Equation of state for potassium in shock waves at high pressures

K V Khishchenko$^{1,2}$

$^1$ Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
$^2$ Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia
E-mail: konst@ihed.ras.ru

Abstract. A simple caloric equation-of-state model, which relates the pressure with density and internal energy, is applied for potassium in the bcc-solid and liquid phases. Thermodynamic characteristics along the principal Hugoniot are calculated for the metal and compared with available data from shock-wave experiments at high pressures.

1. Introduction
Equations of state (EOSs) of materials are necessary elements of simulations of various physical processes at interaction of intense energy fluxes with media [1–4]. Such as high velocity collision of bodies [5–12], interaction of intense laser [13–21] and particle beams [22–31] with matter, fast heating of conductors by high power current pulses [32–40] etc. Accuracy of thermodynamic description of properties over wide range of pressures and densities determine the adequacy of results of the simulations, see e.g. [41]. A semiempirical approach is traditionally used to build wide-range EOS models [1, 42, 43].

This paper is devoted to thermodynamic description of properties of potassium. The metal is used as a heat-transfer medium in power-plants. Particularly, EOS for potassium is of interest for analysis of different working regimes of the power-plants under conditions of intense mechanical and thermal loadings.

A semiempirical EOS in a simple caloric form $P = P(V, E)$ [44,45] is presented for the metal. Here, $P$ is the pressure, $V = \rho^{-1}$ is the specific volume, $\rho$ is the density, $E$ is the specific internal energy. The EOS provides an adequate description of thermodynamic properties of K in the bcc-solid and liquid phase states realized under conditions of shock compression and isentropic expansion at high pressures.

2. EOS model
The EOS model is formulated in the general form as

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

where $E_c$ and $P_c = -dE_c/dV$ are the cold components of energy and pressure at $T = 0$; $\Gamma$ is a coefficient determining the contribution of thermal components of the EOS.
The cold-interaction energy is given by the relation [44–48]

\[ E_c(V) = \frac{B_0cV_0c}{m - n} \left( \frac{\sigma_m^2}{m} - \frac{\sigma_c^2}{n} \right) + E_{sub}, \quad (2) \]

Here, \( \sigma_c = V_0c/V; \) \( V_0c \) and \( B_0c \) are the specific volume and bulk modulus at \( P = 0 \) and \( T = 0. \) Value \( E_{sub} \) has meaning of the sublimation energy and is determined by a normalized condition

\[ E_c(V_0c) = 0, \quad (3) \]

which gives

\[ E_{sub} = \frac{B_0cV_0c}{mn}. \quad (4) \]

The functional dependence of the coefficient \( \Gamma \) upon the volume and internal energy is defined analogously to caloric models [44, 45, 49–53] in the following form:

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

\[ \gamma_c(V) = 2/3 + (\gamma_0c - 2/3) \frac{\sigma_n^2 + \ln^2 \sigma_m}{\sigma_n^2 + \ln^2(\sigma/\sigma_m)}, \quad (6) \]

where \( \sigma = V_0/V; \) \( V_0 \) is the specific volume under normal conditions; \( \gamma_c(V) \) corresponds to the case of low thermal energies, and \( \gamma_i \) characterizes the region of highly-heated condensed substance. The energy \( E_a, \) which sets the thermal energy of a transition of \( \Gamma \) from one limiting case to another, is determined from the results of shock-wave experiments at high pressures.

From equations (1), (5) and (6), a relation of the parameter \( \gamma_0c \) can be obtained:

\[ \gamma_0c = \gamma_i + (\gamma_0c - \gamma_i) \left[ 1 + \frac{E_0 - E_c(V_0c)}{E_a} \right]^2. \quad (7) \]

The functional form (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 \( \sigma. \) The parameters \( \sigma_n \) and \( \sigma_m \) are determined from the requirement of optimum fit to experimental data on shock compressibility of a substance in question.

3. EOS for potassium

Potassium under atmospheric pressure has a body-centered cubic (bcc) structure [54]. It melts at 337 K. Under compression at room temperature, the bcc phase I transforms at pressure 12 GPa to the phase II with a face-centered cubic (fcc) structure. At further increase of pressure at room temperature, more crystalline phases of potassium are observed [55–58].

Shock compressibility of potassium is investigated with use of traditional explosive systems up to 0.1 TPa [59–61]. Shock compression leads to increase of temperature and melting of the phase I.

In this work, EOS for the bcc-solid and liquid phases of potassium is constructed. The EOS coefficients for K obtained within the framework of the model are as follows: \( V_0 = 1.1628 \) cm\(^3\)/g, \( V_0c = 1.1057 \) cm\(^3\)/g, \( B_0c = 3.81484 \) GPa, \( m = 1, \) \( n = 0.7, \) \( \sigma_m = 0.9, \) \( \sigma_n = 0.7, \) \( \gamma_0c = 0.6, \) \( \gamma_i = 0.45 \) and \( E_a = 6 \) kJ/g.

Calculated principal Hugoniot of potassium is presented in figures 1–3 in comparison with data from experiments [59–61]. Calculation of the Hugoniot is performed by solving the equation of energy conservation in the shock-wave front [1]:

\[ E = E_0 + \frac{1}{2}(P_0 + P)(V_0 - V), \quad (8) \]
Figure 1. The principal Hugoniot of potassium: curve corresponds to the present calculations; markers—experimental data (I1—[59], I2—[60], I3—[61]).

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

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 for samples of initial
Figure 3. The cold curve \( (P_c) \) and the principal Hugoniot \( (H) \) of potassium: curves correspond to the present calculations; markers—experimental data (I1—[59], I2—[60], I3—[61]).

Then the shock \( (U_s) \) and particle \( (U_p) \) velocities are calculated using the equations of conservation of mass and momentum in the shock-wave front [1]:

\[
U_s = V_0 \sqrt{(P - P_0)/(V_0 - V)}, \quad U_p = \sqrt{(P - P_0)(V_0 - V)}. \tag{9}
\]

Analysis of the comparison results in figures 1–3 shows that the obtained EOS provides for a reliable description of thermodynamic properties of the metal over a whole investigated range of shock and particle velocities, pressures and compression ratios.

4. Conclusion

The EOS, which has the form of an analytic function, is proposed for potassium in the bcc-solid and liquid phases. This EOS agrees well with available shock-wave data over a wide range of pressures and densities; one can use it effectively in numerical simulations of physical processes in the metal at high energy densities.

Acknowledgments

The work is supported by the Russian Science Foundation (grant No. 14-50-00124).

References

[1] Zel’dovich Ya B and Raizer Yu P 1967 Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena (New York: Academic Press)
[2] Bushman A V, Fortov V E, Kanel’ G I and Ni A L 1993 Intense Dynamic Loading of Condensed Matter (Washington: Taylor & Francis)
[3] Fortov V 2016 Thermodynamics and Equations of State for Matter: From Ideal Gas to Quark–Gluon Plasma (Singapore: World Scientific Publishing)
[4] Lomonosov I V and Fortova S V 2017 High Temp. 55 585–610
[5] Agureikin V A, Anisimov S I, Bushman A V et al 1984 High Temp. 22 761–78
