

EQUATION OF STATE FOR LITHIUM IN SHOCK WAVES

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Summary. An equation of state in the form of an analytic function of the pressure on the specific volume and the internal energy is proposed for lithium in the bcc-solid and liquid phases. The principal Hugoniot adiabat is calculated for the metal and compared with available shock-wave data. The results of the calculations are in good agreement with the data over the whole range of kinematic and dynamic characteristics investigated. This equation of state can be used effectively in simulations of shock-wave processes in lithium at high pressures.

1 INTRODUCTION

Equations of state (EOSs) of materials are necessary in hydrodynamic simulations of physical processes at high energy densities [1–3]. Such processes take place at high-velocity impingement of bodies [4–11], interaction of intense laser [12–23] and particle beams [24–28] with a condensed medium, electrical explosion of conductors under the action of high power current pulses [29–36], etc. The adequacy of the simulation results is determined mainly by accuracy of thermodynamic description of the materials response upon the changes in surrounding conditions over a wide range of pressures and specific volumes [37, 38].

For wide-range EOS modeling, a semiempirical approach is commonly applied [1], where a functional form of a thermodynamic potential is chosen via theoretical considerations, while numerical coefficients in the form are determined using experimental data [39–41].

In the work, a semiempirical EOS for lithium is proposed. This metal is used as a coolant in power plants, especially in molten salt reactors. In particular, EOS for lithium is of interest for numerical modeling of different working regimes of such reactors.

Unlike more complex EOSs of Li [2, 42–45], a simple analytic function $P = P(V, E)$ [46–48] is adapted for the metal, where, P is the pressure, $V = \rho^{-1}$ is the specific volume, ρ is the density, E is the specific internal energy. Thermodynamic characteristics of lithium along the principal Hugoniot adiabat are calculated and compared with available data from shock-wave experiments [49–52].

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2 EOS MODEL

The EOS model is formulated in the general form as

$$P(V, E) = P_c(V) + \frac{\Gamma(V, E)}{V} [E - E_c(V)]. \quad (1)$$

Here, E_c and $P_c = -dE_c/dV$ are the cold components of internal energy and pressure at $T = 0$ given by polynomials [53–58]:

$$E_c(V) = \frac{B_{0c} V_{0c}}{m-n} \left(\frac{\sigma_c^m}{m} - \frac{\sigma_c^n}{n} \right) + E_{\text{sub}} \quad (2)$$

and

$$P_c(V) = \frac{B_{0c} \sigma_c}{m-n} (\sigma_c^m - \sigma_c^n), \quad (3)$$

$\sigma_c = V_{0c}/V$; V_{0c} and B_{0c} are the specific volume and bulk modulus at $P = 0$ and $T = 0$. The quantity E_{sub} has meaning of the sublimation energy; it is determined by a normalization condition $E_c(V_{0c}) = 0$, which gives

$$E_{\text{sub}} = \frac{B_{0c} V_{0c}}{mn}. \quad (4)$$

Parameters m and n are determined using shock-wave data for solid samples.

The coefficient Γ as a function of the volume and internal energy is defined analogously to caloric models [56–61] in the following form:

$$\Gamma(V, E) = \gamma_i + \frac{\gamma_c(V) - \gamma_i}{1 + \sigma^{-2/3} [E - E_c(V)] / E_a}, \quad (5)$$

where

$$\gamma_c(V) = 2/3 + (\gamma_{0c} - 2/3) \frac{\sigma_n^2 + \ln^2 \sigma_m}{\sigma_n^2 + \ln^2(\sigma/\sigma_m)}, \quad (6)$$

$\sigma = V_0/V$; V_0 is the specific volume under normal conditions; $\gamma_c(V)$ corresponds to the case of low thermal energies, and γ_i characterizes the region of highly-heated matter. The value of E_a defines the thermal energy of the transition of Γ from one limiting case to the other; it is determined from the results of shock-wave experiments at high pressures. From equations (1), (5) and (6), one can obtain a relation of the parameter γ_{0c} with values of the Grüneisen coefficient $\gamma = V(\partial P/\partial E)_V$, the internal energy and the specific volume under normal conditions (γ_0 , E_0 and V_0 , respectively):

$$\gamma_{0c} = \gamma_i + (\gamma_0 - \gamma_i) \left[1 + \frac{E_0 - E_c(V_0)}{E_a} \right]^2. \quad (7)$$

Therefore, the interpolational function (6) ensures validity of the condition $\gamma(V_0, E_0) = \gamma_0$, and gives the asymptotic value $\gamma_c = 2/3$ in the limiting cases of low and high compression ratios σ . The parameters σ_n and σ_m are determined from the requirement of optimum fit to experimental data on shock compressibility of a substance in question.

3 EOS FOR LITHIUM

Lithium in the solid phase under atmospheric pressure has a body-centered cubic (bcc) structure ($T > 75$ K) [62]; it melts at 454 K. Under static compression at room temperature, the bcc phase transforms at pressure 6.9 GPa [63] to the phase with a face-centered cubic (fcc) structure. At further increase of pressure at room temperature, more crystalline phases of lithium are observed [64–66].

Shock compressibility of lithium is studied with the use of traditional explosive systems up to 70 GPa [49–52]. Shock compression leads to increase of temperature and melting of the bcc phase [44].

In this work, the unified EOS for the bcc-solid and liquid phases of lithium is constructed. The EOS coefficients are as follows: $V_0 = 1.8868 \text{ cm}^3/\text{g}$, $V_{0c} = 1.8422 \text{ cm}^3/\text{g}$, $B_{0c} = 11.887 \text{ GPa}$, $m = 0.67$, $n = 0.48$, $\sigma_m = 0.9$, $\sigma_n = 1$, $\gamma_{0c} = 0.6$, $\gamma_l = 0.45$ and $E_a = 5 \text{ kJ/g}$.

Calculated principal Hugoniot adiabat of lithium is presented in figures 1–3 in comparison with experimental data [49–52]. Calculation of the Hugoniot adiabat is performed by solving the equation of energy conservation in the shock front [1]:

$$E = E_0 + \frac{1}{2}(P_0 + P)(V_0 - V), \quad (8)$$

where the left-hand side is closed by the EOS function $E = E(P, V)$. Equation (8) and the EOS determine the specific volume as a function of pressure along the Hugoniot adiabat for samples of initial density $\rho_0 = V_0^{-1}$. The shock (U_s) and particle (U_p) velocities are calculated using the equations of conservation of mass and momentum in the shock front [1]:

$$U_s = V_0 \sqrt{(P - P_0)/(V_0 - V)}, \quad (9)$$

$$U_p = \sqrt{(P - P_0)(V_0 - V)}. \quad (10)$$

As one can see in figures 1–3, the obtained EOS provides for reliable description of thermodynamic properties of the metal over the entire range of shock and particle velocities, pressures and compression ratios investigated.

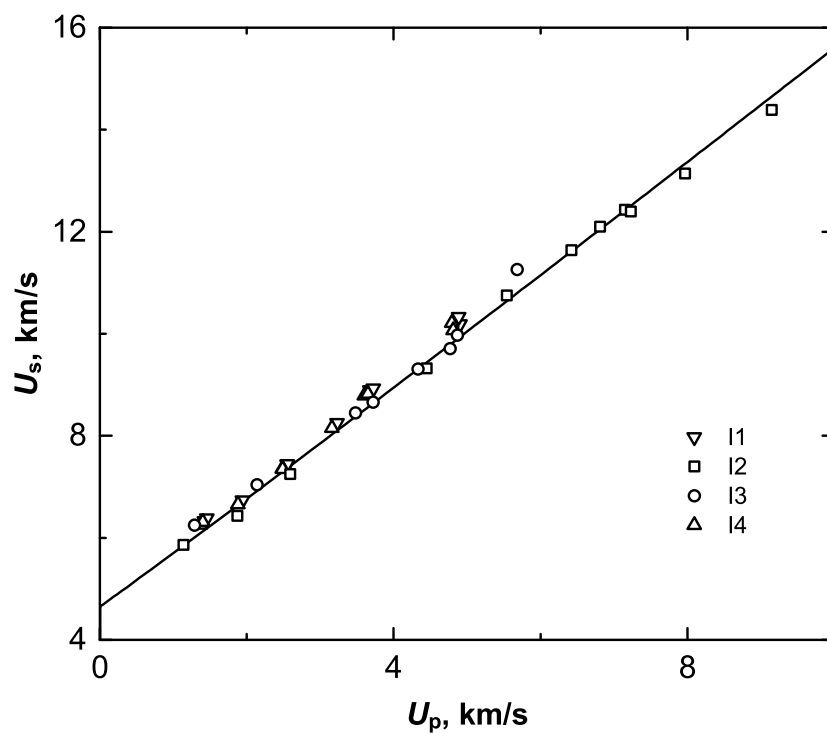


Figure 1. The principal Hugoniot adiabat of lithium: curve corresponds to the present calculations; markers—experimental data (I1—[49], I2—[50], I3—[51], I4—[52]).

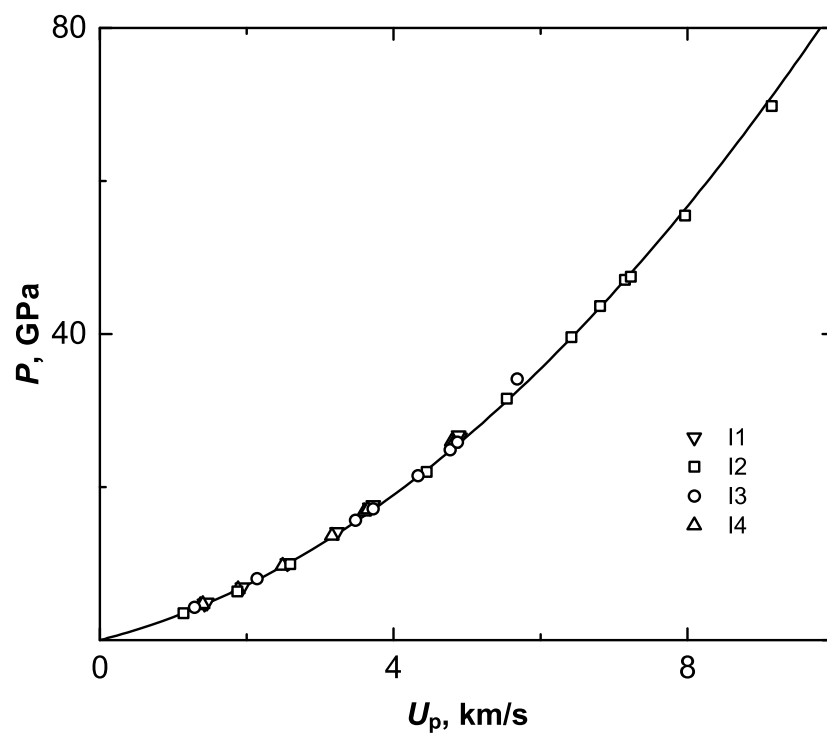


Figure 2. The principal Hugoniot adiabat of lithium: notations are analogous to figure 1.

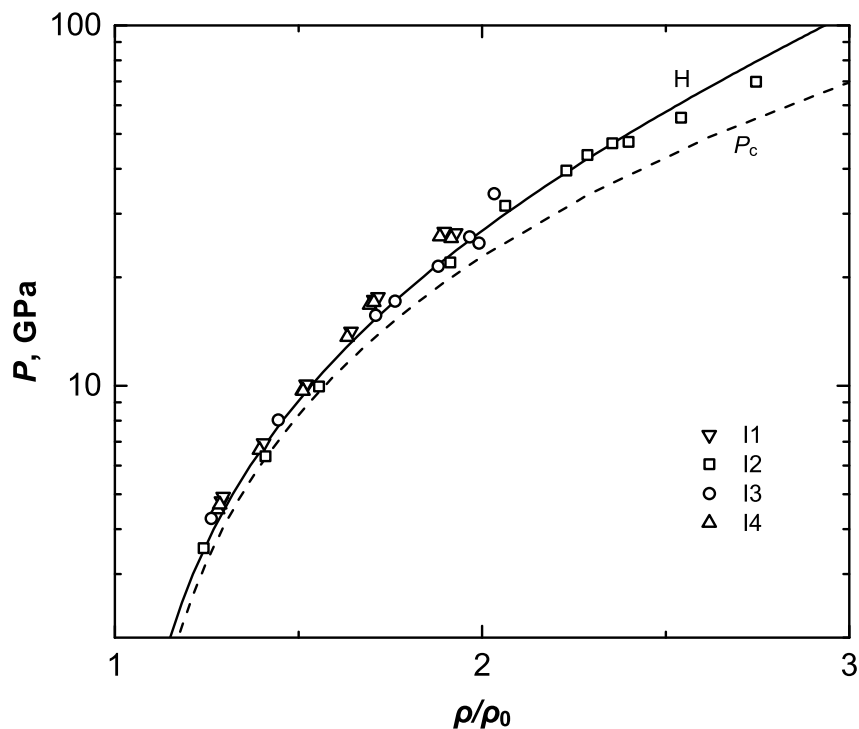


Figure 3. The cold curve (P_c) and the principal Hugoniot adiabat (H) of lithium: curves correspond to the present calculations; markers—experimental data (I1—[49], I2—[50], I3—[51], I4—[52]).

4 CONCLUSIONS

The EOS in the form of an analytic function $P = P(V, E)$ is created for lithium in the bcc-solid and liquid phases. This EOS agrees well with available shock-wave data; it can be used effectively in numerical simulations of dynamic processes in the metal at high pressures.

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