Static and shock compressibility of TATB molecular crystal

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Abstract. The paper presents analysis of experimental data on hydrostatic and shock-wave compression of TATB energy-saturated material. The semi-empirical Mie–Grüneisen equation of state was used to describe thermodynamic properties of metastable molecular crystals without considering phase transitions. The equation of state describes experimental data on isothermal compression of a molecular crystal, and this data are obtained using the powder diffraction method. The Hugoniot curve expression plausibly describes shock-compression data on the studied material having various initial porosities.

Despite its practical significance, thermodynamics of high-molecular substances, in particular, metastable chemical compounds referred to as energy-saturated materials (ESM), has been understood insufficiently. The study of equation of state is an actual problem [1–3].

In the present paper, hydrostatic and shock compression data on low-sensitive, energy-related materials, are used to derive semi-empirical Mie–Grüneisen equation of state (EOS).

Experimental data on hydrostatic compression of TATB (triaminotrinitrobenzene) ESM up to the pressures of $\sim 6.5$ GPa at $T_0 = 293$ K were obtained at the Experimental Station of Diffractometry in the hard x-ray range of the accelerator complex VEPP-3 at the Budker Institute of Nuclear Physics of the Siberian Branch RAS (Novosibirsk, Russia) using the powder diffraction method with compression of material under study in the diamond anvil cell [4,5]. The diffractograms were used in x-ray crystallographic analysis considering an actual crystallographic model. This study was performed to determine the ESM crystal structure parameters and the cell volume values versus the pressure applied [6]. Figure 1 shows correlation between hydrostatic pressure $P_x(\sigma)$ and ESM crystal volume fraction. The data obtained in [7] are plotted for comparison.

Figure 1 shows shock compression data obtained with piezoresistive and radiointerferometer methods [8]: the data obtained using the optical lever method [9] are also demonstrated. Resulting Hugoniot curves [8,9] correspond to the studied ESM having initial porosity $\approx 1.01$. 
The approach described in [10–12] is used to approximate experimental data. The pressure is represented by the sum of elastic and thermal pressures [8]:

$$P = P_x + P_t = P_x + \Gamma \rho_0(\varepsilon - \varepsilon_x),$$

(1)

where $P_x = \rho_0 C_0 (\sigma^n - 1)/n$ is the elastic pressure; $\Gamma$ is the Gr"uneisen constant; $\varepsilon$ is the internal matter energy; $\varepsilon_x$ is the elastic compression energy; $\rho_0$ is the initial density of matter; $\sigma = \rho/\rho_0$ is the compression ratio; $\rho$ is the current density of matter.

The Hugoniot curve expression according to [10] is as follows:

$$P = P_0 C_0^2 \frac{n \sigma^n [h - (n + 1)/(n - 1)] + \sigma 2n/(n - 1) - (h + 1)}{h - k\sigma},$$

(2)

where $h = 2/\Gamma + 1$ is the ultimate compression ratio; $k = \rho_{cr}/\rho_0$ is the porosity ratio; $\rho_{cr}$ is the crystalline material density at $T = 293$ K.

The EOS parameters $n$, $h$, and $C_0$ were found using the nonlinear regression method by best description of hydrostatic and shock compression data. The results [13] corresponding to the shock-compressed material having porosity of about 1.05 were used to describe coefficients found by approximation. Figure 2 shows results of experimental data on ESM having porosity of 1.01 and 1.05 approximated by the $P(\sigma, k)$ equation (2). The whole data set was used to find the approximation coefficients $n = 6.0 \pm 0.2$ and $h = 2.6 \pm 0.4$, and the sound velocity value, $C_0 \approx 3000$ m/s was determined in [6].
Figure 2. Surface $P(\sigma, k)$ (2) approximated experimental data on shock compressibility of ESM having various initial porosity: circles correspond to data for $k = 1.01$ [8, 9] and 1.05 [13].

The suggested equation of state is anticipated to improve description of thermodynamic properties for energy-saturated material in numerical simulation of shock-wave and detonation processes.

References

[1] Bushman A V, Lomonosov I V, Fortov V E and Khishchenko K V 1994 Khim. Fiz. 13(1) 64–81
[2] Bushman A V, Lomonosov I V, Fortov V E and Khishchenko K V 1994 Khim. Fiz. 13(5) 97–106
[3] Lomonosov I V, Fortov V E and Khishchenko K V 1995 Khim. Fiz. 14(1) 47–52
[4] Badretdinova L K, Kostitsin O V, Smirnov E B, Stankevich A V, Ten K A, Tolochko B P and Shakirov I R 2014 XII Zababikhin Scientific Talks (Snezhinsk) pp 23–27
[5] Ten K A, Prunel E R, Lukyanchikov L A, Tolochko B P, Sharaftudinov M R, Shmakov A N, Aminov Y A, Muzyria A K, Kostitsin O and Smirnov E B 2012 XI Zababikhin Scientific Talks (Snezhinsk)
[6] Badretdinova L K, Kostitsyn O V, Smirnov E B, Stankevich A V, Ten K A and Tolochko B P 2015 Bull. Russ. Acad. Sci.: Phys. 79 15–19
[7] Stevens L L, Velisavljevic N, Hooks D E and Dattelbaum D M 2008 Propellants, Explos., Pyrotech. 33 286–295
[8] Smirnov E B, Kostitsin O V, Shcherbakov V N, Prosvirnin K M, Kiselev A N and Akhlustin I A 2014 Physics of Extreme States of Matter—2014 ed Fortov V E et al (Moscow: JIHR RAS)
[9] Shorohov E V and Litvinov B V 1995 Shock Waves at Marseille III: Shock Waves in Condensed Matter and Heterogeneous Media ed Brun R and Dumitrescu L Z (Berlin, Heidelberg: Springer) pp 295–298
[10] Zababakhin E I 1997 Some Problems of the Gasdynamics of Explosions (Snezhinsk: RFNC VNIITF)
[11] Zharkov V N and Kalinin V A 1968 Equations of State for Solids at High Pressures and Temperatures (Moscow: Nauka)
[12] Bushman A V and Fortov V E 1983 Phys. Usp. 26 465–496
[13] Levashev P R, Khishchenko K V, Lomonosov I V and Fortov V E 2004 AIP Conf. Proc. 706 87–90