Equation of state for iridium at high pressures

K V Khishchenko\textsuperscript{1,2,3}

\textsuperscript{1} Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
\textsuperscript{2} Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
\textsuperscript{3} South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia

E-mail: konst@ihed.ras.ru

Abstract. An equation of state for iridium is proposed in a wide range of density and internal energies. The results of calculations using this equation of state are compared with the available experimental data for this metal at high pressures. The proposed equation of state can be used to simulate adiabatic processes in iridium under shock-wave loading.

1. Introduction
Equations of state (EOSs) of materials are required for hydrodynamic modeling of processes with high energy concentration [1–3]. Such processes take place, for example, during a high-speed collision of bodies [4–6], when a substance is exposed to intense laser radiation [7–10] or beams of high-energy particles [11–13], during an electric explosion of conductors [14–17]. The EOS essentially determines the correspondence of the results of numerical modeling to the physical characteristics of flows arising in the modeled process [2, 18, 19].

Iridium is a refractory metal with high hardness and corrosion resistance, which is used, in particular, to coat x-ray reflecting mirrors [20] and as a target material for the production of antiprotons [21]. The EOS for this metal in a wide range of pressures ($P$), specific volumes ($V = \rho^{-1}; \rho$ is the density) and internal energies ($E$) is necessary to simulate various processes under intense pulsed action, accompanied by the formation of shock waves.

In this work, an EOS for iridium is proposed in the form of a pressure function depending on the specific volume and internal energy. The calculation results are presented in comparison with the available experimental data in the high-pressure region.

2. EOS model
The EOS for matter is developed on the basis of the model [22–24], in which thermodynamic functions are related by the following general dependence:

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

(1)

Here, $E_c$ and $P_c$ are internal energy and pressure at zero temperature, $T = 0$; $\Gamma$ is the ratio of thermal pressure to thermal energy density.
The energy $E_c$ on the cold compression curve for $V \leq V_{0c}$ (where $V_{0c}$ is the specific volume of matter at $P = 0$ and $T = 0$) is given by a transcendental function:

$$E_c(V) = 3V_{0c} \left( \frac{a_0}{3} \ln \sigma_c - \sum_{i=1}^{\infty} \frac{a_i}{i} \sigma_c^{-i/3} + \sum_{i=1}^{\infty} \frac{b_i}{i} \sigma_c^{i/3} + \sum_{i=1}^{\infty} \frac{a_i}{i} - \sum_{i=1}^{\infty} \frac{b_i}{i} \right), \quad (2)$$

where $\sigma_c = V_{0c}/V$. This expression satisfies the following condition:

$$E_c(V_{0c}) = 0. \quad (3)$$

The value of the coefficient $b_2$ is selected from the model of an ideal fermion gas in the limit of high compression ratios:

$$b_2 = 3^{2/3} \pi^{-1} \frac{4^{4/3}}{Z^{5/3}} \frac{\alpha_0^2}{a_0^3} E^2 \frac{[A m_u V_{0c}]}{V_{0c}}^{5/3}, \quad (4)$$

where $a_0$ is the Bohr radius; $E_H$ is the Hartree energy; $m_u$ is the unified atomic mass unit; $A$ is the relative atomic mass; $Z$ is the atomic number. The values of the remaining coefficients $b_1$ and $a_i$ in function (2) are determined from the requirement for a minimum root-mean-square deviation of cold pressure $P_c = -dE_c/dV$ from the results of calculations by the Thomas–Fermi model with quantum and exchange corrections [25] in a certain range of compression ratios when the conditions for pressure, bulk modulus $B_c = -VdP_c/dV$ and its derivative with respect to pressure $B'_c = dB_c/dP_c$ are met at $T = 0$ and $\sigma_c = 1$:

$$P_c(V_{0c}) = 0, \quad (5)$$
$$B_c(V_{0c}) = B_{0c}, \quad (6)$$
$$B'_c(V_{0c}) = B'_{0c}. \quad (7)$$

The energy $E_c$ for $V > V_{0c}$ is given by an algebraic function:

$$E_c(V) = V_{0c} \left( \frac{a_m}{m} \sigma_c^m + \frac{a_n}{n} \sigma_c^n - \frac{a_m}{m} + \frac{a_n}{n} \right) + E_{sub}, \quad (8)$$

where $E_{sub}$ is the sublimation energy at zero temperature. This relation satisfies condition (5). Conditions (3), (6) and (7) are required additionally. Taking this into account, two parameters ($l$ and $n$) remain free in expression (8).

The thermal contribution to the EOS is determined by the coefficient $\Gamma$, which depends upon the specific volume and internal energy:

$$\Gamma(V, E) = \gamma_1 + \frac{\gamma_c(V) - \gamma_1}{1 + \sigma^{-2}(E - E_c(V))/E_a}, \quad (9)$$

where $\sigma = V_0/V$; $V_0$ is the specific volume of matter under normal conditions ($P = P_0$, $E = E_0$); $\gamma_1$ is a constant characterizing hot matter; $\gamma_c$ is a function of the specific volume corresponding to the Grüneisen coefficient at zero temperature; $E_a$ is the characteristic thermal energy that delimits the cases of hot and cold matter. Dependency $\gamma_c(V)$ is taken similarly to work [26]:

$$\gamma_c(V) = 2/3 + (\gamma_{0c} - 2/3) \frac{\sigma_n^2 + \ln^2 \sigma_m}{\sigma_n^2 + \ln^2 (\sigma/\sigma_m)}, \quad (10)$$

where $\gamma_{0c}$ is the Grüneisen coefficient at $T = 0$ and $V = V_0$; $\sigma_n$ and $\sigma_m$ are free parameters.

3. Calculation results

The shock compressibility of iridium was studied using conventional explosive devices up to pressures of 292 GPa [27, 28]. The use of special hemispherical explosive devices [29] made it possible to obtain a pressure of 617 GPa in iridium under shock loading [28].
Figure 1. Shock adiabat of iridium: line—the result of calculation according to the presented EOS; markers—experimental data (I1—[27]; I2—[28]).

Figure 2. Shock adiabat of iridium: the designations are the same as in figure 1.

Comparison of the calculated shock adiabat with data [27, 28] for iridium is illustrated in figures 1–3. Figure 3 also shows the calculated cold curve of the metal in comparison with the results of static compression experiments at room temperature [30].
Figure 3. Shock adiabat (H), cold curve ($P_c$) and room-temperature isotherm ($P_r$) of iridium: black solid and dash-dot lines—shock adiabat and cold curve calculated using the presented EOS; green dash-dot line—room-temperature isotherm [30]; markers—experimental data upon shock (I1—[27]; I2—[28]) and isothermal (I3—[30]) compression.

Analysis of figures 1–3 allows one to conclude that there is a fairly good description of the properties of iridium in the entire investigated range of velocities of the shock front and matter behind this front, pressures and compression ratios.

4. Conclusion
Thus, the developed equation of state for iridium is in good agreement with the experimental data available at high pressures. This equation of state can be used for numerical simulation of hydrodynamic processes in this material in shock waves.

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