Уравнение состояния рутения при высоких давлениях и температурах

К. В. Хищенко[1,2,3,4,*]

[1]Объединенный институт высоких температур РАН, Москва, Россия
[2]Московский физико-технический институт, Долгопрудный
[3]Федеральный исследовательский центр проблем химической физики и медицинской химии РАН, Черноголовка
[4]Южно-Уральский государственный университет, Челябинск

**konst@ihed.ras.ru*

XVI Забабахинские научные чтения
29 мая – 2 июня 2023 г., Снежинск, Россия

Equation of state for ruthenium at high pressures and temperatures

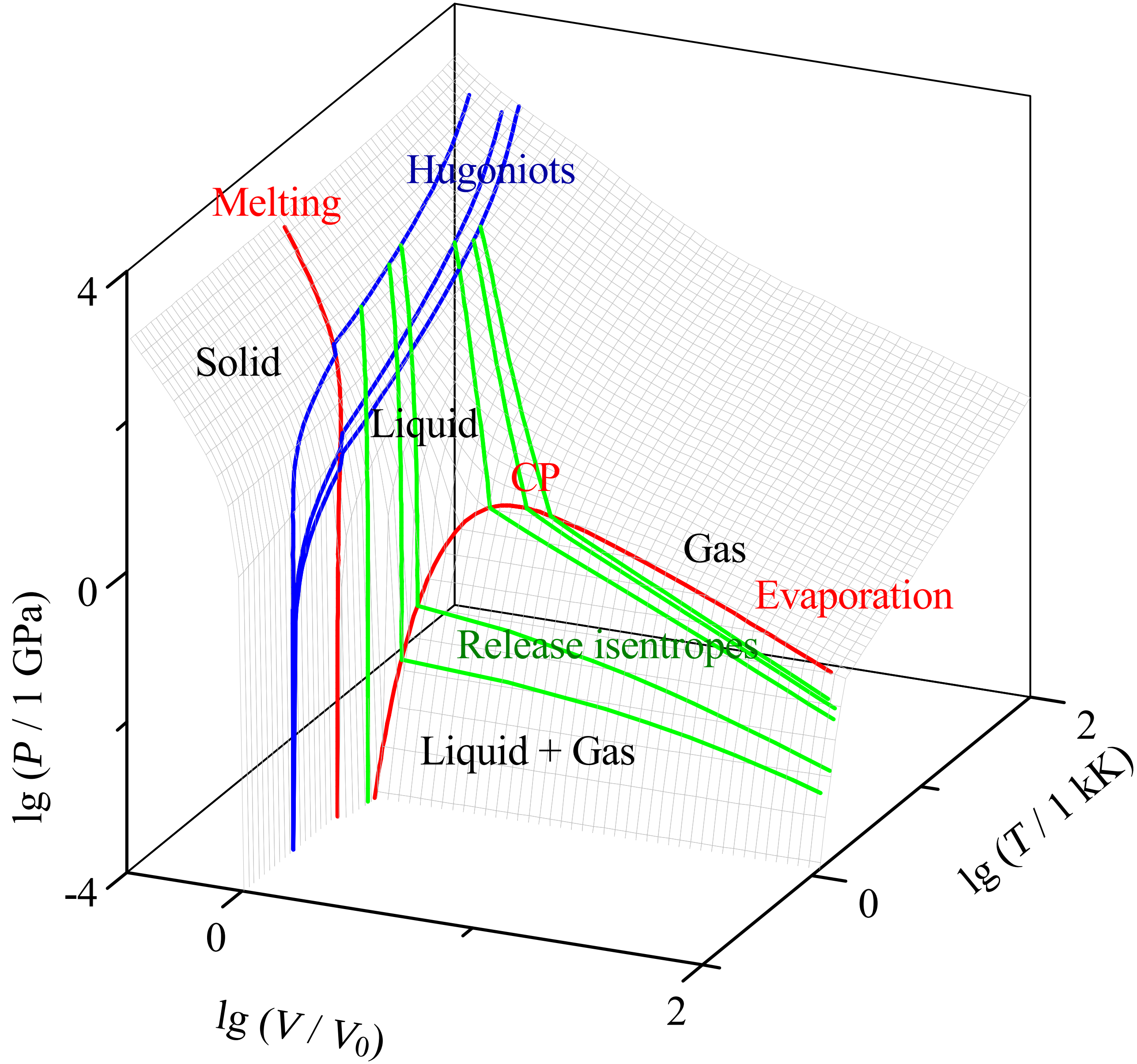
K. V. Khishchenko[1,2,3,4,*]

[1]Joint Institute for High Temperatures RAS, Moscow, Russia
[2]Moscow Institute of Physics and Technology, Dolgoprudny, Russia
[4]Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS, Chernogolovka, Russia
[3]South Ural State University, Chelyabinsk, Russia

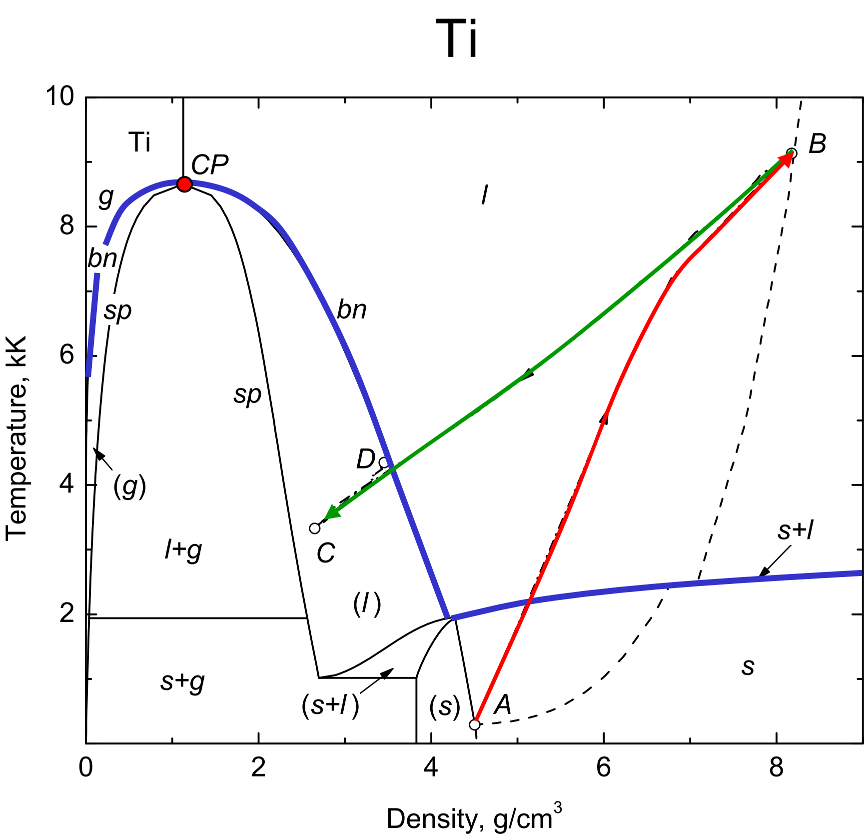
**konst@ihed.ras.ru*

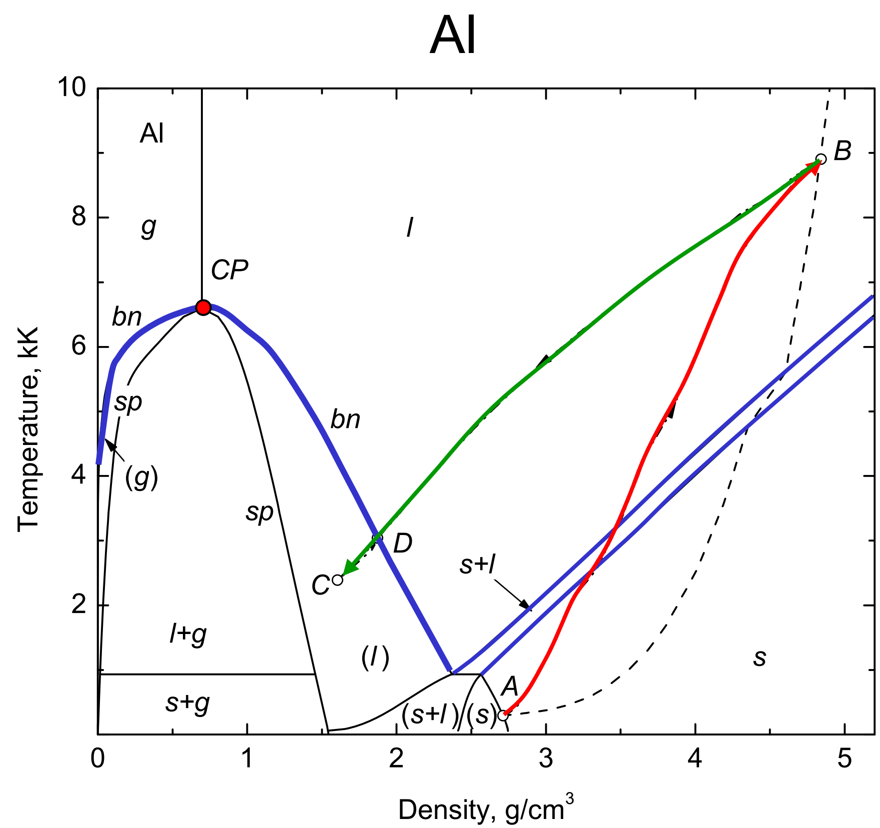
XVI Zababakhin Scientific Talks
May 29 – June 2, 2023, Snezhinsk, Russia

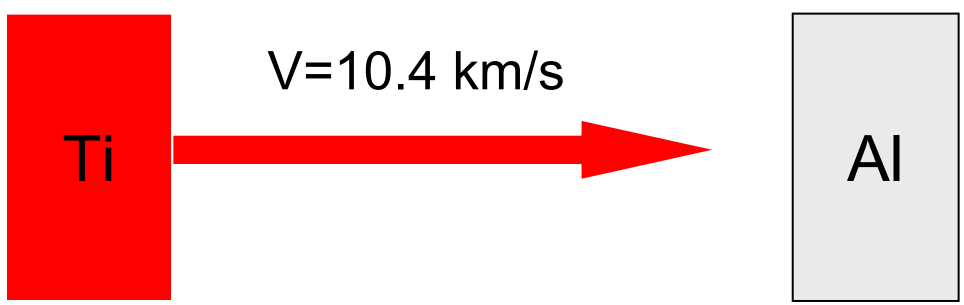
Pressure versus volume and temperature for zinc



Ti - Al Impact at 10.4 km/s







Equation of State Modeling

Equation of State Model

General form

$$F(V,T) = F_c(V) + F_a(V,T) + F_e(V,T)$$

Solid phase. Elastic component (EOS at *T* = 0 K)

at $V < V_{0c}$:

$$F_c(V) = 3V_{0c}\sum_{i=1}^{2}\frac{a_i}{i}\left(\sigma_c^{i/3}-1\right) - 3V_{0c}\sum_{i=1}^{3}\frac{b_i}{i}\left(\sigma_c^{-i/3}-1\right) + b_0 V_{0c}\ln\sigma_c$$

at $V > V_{0c}$:

$$F_c(V) = V_{0c}\left[A\left(\sigma_c^m/m - \sigma_c^n/n\right) + B\left(\sigma_c^l/l - \sigma_c^n/n\right)\right] + E_{sub}$$

at $V = V_{0c}$:

$$\sigma_c = V_{0c}/V$$

$$F_c(V_{0c}) = F_{0c}$$

$$P_c(V_{0c}) = -dF_c/dV = 0$$

$$B_c(V_{0c}) = -VdP_c/dV = B_{0c}$$

$$B_c'(V_{0c}) = dB_c/dP_c = B_{0c}'$$

$$B_c''(V_{0c}) = -d(V\,dB_c/dV)/dB_c = B_{0c}''$$

Equation of State Model

General form

$$F(V,T) = F_c(V) + F_a(V,T) + F_e(V,T)$$

Solid phase. Thermal lattice components

$$F_a(V,T) = F_a^{acst}(V,T) + \sum_{\alpha=1}^{3(\nu-1)} F_{a\alpha}^{opt}(V,T)$$

$$F_a^{acst}(V,T) = \frac{RT}{\nu}\left[3\ln\left(1 - e^{-\theta^{acst}/T}\right) - D\left(\theta^{acst}/T\right)\right] - \beta_{acst}\frac{T^2/\theta^{acst}}{e^{\theta^{acst}/T} - 1}$$

$$F_{a\alpha}^{opt}(V,T) = \frac{RT}{\nu}\ln\left(1 - e^{-\theta_\alpha^{opt}/T}\right) - \beta_{opt\alpha}\frac{T^2/\theta_\alpha^{opt}}{e^{\theta_\alpha^{opt}/T} - 1} \qquad D(x) = \frac{3}{x^3}\int_0^x \frac{t^3 dt}{e^t - 1}$$

$$\frac{\theta^{acst}(V)}{\theta_0^{acst}} = \frac{\theta_\alpha^{opt}(V)}{\theta_{0\alpha}^{opt}} = \sigma^{2/3}\exp\left\{(\gamma_0 - 2/3)\frac{\sigma_n^2 + \ln^2\sigma_m}{\sigma_n}\operatorname{arctg}\left[\frac{\sigma_n \ln\sigma}{\sigma_n^2 - \ln(\sigma/\sigma_m)\ln\sigma_m}\right]\right\}$$

Equation of State Model

General form

$$F(V,T) = F_c(V) + F_a(V,T) + F_e(V,T)$$

Fluid phase. Elastic component (EOS at *T* = 0 K)

at $V < V_{m0}$:

$$F_c^{(l)}(V) = F_c^{(s)}(V) + 3RT_{m0}\frac{2\sigma_m^2}{1+\sigma_m^3}\left[\frac{3A_m}{5}\left(\sigma_m^{5/3}-1\right)+C_m\right]$$

at $V_{m0} < V < V_{cr}$:

$$F_c^{(l)}(V) = F_c^{(s)}(V) + V_{m0}\sum_{i=1}^{7}\frac{a_{mi}}{\alpha_{mi}}\left(\sigma_m^{\alpha_{mi}}-1\right)+E_{m0}$$

$$\sigma_m = V_{m0}/V$$

at $V_{cr} < V$:

$$F_c^{(l)}(V) = F_c^{(s)}(V) + 3V_{cr}\sigma_v\sum_{i=1}^{3}\frac{b_{mi}}{i}\left(\sigma_v^{i/3}-1\right)$$

$$\sigma_v = V_{cr}/V$$

Equation of State Model

General form

$$F(V,T) = F_c(V) + F_a(V,T) + F_e(V,T)$$

Fluid phase. Thermal atomic components

$$F_a(V,T) = C_a(V,T)T\ln\left(1 - e^{-\theta^{liq}/T}\right) + 3RT\frac{B_m}{D_m + \left(\theta^{liq}/T\right)^{\alpha_m}}$$

$$C_a(V,T) = \frac{3}{2}R\left[2 - \frac{1}{1 + \theta^{liq}/T}\right]$$

$$\theta^{liq}(V,T) = T_{sa}\sigma^{2/3}\left[\theta_l(V) + \frac{1 - \theta_l(V)}{1 + \sqrt{T_{ca}\sigma_m^{2/3}/T}}\right]$$

$$\frac{\theta_l(V)}{\theta_{0l}} = \exp\left\{(\gamma_{0l} - 2/3)\frac{B_l^2 + D_l^2}{B_l}\operatorname{arctg}\left(\frac{B_l\ln\sigma}{B_l^2 + D_l(\ln\sigma + D_l)}\right)\right\}$$

Equation of State Model

General form

$$F(V,T) = F_c(V) + F_a(V,T) + F_e(V,T)$$

Thermal electron component is from Ref. [A. V. Bushman, V. E. Fortov, G. I. Kanel', A. L. Ni, *Intense Dynamic Loading of Condensed Matter* (Taylor & Francis, Washington, 1993).]

$$F_{\mathrm{e}}(V,T) = -C_{\mathrm{e}}(V,T)T\ln\left\{1 + \frac{B_{\mathrm{e}}(T)T}{2C_{\mathrm{ei}}}\sigma^{-\gamma_{\mathrm{e}}(V,T)}\right\}$$

$$C_{\mathrm{e}}(V,T) = \frac{3R}{2}\left\{Z + \frac{\sigma_z T_z^2(1-Z)}{(\sigma+\sigma_z)(T^2+T_z^2)}\right\}\exp(-\tau_{\mathrm{i}}(V)/T) \qquad C_{\mathrm{ei}} = \frac{3RZ}{2}$$

$$B_{\mathrm{e}}(T) = \frac{2}{T^2}\int\int_0^T \beta(\tau)d\tau dT \qquad \beta(T) = \beta_{\mathrm{i}} + (\beta_0 - \beta_{\mathrm{i}} + \beta_{\mathrm{m}}T/T_{\mathrm{b}})\exp(-T/T_{\mathrm{b}})$$

$$\tau_{\mathrm{i}}(V) = T_{\mathrm{i}}\exp(-\sigma_{\mathrm{i}}/\sigma) \qquad \gamma_{\mathrm{e}}(V,T) = \gamma_{\mathrm{ei}} + (\gamma_{\mathrm{e0}} - \gamma_{\mathrm{ei}} + \gamma_{\mathrm{m}}T/T_{\mathrm{g}})\exp(-T/T_{\mathrm{g}})$$

Phase Equilibration

● Phase equilibrium boundary at given temperature T is determined by conditions

$$G^{(1)}(V_1, T) = G^{(2)}(V_2, T)$$
$$P^{(1)}(V_1, T) = P^{(2)}(V_2, T)$$

where $G^{(i)}$ and $P^{(i)}$ are the Gibbs energy and pressure functions defined by EOS of phase i = 1 and 2;
V_1 and V_2 are specific volumes of competitive phases 1 and 2

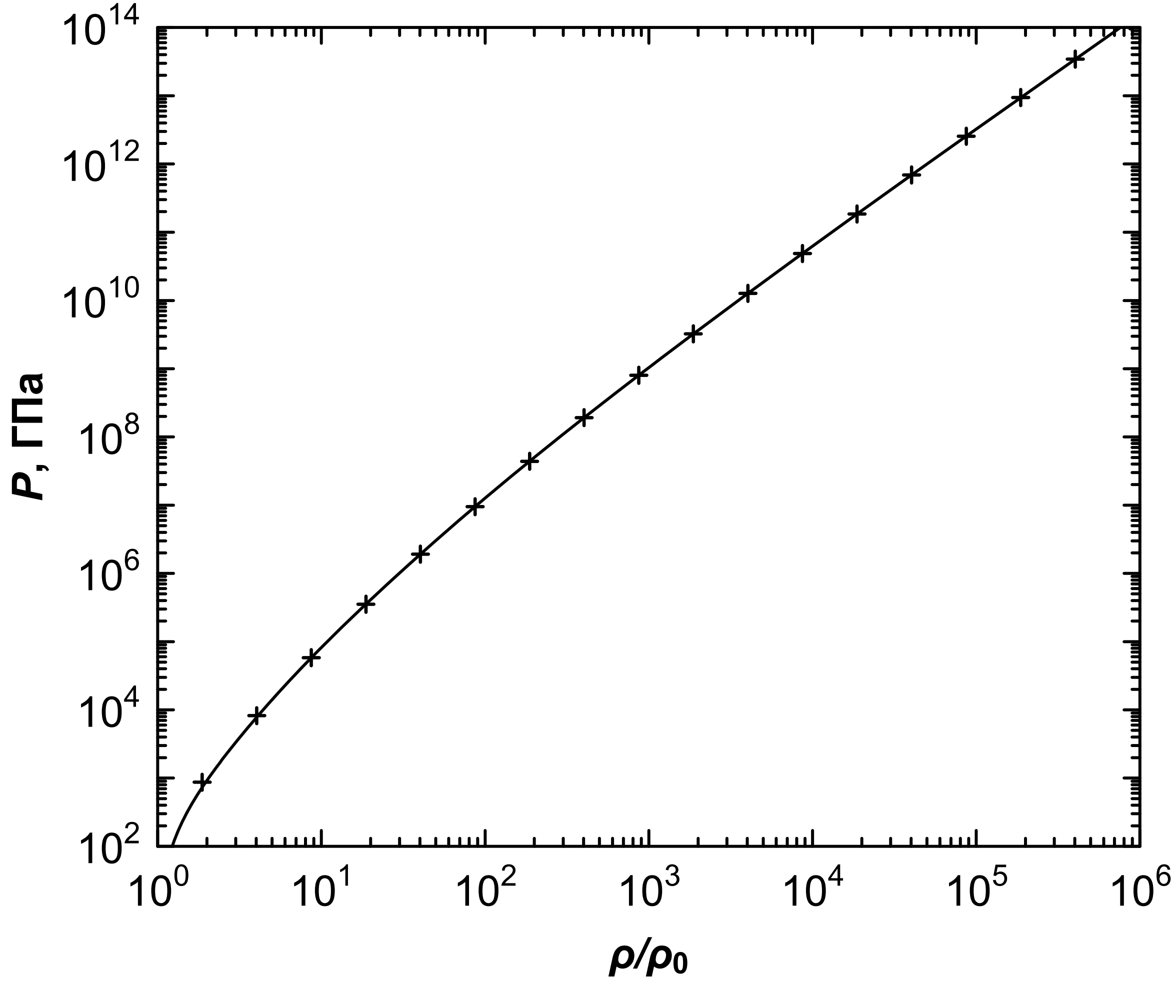
● Phase equilibrium boundary at given pressure P is determined by conditions

$$G^{(1)}(V_1, T) = G^{(2)}(V_2, T)$$
$$P^{(1)}(V_1, T) = P$$
$$P^{(2)}(V_2, T) = P$$

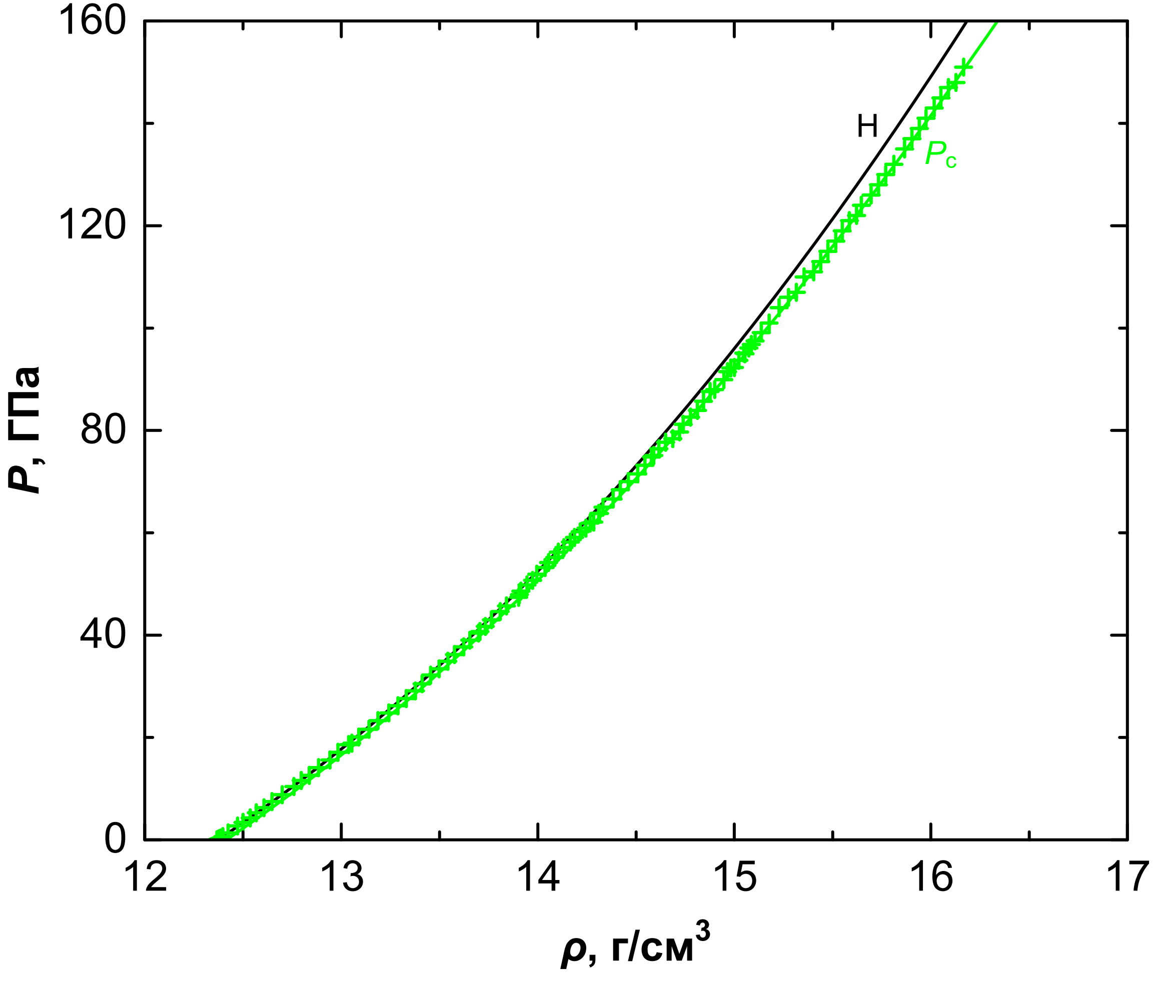
where $G^{(i)}$ and $P^{(i)}$ are the Gibbs energy and pressure functions defined by EOS of phase i = 1 and 2;
V_1 and V_2 are specific volumes of competitive phases 1 and 2;
T is the temperature of phase equilibrium

Calculation Results

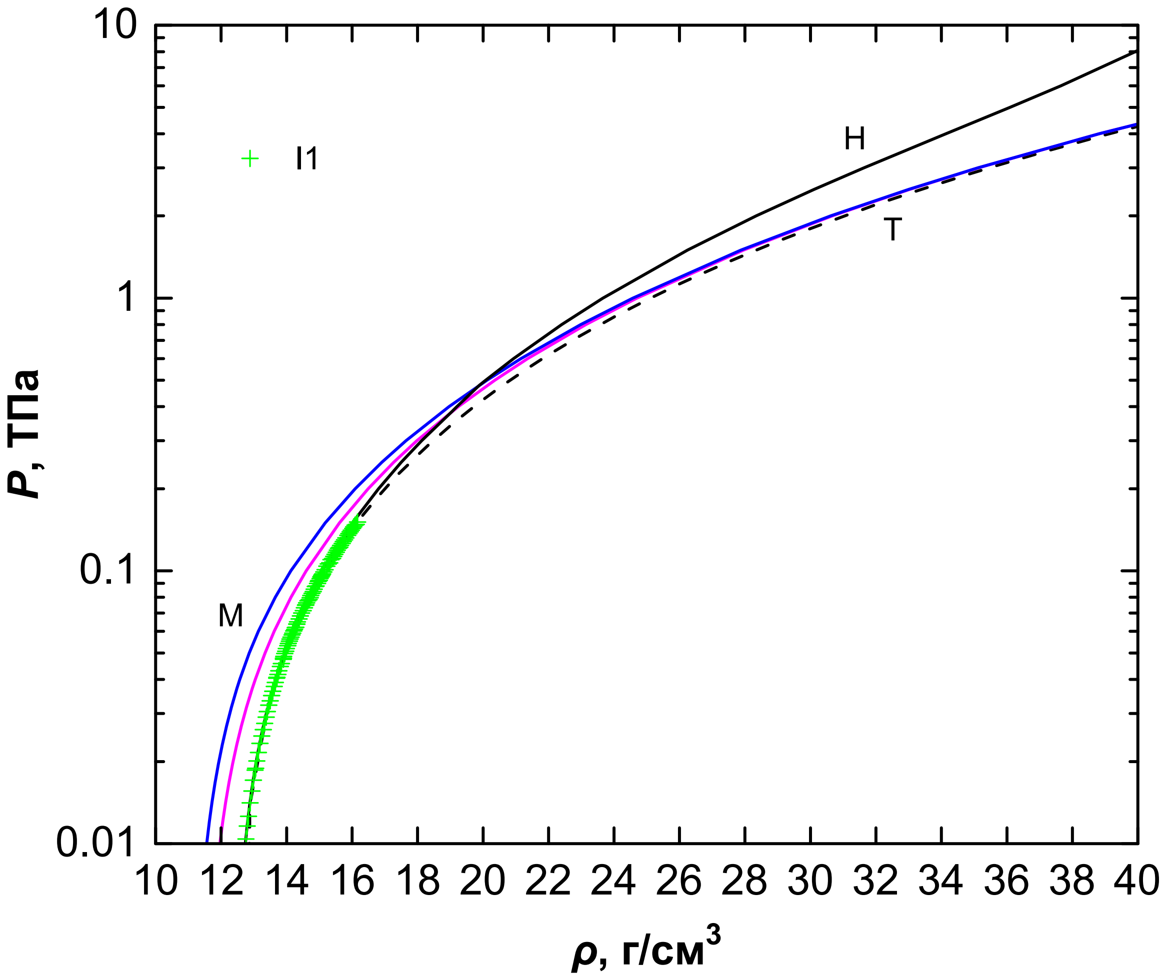
Ruthenium at $T = 0$



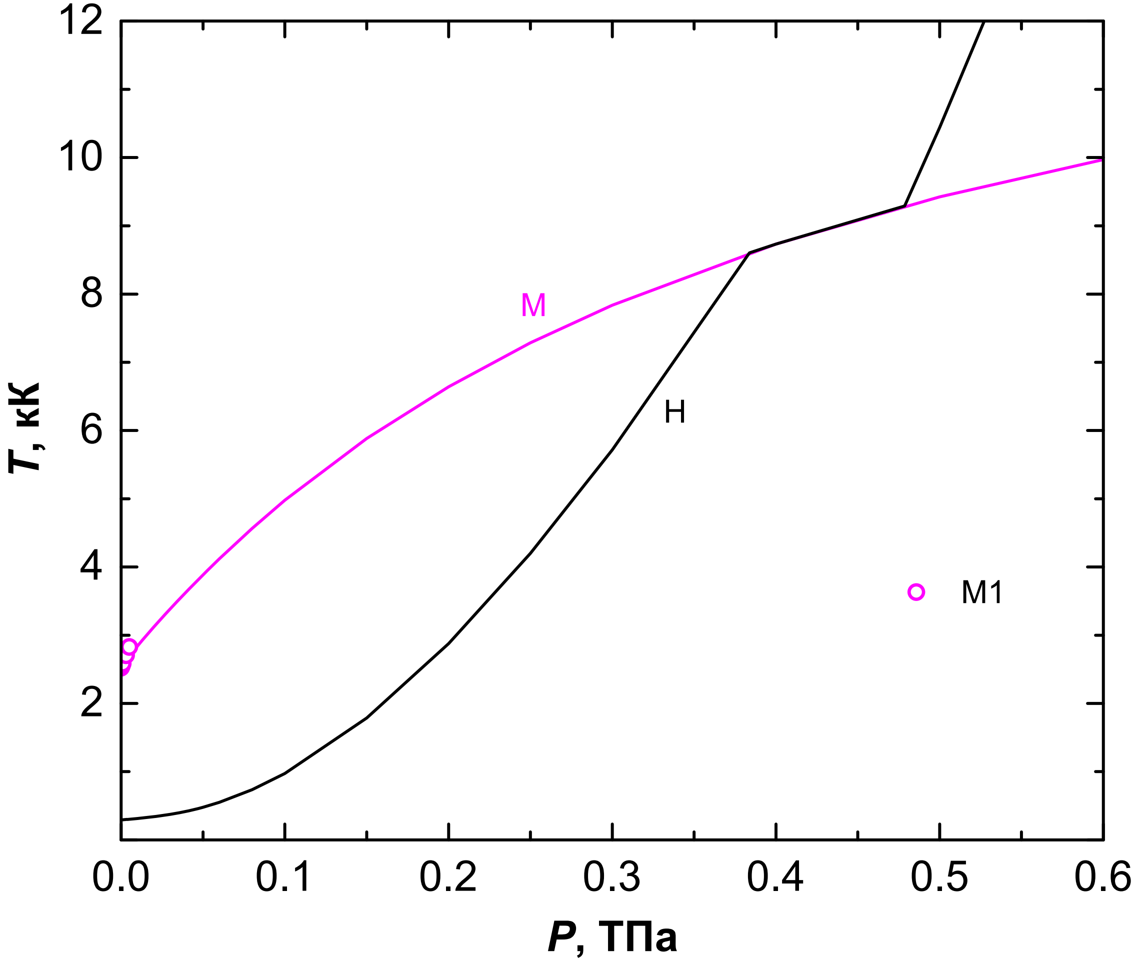
Ruthenium at T = 293 K



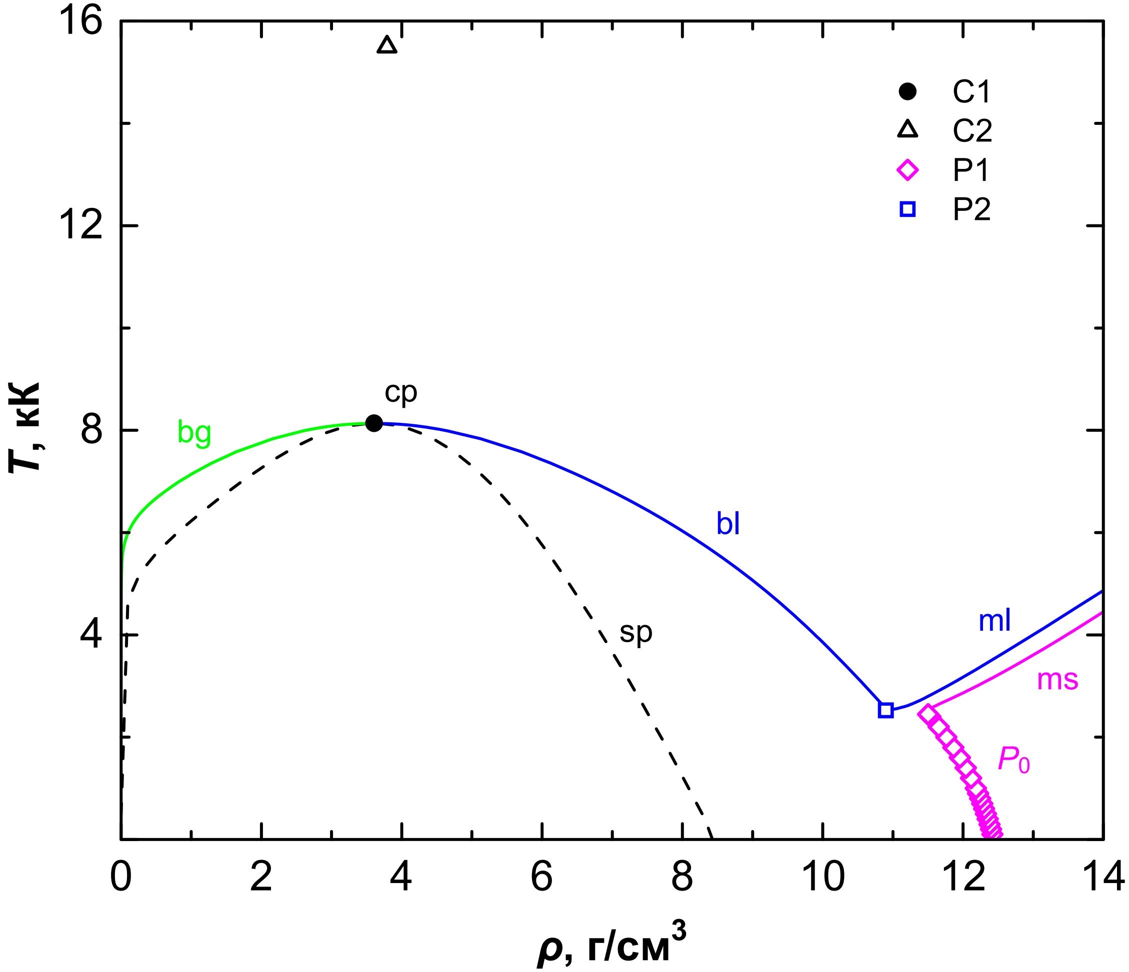
Ruthenium Phase Diagram



Ruthenium Phase Diagram



Ruthenium Phase Diagram



Conclusions

- A thermodynamic approach is proposed for modeling of equation of state of structural materials over a broad region of the phase diagram.
- Multiphase equation of state for ruthenium is developed with taking into account melting and evaporation. This equation of state is in a good agreement with experimental data.
- Obtained equation of sate can be used in numerical simulations of processes in matter under extreme conditions of high temperatures and high pressures.

Спасибо