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Equations of state for rubidium and cesium at high pressures in shock waves

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

1. Introduction
Equations of state (EOSs) for substances over wide range of pressures and densities are needed for numerical simulations of processes at powerful interactions with condensed matter [1–3]. Such processes occur, in particular, when intense laser [4–9] and particle [10–13] beams, high current pulses [14–20], detonation products from chemical explosives [21–24] and high-velocity bodies [25–28] influence upon materials. In some experimental studies, numerical simulations are often necessary for interpretation of results of complex measurements at extreme conditions [29–33].

Alkali elements rubidium and cesium are used as working fluids in turboelectric generators and heat-transfer media in power plants. EOSs for these metals are of interest for simulating various working regimes of such systems at intense mechanical and thermal actions.

In this work, a semiempirical approach is used for thermodynamic description of properties of rubidium and cesium at high energy densities. A simple caloric form of EOS [34–36] is adapted for these two metals in the bcc-solid and liquid phases. The EOS-calculation results are compared with available data from shock-wave experiments [37, 38].

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

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

where \( P \) is the pressure; \( V = \rho^{-1} \) is the specific volume; \( \rho \) is the density; \( E \) is the specific internal energy; \( E_c \) is a cold component of the energy at zero temperature \( T = 0 \); \( P_c = -\frac{dE_c}{dV} \) is the corresponding cold pressure at \( T = 0 \); \( \Gamma \) is a coefficient determining the contribution of thermal components of the EOS.
The cold energy is given by the relation \[39–43\]

\[ E_c(V) = B_{0c}V_{0c} \left( \frac{\sigma_m^{n}}{m} - \frac{\sigma_n^{n}}{n} \right) + E_{\text{sub}}. \]  

(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 \( E_{\text{sub}} \) has meaning of the sublimation energy and is determined by a normalizing condition

\[ E_c(V_{0c}) = 0, \]  

(3)

which gives

\[ E_{\text{sub}} = B_{0c}V_{0c}. \]  

(4)

The coefficient \( \Gamma \) as a function of the specific volume and internal energy is defined analogously to caloric models \[42–48\] in the following form:

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

(5)

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

(6)

where \( \sigma = V_0/V; \) \( V_0 \) is the specific volume under normal conditions \( P = 0.1 \) MPa, \( E = E_0; \) the function \( \gamma_c(V) \) corresponds to the case of low thermal energies, and the constant \( \gamma_i \) characterizes the case 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), one can obtain a relation of the quantity \( \gamma_{0c} \) with values of the Grüneisen coefficient \( \gamma = V(\partial P/\partial E)_V \), the specific internal energy and the specific volume under normal conditions (\( \gamma_0, E_0 \) and \( V_0 \)):

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

(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 generally found from the condition of optimum description of experimental data on shock compressibility of substances.

3. EOSs for the two metals

Under normal pressure, the solid phases of rubidium and cesium have a body-centered cubic (bcc) structure \[49\]; Rb melts at 312 K, Cs—at 301 K. Under compression at room temperature, the bcc phase I transforms at pressure 7 (Rb) and 2.26 GPa (Cs) to the phase II with a face-centered cubic (fcc) structure. With a further increase in pressure at room temperature, other crystalline phases of rubidium and cesium are also observed \[49–52\].

Shock compressibility of rubidium and cesium is studied with the use of traditional explosive systems up to about 40 GPa \[37, 38\]. Shock compression of these metals leads to an increase in temperature and melting of the phase I.

In this work, EOSs for the bcc-solid and liquid phases of rubidium and cesium are constructed. The EOS coefficients for Rb and Cs obtained within the framework of the model are listed in table 1.

Calculated principal Hugoniots of Rb and Cs are displayed in figures 1 and 2 in comparison with data from shock-wave experiments \[37, 38\]. Analysis of the comparison results in figures 1 and 2 shows that the obtained EOSs provide for a reliable description of thermodynamic properties of these two metals over a whole investigated range of shock and particle velocities \( (U_s \) and \( U_p \)), pressures and densities.
Figure 1. The principal Hugoniots of rubidium (red) and cesium (blue): curves correspond to the present calculations; markers—experimental data (R1 and C1—[37]; R2 and C2—[38]).

Figure 2. The principal Hugoniots of rubidium and cesium: notations are analogous to figure 1.
Table 1. The EOS coefficients for rubidium and cesium.

| Metal | $V_0$ (cm$^3$/g) | $V_{0c}$ (cm$^3$/g) | $B_{0c}$ (GPa) | $m$ | $n$ | $\sigma_m$ | $\sigma_n$ | $\gamma_{0c}$ | $\gamma_i$ | $E_a$ (kJ/g) |
|-------|-----------------|-----------------|---------------|-----|-----|-----------|-----------|-----------|----------|-------------|
| Rb    | 0.65359         | 0.61659         | 2.17169       | 1   | 1.5 | 0.9      | 1         | 0.8       | 0.45     | 6          |
| Cs    | 0.54765         | 0.51182         | 0.41743       | 1   | 3.6 | 0.9      | 1         | 0.9       | 0.45     | 6          |

4. Conclusion
EOSSs in the form of an analytic function are proposed for rubidium and cesium in the bcc-solid and liquid phases. These EOSs agree well with available shock-wave data; one can use the EOSs effectively in numerical simulations of physical processes in the metals at high pressures.

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