

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 ~ 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 ≈ 1.01 .



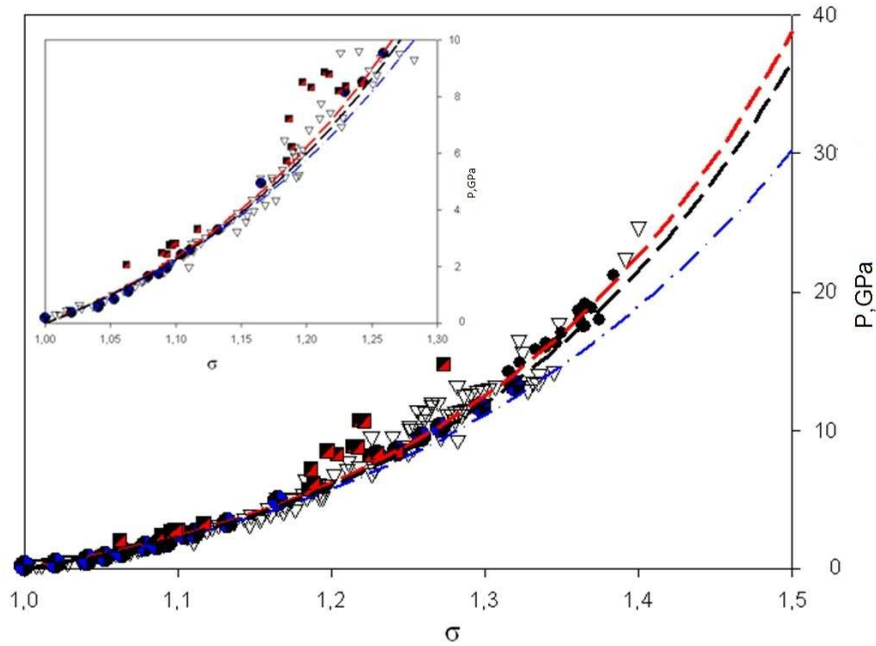


Figure 1. TATB ESM static and dynamic experimental data and results of the data fitting: black downtriangle—shock-wave data for $k = 1.01$ [9]; black dashed line—approximation of shock-wave data on $k = 1.01$ [9]; black-blue solid circles—ESM isotherm data [6]; blue dash-dot line—the isotherm approximation; black open circles—ESM isotherm data [7]; black-red solid squares—shock-wave data for $k = 1.05$ [13]; red dashed line—approximation of shock-wave data on $k = 1.05$ [13]; black solid circles—shock-wave data [8].

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]:

$$P = P_x + P_t = P_x + \Gamma \rho_0 (\varepsilon - \varepsilon_x), \quad (1)$$

where $P_x = \rho_0 C_0 (\sigma^n - 1)/n$ is the elastic pressure; Γ is the Grüneisen constant; ε is the internal matter energy; ε_x is the elastic compression energy; ρ_0 is the initial density of matter; $\sigma = \rho/\rho_0$ is the compression ratio; ρ is the current density of matter.

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

$$P = \frac{\rho_0 C_0^2}{n} \frac{\sigma^n [h - (n+1)/(n-1)] + \sigma 2n/(n-1) - (h+1)}{h - k\sigma}, \quad (2)$$

where $h = 2/\Gamma + 1$ is the ultimate compression ratio; $k = \rho_{cr}/\rho_0$ is the porosity ratio; ρ_{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].

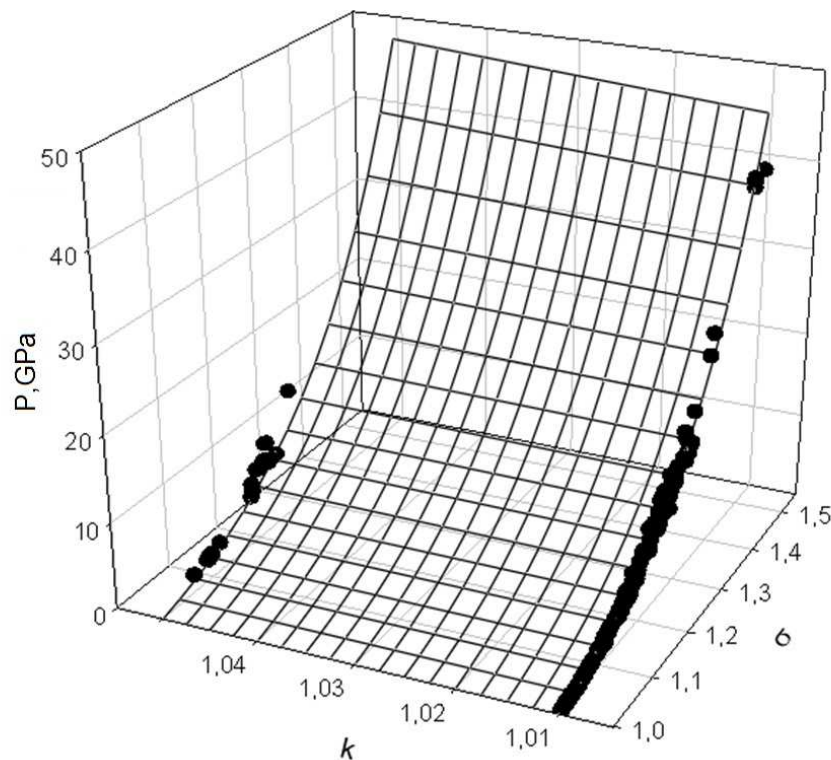


Figure 2. Surface $P(\sigma, k)$ (2) approximated experimental data on shock compressibility of ESM having various initial porosity: circles correspond to data for $k = 1.01$ [8,9] and 1.05 [13].

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.

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