Equation of state for rhenium at high pressures

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Abstract. In this work, the equation of state for rhenium is proposed as a relationship between pressure, internal energy and density. The consistency of calculation results with experimental data at high energy densities is demonstrated. The equation of state can be used in numerical simulations of dynamic processes in this metal.

1. Introduction
The development of experimental methods for generating extreme conditions of high pressures and high temperatures in a substance requires thermodynamic models of the behavior of various media [1]. In particular, the refractory metal rhenium is used in high-temperature measurements at resistive heating [2], as well as in high-pressure investigations in diamond-anvil cells [3–9]. The equation of state (EOS) for this material is needed for numerical simulations of related and other processes [10–12].

In the present work, the equation of state for rhenium is developed in the form of a relationship between specific internal energy $E$, specific volume $V = \rho^{-1}$ ($\rho$ is the density) and pressure $P$. The calculation results are compared with the available high-pressure data for this metal from static [6, 7] and dynamic [13, 14] experiments.

2. EOS model
The accepted EOS model [15] is based on the quasi-harmonic approximation, which is expressed by the equation

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

Here, $E_c$ is the internal energy at zero temperature $T = 0$; $P_c = -dE_c/dV$ is the corresponding pressure. The coefficient $\Gamma$ represents the ratio of the thermal pressure $P - P_c$ to the thermal energy density $[E - E_c]/V$.

The cold energy depends on the volume as

$$E_c(V) = \frac{B_0 V_0 c^m}{m - n} \left( \frac{\sigma_c^m}{m} - \frac{\sigma_c^n}{n} \right) + E_{sub},$$

where $\sigma_c = V_0 c/V$; $V_0 c$ is the specific volume of the substance at $T = 0$ and $P = 0$; $B_0 c$ is the bulk modulus $B_c = -VdP_c/dV$ at $T = 0$ and $P = 0$; $E_{sub} = B_0 V_0 c/(mn)$; $m$ and $n$ are parameters.
The coefficient $\Gamma$ depends on the volume and the internal energy as

$$\Gamma(V, E) = \gamma_1 + \frac{\gamma_c(V) - \gamma_1}{1 + \sigma^{-2/3} \frac{E - E_c(V)}{E_a}}. \quad (3)$$

Here, $\gamma_c$ is the Grüneisen coefficient at $T = 0$; $\gamma_1$ is the constant value of the Grüneisen coefficient corresponded to the case of high thermal energy densities; $\sigma = V_0/V$; $V_0$ is the specific volume of the substance under normal conditions at $T = T_0$ and $P = P_0$. The parameter $E_a$ determines the behavior of $\Gamma$ between the cases of low and high thermal energy densities.

The cold Grüneisen coefficient depends on the volume as

$$\gamma_c(V) = 2/3 + (\gamma_{0c} - 2/3) \frac{\sigma_m^2 + \ln^2 \sigma_m}{\sigma_n^2 + \ln^2 \sigma_m}, \quad (4)$$

where $\gamma_{0c}$ is the value of $\gamma_c$ at $V = V_0$; $\sigma_m$ and $\sigma_n$ are parameters.

3. EOS for rhenium

Under normal pressure, the solid phase of rhenium has a hexagonal close packed (hcp) structure; it melts at $T = 3463$ K [16]. At normal temperature, quasi-hydrostatic compression of rhenium is studied up to 280 GPa [3–8]; some compression experiments are known up to about 640 GPa [6]; at those, rhenium remains in the hcp phase.
Shock compression of rhenium is studied with the use of traditional explosive systems up to 280 GPa [13,14]. Using special explosive systems, pressures up to 590 GPa was realized in shock waves [14].

Results of the Hugoniot calculations for rhenium are shown in figures 1 and 2 in comparison with shock-wave data [13,14]. As one can see in figures 1 and 2, the EOS agrees well with the data over the entire range of measured shock-front and particle velocities, $U_s$ and $U_p$, respectively.

Figure 3 shows the diagram of states of rhenium studied at high pressures. Calculated curves of shock compression are in a good agreement with data from dynamic experiments [13,14]. The calculated cold curve also agrees with data from static experiments at room temperature [7] and corresponding fitted isotherm [17]. It is strange that the data from experiments with both conventional and double-stage diamond-anvil cells [6] not only do not agree with other data on static compression [7,8], but also clearly contradict the data on dynamic compression [13,14]. The pressure in those experiments at room temperature [6] is estimated to be much higher than at the same densities (or the density is estimated to be much less than at the same pressures) in dynamic experiments [13,14], although this is hardly possible, since entropy and temperature normally increase at shock compression [18–21] and, therefore, the pressure (respectively, in a shock-wave experiment) should be greater than at the same density (for the same phase) at initial room temperature [22].

The coefficients of EOS for rhenium in the framework of equations (1) to (4) are as follows:

$V_0 = 0.047551$ cm$^3$/g, $V_{0c} = 0.047383$ cm$^3$/g, $B_{0c} = 359.242255$ GPa, $m = 1.13$, $n = 1.15$, $\sigma_m = 0.9$, $\sigma_n = 0.7$, $\gamma_{0c} = 1.75$, $\gamma_i = 0.45$ and $E_a = 55$ kJ/g.
Figure 3. The Hugoniot adiabats for samples with different initial densities $\rho_{00}$ (H), the room-temperature isotherm ($P_r$) and the cold curve ($P_c$) of rhenium: solid lines—adiabats from the present EOS; black dash-dot line— isotherm $T = 0$ from the present EOS; green dash-dot line— isotherm $T = 300$ K [17]; markers—data from experiments on shock loading at $\rho_{00} = 20.99$ (I1—[13]), 20.53 (I2—[13]) and 21.03 g/cm$^3$ (I3—[14]) and static compression at room temperature (I4—[6]; I5—[7]); $\rho_0 = 21.03$ g/cm$^3$.

4. Conclusion
The EOS $P(V, E)$ has been proposed, which adequately describes experimental data upon the shock and static compression of rhenium at high pressures. This EOS can be used in the numerical simulation of various processes in the interaction of intense energy fluxes with matter.

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