SHOCK ADIABATS OF OXIDES OF THE ALKALINE-EARTH METALS

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The analysis of the shock adiabats of ionic crystals (alkali-halide compounds, oxides) is a necessary link in the passage to the examination of the behavior of many inorganic materials (minerals, mountain rocks) under shock compression [1-3]. The shock compression parameters of the majority of alkali-halide crystals have been determined well both experimentally [4] and theoretically [5, 6]. The behavior of oxides under shock loading conditions has been investigated much less. On the basis of a proposed semiempirical binding energy function which takes account of pairwise and triple ion interactions, the shock adiabats are analyzed in this paper for oxides of the alkaline-earth metals MgO, CaO, SrO, BaO in the phases B1 (NaCl lattice) and B2 (CsCl lattice).

The shock adiabat $P_H(V)$ is computed by means of the formula [7]

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

where U(V), $P_x(V)$ are the energy and pressure on the zero isotherm, $\gamma(V)$ is the Gruneisen factor, and V_0, E_0 are the volume and internal energy of the free crystal. Utilization of a quantum-mechanical method of computing U(V) [5], on the basis of a pairwise approximation of the binding forces is less justified in oxides tha in alkali-halide crystals since substantial deviations from the Cauchy relationships between the second-order elastic moduli are observed there. These deviations are due primarily to three-particle interactions.

Taking account of the three-particle interactions, the crystal binding energy function formed by particles of different species has the form

$$U=\frac{1}{2}\sum_{\substack{ll'\\kk'}}\varphi\left(r^{ll'kk'}\right)+\frac{1}{6}\sum_{\substack{ll'l''\\kk'k''}}\psi\left(r^{ll'kk'},\,r^{l''lk''k},\,r^{l''l'k''k'}\right),\tag{2}$$

where $r^{\ell\ell'kk'}$ is the spacing between particles of the species k and k′ that are in the elementary cells, l and l', φ, ψ are, respectively, the potentials of the pairwise and three-particle interactions. We approximate the pairwise interaction by the Born-Maier potential

$$\varphi(r)=\frac{e_ke_{k'}}{r}+A_{kk'}\exp\left(-\frac{r}{\rho}\right)-\frac{c_{kk'}}{r^6}-\frac{d_{kk'}}{r^8},$$

where e_k, e_k' are the ion charges, $c_{kk'}$, $d_{kk'}$ are, respectively, the dipole–dipole and dipole–quadrupole interaction constants whose values for the oxides are presented in [8], and $A_{kk'}$, ρ are parameters. A potential whose functional form is proposed in [9]

$$\psi=B_{kk'k''}\exp\left(-\frac{r^{ll'kk'}+r^{l''lk''k}+r^{l'l''k'k''}}{3\rho}\right)$$

is used to approximate the triple interactions, where $B_{kk'k''}$ are parameters, and ρ has the same numerical value as in the pairwise potential. Triplets of ions formed by two ions of the same sign and one ion of the opposite sign were taken into account in the last term in (2) in the summation over the crystal lattice. The configuration of such triplets for the NaCl lattice (under normal conditions oxides of the alkaline-earth metals have this kind of structure) is an isosceles right triangle, whose two sides equal the shortest distance R between the ions, and the third side is $\sqrt{2}R$. Experimental characteristics of the free oxides, the binding energy, the equilibrium volume [8], and the second-order elastic modulus [10-13] were used to determine the four unknown parameters of the binding energy function.

The equations of state of hydrostatic compression of oxides of the alkaline-earth metals in the B1 and B2 phases, computed on the basis of the binding energy function obtained, are in good agreement with existing experimental data [14-16]. The Gruneisen coefficients $\gamma(V)$ were calculated by the Slater–Landau (SL), Dugdale–Macdonald (DM), Zubarev–Vashchenko (ZV) formulas to compute the shock adiabats. Good agreement between the computed values $\gamma(V_0)$ and experiment for MgO is obtained in a computation using SL, and for CaO, SrO using ZV. We know of no experimental values of $\gamma(V_0)$ for BaO. The computed values of $\gamma(V_0)$ are presented in Table 1. Computation of the shock adiabats for the phase B2 was by means of (1) with parameters of the initial state of the lattice B1 with U(V), $P_x(V)$, $\gamma(V)$ referred to the phase B2. In the case of MgO the shock compression pressure $P_H(V)$ as computed by using the $\gamma(V)$ according to Slater–Landau, and according to Zubarev–Vashchenko for CaO, SrO, BaO. Computed pressures on the zero isotherm $P_x(V)$ and

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TABLE 1

Crystal	$\gamma(V_0)$			Experiment
	SL	DM	ZV	
MgO	1,58	1,25	0,92	1,54
CaO	1,78	1,45	1,12	1,19
SrO	1,79	1,46	1,13	1,11
BaO	1,87	1,54	1,21	—

TABLE 3

Crystal	Phase B1		Phase B2	
	a, km/sec	b	a, km/sec	b
MgO	7,25	1,17	5,10	1,71
CaO	6,30	1,26	4,63	1,63
SrO	3,97	1,27	2,61	1,59
BaO	2,68	1,27	2,62	1,54

TABLE 2

Crystal	Phase B1			Phase B2		
	V_0/V	P_x, kbar	P_H, kbar	V_0/V	P_x, kbar	P_H, kbar
MgO	1,17	372	376	1,61	1619	1686
	1,20	473	481	1,72	2117	2431
	1,28	708	733	1,78	2404	2904
	1,32	845	884	1,84	2720	3464
	1,51	1554	1730	1,91	3068	4133
	1,75	2603	3209	1,97	3450	4942
	1,88	3299	4378	2,04	3870	5932
CaO	1,17	310	313	1,51	866	918
	1,20	397	403	1,56	1025	1122
	1,28	604	622	1,61	1203	1359
	1,32	726	755	1,72	1620	1956
	1,42	1015	1081	1,84	2136	2773
	1,57	1586	1770	1,97	2771	3916
	1,88	3044	3866	2,04	3141	4660
SrO	1,17	233	236	1,46	540	559
	1,20	298	304	1,51	648	695
	1,28	455	469	1,61	903	1033
	1,37	651	685	1,72	1222	1490
	1,46	895	968	1,84	1615	2120
	1,68	1575	1840	1,97	2102	3005
	1,88	2309	2943	2,04	2386	3582
BaO	1,17	198	201	1,38	260	267
	1,20	254	259	1,46	408	449
	1,28	390	404	1,56	594	696
	1,37	562	596	1,67	829	1033
	1,46	779	851	1,78	1121	1502
	1,68	1391	1661	1,90	1485	2165
	1,88	2061	2726	2,04	1936	3135

the shock compression pressure $P_H(V)$ of the oxides as functions of the relative compression V_0/V are presented in Table 2. The shock adiabats of MgO, CaO, BaO are represented in Figs. 1-3 (experimental data: 1 from [17], 2 from [1], 3 from [15]). In the case of MgO and CaO the experimental points from [1, 17] are in good agreement with the computed curve of $P_H(V)$ for the B1 phase; the passage to the compact B2 phase was not established experimentally. In the case of BaO the phase transition holds in the low pressure area [3, 15]. The computed shock adiabats of the B1 and B2 lattices for BaO are close to the experimental points referring to static compression [15] in the above-mentioned domain. There are no experimental data on the shock compression of SrO in the literature. Good agreement between experiment $P_x(V)$ and $\gamma(V_0)$, as well as the utilization of the experimental characteristics of the free state in determining the binding energy function parameters,allow the hope that the computed shock adiabats for SrO would, as for MgO and CaO, describe the actual behavior of this crystal under shock compression conditions sufficiently correctly.

The shock adiabats obtained for the crystal under consideration allowed the computation of a relationship between the shock velocity D and the mass velocity u. The following relations from the conservation laws were used in the computations

$$D(v) = v_0 \sqrt{P_H/(v_0 - v)}, \quad u(v) = \sqrt{P_H(v_0 - v)},$$

where P_H and v (the specific volume) are taken from our computations. The relation between D and u is interpolated in a broad range of velocities by a function of the form

$$D = a + bu. \tag{3}$$

The parameters *a* and b found from the computed velocities D and u by least squares are presented in Table 3 for the B1 and B2 phases of the oxides. The location of experimental points relative to the computed line (3) is shown in Fig. 4 for the crystals MgO and CaO (1 from [17], 2 from [1]). The experimental points stack up well on the computed lines (3) corresponding to the B1 phase of the oxides MgO and CaO.

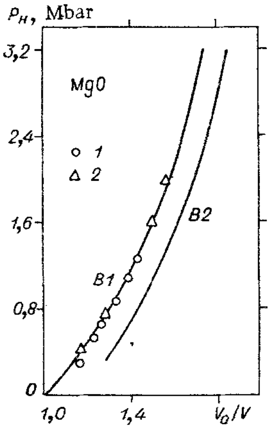

Fig. 1

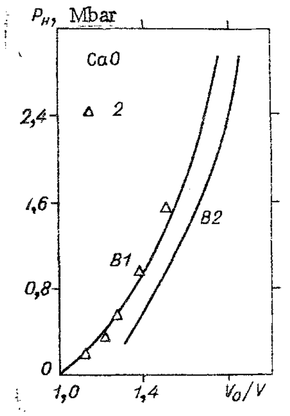

Fig. 2

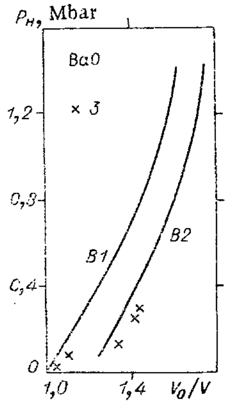

Fig. 3

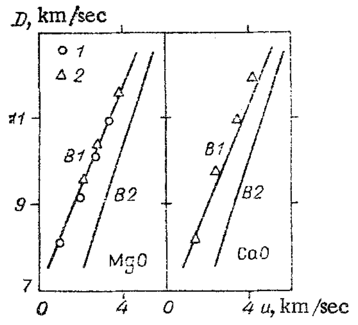

Fig. 4

The results obtained can be used in interpreting experimental results on the shock compression of oxides, as well as to construct the additive equations of state for minerals and mountain rocks.

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STRESSED STATE OF A CEMENTED POROUS MEDIUM WITH AN UNDERGROUND EXPLOSION

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The investigation of the behavior of a cemented porous medium with an underground explosion is of considerable interest. This is connected with the fact that many rocks (e.g., gas-and-oil-saturated collectors) are cemented porous media, saturated by a gas or a liquid. At the same time, many important questions connected with the action of explosive loads on such media have been insufficiently studied. In [1, 2] a model was formulated, and experimental investigations were made of an underground explosion in soft soils. Explosion in a brittle medium was studied in [3, 4]. However, it is well known that cemented porous media differ in a number of special characteristics [5]: an increased compressibility in comparison with excavated rock, a considerable porosity (in distinction from soft soils), etc. For practical applications, an important question is that of the residual stresses, arising at the moment of the breakdown of the underground cavity, which will determine the rheological behavior of the medium in the vicinity of the explosion. The present article describes a method and the results of experimental investigations of an underground explosion in porous cement blocks.

1. Experimental explosions were carried out in cement blocks with a diameter of 790 mm and a height of 890 mm. The blocks were put into metallic casings with a wall thickness of 10 mm. The power of the explosion was selected from the condition that the time of the formation of the cavity must be less than twice the time of the passage of the wave of the compression up to the limits of the block. The experiments were made using charges of TG-20/80 with a weight of 12 g, having a cylindrical form with a height equal to their diameter. The blocks were prepared by filling metallic casings with a cement solution with VTs-0.5. Before the solution was poured, a tube was installed in the center of the vessel; when the tube was removed from the hardening solution, a hole was formed, into which the charge was lowered. The charge was installed at the center of the block and sand was poured in to a height of 40 cm. The remaining part of the charging hole was sealed by a compound based on an epoxide resin. To determine the physicomechanical properties of the medium at the moment of the explosion, samples were taken. The mean values of the properties of the medium are given in Table 1. To make dynamic measurements, before the solution was poured, wire-type strain-gauge pickups were installed radially and azimuthally with respect to the front of the wave. The overall dimensions of the pickups were: diameter 4 mm, length 10 mm. Micromodular stabilitrons were used as converters. The principle of the action of a pickup consisted in the following. The pressure is transmitted to the silicon crystal of a diode, whose sensing layer is a p–n transition. A direct current is passed through the diode from a current generator. An increase or decrease in the thickness of the p–n transition with the action of a load on the crystal brings about a change in the voltage drop at the p–n-transition, which is recorded using an amplification device. After an analysis of the oscillograms of the stresses in the compression wave, the following dependence of the maximal radial σ_{rm} and azimuthal $\sigma_{\varphi m}$ stresses on the distance were obtained

$$\sigma_{rm}=71.4\,(W^{1/3}/r)^{2.5},\quad \sigma_{\varphi m}=59.7\,(W^{1/3}/r)^{2.75},$$

where W is in kg, r is in m, σ is in kg/cm^2.

Figure 1 shows a typical oscillogram of the stresses at different points from the center of the charge, where the crosses denote the residual stresses; 0 denotes zero explosion; 2φ, 5r are the number of the pickup and the recorded azimuthal components of the stresses, respectively; r is the distance from the pickup to the charge. On some oscillograms there are residual stresses differing in sign. It is well known that, with the hardening of a cement solution there arises a compressive stress, which, in the experiments, was around 200 kg/cm^2, and with respect to which the parameters of the wave were recorded. The appearance of negative stresses beyond the zone of the breakdown is explained by discharging of the pickups from the phonon pressure due to the appearance of elongational stresses in the medium.

Figures 2 and 3 show the distribution of the residual radial σ_r and azimuthal σ_φ stresses, where 1 is the measured, and 2 the reduced stress. Since the explosions took place in blocks whose yield points differed somewhat in value, on the axis of ordinates there are plotted the ratios of the actually recorded residual stresses to the crushing strength of the

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