,32	1371	3,60	3,92	1,40	+0,010
21	Zn	2,00	683	4,64	3,09	1,66	—0,047
22	Ga	3,73	582	3,44	3,14	1,36	—0,017
23	Ge	5,18	754	3,44	3,72	1,36	—0,053
24	As	4,03	394	2,76	2,62	1,19	—0,072
25	Se	2,87	93,0	1,76	1,39	0,94	+0,036
26	Rb	0,96	35,9	3,32	1,53	1,33	+0,032
27	Sr *	1,83	116	3,32	2,11	1,33	—0,019
28	Y *	4,77	415	2,92	3,01	1,23	—0,018
29	Zr *	6,67	984	3,20	3,89	1,30	—0,043
30	Nb	7,75	1533	3,24	4,24	1,31	+0,003
31	Mo	6,85	2707	4,16	5,15	1,54	—0,030
32	Tc	6,54	3026	4,24	5,14	1,56	+0,016
33	Ru	6,51	3292	4,32	5,17	1,58	+0,040
34	Rh	5,41	2750	4,28	4,71	1,57	—0,001
35	Pd	3,31	1923	4,08	4,01	1,67	—0,029
36	Ag	2,64	1036	4,08	3,14	1,52	+0,010
37	Cd	0,99	535	5,28	2,49	1,82	—0,042
38	In	2,12	416	3,48	2,38	1,37	+0,066
39	Sn	2,54	543	3,64	2,73	1,41	+0,034
40	Sb	2,15	378	3,44	2,37	1,36	—0,079
41	Te	1,53	233	3,32	1,93	1,33	—0,074
42	Cs *	0,95	22,8	3,04	1,10	1,26	+0,013
43	Ba *	1,29	100	3,16	1,66	1,29	—0,078
44	La *	3,00	303	2,72	2,22	1,18	—0,040
45	Ce(γ)*	2,91	197	2,12	1,71	1,03	—0,019
46	Pr *	2,52	307	2,84	2,12	1,21	—0,069
47	Nd *	2,27	324	3,04	2,15	1,26	—0,061
48	Sm *	1,37	383	4,08	2,26	1,52	—0,172
49	Eu *	1,15	154	2,76	1,40	1,19	+0,070
50	Gd *	2,53	401	3,00	2,25	1,25	—0,075
51	Tb *	2,44	402	2,96	2,17	1,24	—0,045
52	Dy *	1,76	409	3,62	2,19	1,38	—0,099
53	Ho *	1,82	400	3,32	2,10	1,33	—0,071
54	Er *	1,89	462	3,48	2,26	1,37	—0,070

continued on next page

TABLE 1 (continued)

1	2	3	4	5	6	7	8
55	Tm *	1,37	402	3,76	2,08	1,44	—0,096
56	Yb *	0,88	136	3,16	1,39	1,29	—0,074
57	Lu *	2,44	442	2,88	2,13	1,22	—0,057
58	Hf *	3,46	1163	3,40	2,98	1,35	—0,045
59	Ta	4,32	1943	3,48	3,41	1,37	—0,001
60	W	4,61	3081	3,96	4,00	1,49	—0,019
61	Re	4,18	3634	4,32	4,16	1,58	+0,016
62	Ir	3,48	3600	4,56	4,01	1,64	—0,008
63	Pt	2,89	2643	4,36	3,51	1,59	+0,029
64	Au	1,55	1799	4,76	3,05	1,69	+0,037
65	Hg	0,305	328	6,04	1,57	2,01	—0,139
66	Tl	0,89	380	4,04	1,79	1,51	+0,012
67	Pb	0,94	460	4,40	2,01	1,60	+0,046
68	Bi	0,99	336	3,96	1,85	1,49	—0,135
69	Ra	0,716	135	3,80	1,52	1,45	—0,125
70	Th	2,48	577	2,96	2,19	1,24	+0,003
71	U	2,19	1131	3,52	2,45	1,38	+0,008
72	Pu	1,43	628	3,16	1,78	1,29	+0,246
73	LiF	10,76	698	3,32	5,14	1,33	+0,008
74	LiCl	4,41	315	3,92	3,90	1,48	—0,017
75	NaF	6,57	486	3,44	4,15	1,36	+0,003
76	NaCl	3,91	245	3,60	3,36	1,40	—0,003
77	KF	4,07	319	3,72	3,55	1,43	—0,040
78	KCl	2,95	174	3,64	2,96	1,41	—0,043
79	AgCl	1,56	441	4,76	2,81	1,69	—0,074
80	MgO	15,0	1660	3,72	6,80	1,43	—0,016

where γ_0 is the Gruneisen coefficient of the free material. Using an expression corresponding to the quadratic approximation (3)

$$p_H(V) = \frac{a^2(1-x)}{V_0\{[1-b(1-x)]^2 - 2ac(1-x)^2\}},$$

with the aid of Eqs. (1), (4) we find the shock adiabat parameters:

$$a^2 = \frac{2E_0\alpha^2}{9} = K_S V_0; \tag{5}$$

$$b = \frac{\alpha+2}{4} = \frac{1}{4}\left(\sqrt{9V_0K_S/2E_0} + 2\right); \tag{6}$$

$$c = \left(\gamma_0 - \frac{25\alpha^2+36\alpha-92}{36\alpha+72}\right)\frac{\alpha+2}{8\alpha(2E_0)^{1/2}}. \tag{7}$$

Equation (2) corresponds to the expressions

$$a^2 = n(n-1)E_0 = K_S V_0; \tag{5a}$$

$$b = \frac{1}{2}(n+1) = \frac{3}{4} + \frac{1}{2}\sqrt{\frac{1}{4} + V_0K_S/E_0}; \tag{6a}$$

$$c = \left[\gamma_0 - \frac{3}{2}(n-1)\right]\frac{n+1}{12[n(n-1)E_0]^{1/2}}. \tag{7a}$$

The shock adiabats of chemical elements and ionic compounds were calculated with Eqs. (5)-(7), with E_0 for the ionic compounds being taken as the energy required for liberation of isolated neutral molecules from the crystal. The E_0 values used were determined from

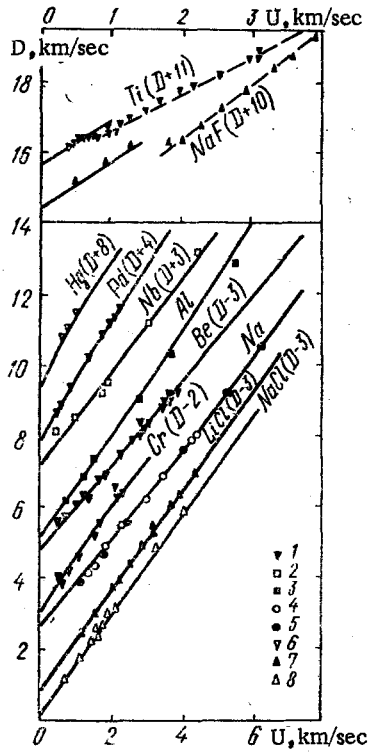

Fig. 1

thermodynamic data [6], while K_S values were taken from ultrasound measurements [7-10], and thermodynamic values of the coefficient γ_0 were taken from [1, 10, 11]. The calculated values of a, b, c, for Eq. (1) and calculated coefficients α and experimental E_0 and K_S values are presented in Table 1. Calculations with Eq. (2) give b values elevated by an average of 20%. As is evident from Table 1 the values of the parameter b lie in the range of 0.94 (Se) to 2.01 (Hg). The c values for the majority of materials are quite small, which corresponds to good approximation of the shock adiabat by a linear expression

$$D = a + bU. \tag{8}$$

The lower part of Fig. 1 shows a comparison of typical calculation results with experimental results for materials whose shock adiabats have no marked inflection corresponding to a phase transition (solid lines, calculations after Table 1, experimental data as follows: 1, [8]; 2, [9]; 3, [12]; 4, [13]; 5, [14]; 6, [15]; 7, [16]; 8, [17]). As is evident from Fig. 1, there is good agreement between calculation and experiment over a wide velocity range. We note that at megabar pressures the quadratic Eq. (3) becomes insufficiently accurate, and it may be necessary to calculate subsequent terms in the expansion of shock wave velocity D in powers of mass velocity U. The upper part of the figure shows typical materials which do undergo a phase transition in the pressure range considered (solid lines, calculation with Table 1, dashes, linear interpolation for the high-pressure phase [8, 16]). As is evident from Fig. 1, the calculated curves agree well with experiment for Ti and NaF, corresponding to the low-pressure phase. The deviation from the experimental points at U = 0.8 km/sec (Ti) and U = 1.51 m/sec (NaF) is related to the beginning of the phase transition. When shock compression data are processed with an interpolation formula of the form of Eq. (8), assignment of experimental points to one or the other phase is usually difficult, which leads to inaccuracy in determination of the parameter b and large scattering in values presented by various authors. The semiempirical adiabats calculated in this study permit refinment of phase transition parameters and more accurate interpretation of available experimental data.

The method described does not give a proper description of the experimental shock adiabats of elements (denoted in Table 1 by an asterisk) which experience electron transitions under pressure [9, 18-20], leading to an increase in values of the parameter b by an average of 1.5 times. This is because the model used does not consider continuous displacement of outer electrons into unfilled inner levels which is accompanied by an anomolously flat path in the lower branch of the adiabat [9, 18]. Consideration of such a process should be made on the

basis of a quantum-mechanical analysis of the electronic structure [21]. The results presented in Table 1 for elements which experience electron transitions may be used to estimate the contribution of electron readjustments to the equation of state.

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