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EQUATION OF STATE FOR NIOBIUM AT HIGH PRESSURES

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Summary. An analytical function of pressure on specific volume and internal energy is developed for niobium. This function allows one to adequately describe the thermodynamic properties of this metal in a wide range of densities and pressures. A comparison of the calculated shock adiabat with experimental data at high dynamic pressures is made. The equation of state proposed for niobium can be used to model physical phenomena at high energy densities.

1 INTRODUCTION

The problem of a thermodynamic description of the properties of matter is of interest for both fundamental and applied investigations [1]. For the analysis and numerical simulation of physical processes at high energy densities, equations of state (EOSs) for materials are needed over the entire range of parameters that are realized in these processes [2]. For example, at high velocity impact [3–5], under the action of intense laser [6–8] and particle beams [9, 10], at an electrical explosion of conductors [11, 12], this range continues from normal conditions up to extremely high pressures and specific internal energies.

Niobium is a refractory material, has a low thermal neutron capture cross section. In particular, the EOS for this metal is required when modeling the operating modes of some nodes at nuclear power plants.

In this work, the EOS for niobium is proposed in the form of an analytic function of pressure on specific volume and internal energy. In this form, the EOS can be used in hydrodynamic simulations of adiabatic processes. To illustrate the quality of the EOS, the calculated shock adiabat of niobium is compared with experimental data at high pressures.

2 EOS MODEL

The model is formulated in the framework of the quasi-harmonic approximation. The general form of the EOS [13] is as follows:

$$P(V,E) = P_{\mathrm{c}}(V) + \frac{\Gamma(V,E)}{V}[E - E_{\mathrm{c}}(V)], \tag{1}$$

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where P is the pressure; V is the specific volume, $V = 1/\rho$; ρ is the density; E is the specific internal energy; E_c is the specific internal energy at zero temperature, $T = 0$; P_c is the corresponding pressure at $T = 0$: $P_c = -dE_c/dV$.

The coefficient Γ is the ratio of thermal pressure to thermal energy density: $V[P-P_c]/[E-E_c]$. Its dependence on volume and internal energy is chosen as follows:

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

where $\sigma = V_0/V$; V_0 is the specific volume under normal conditions, $E = E_0$ and $P = P_0$; γ_c is the Grüneisen coefficient $\gamma = V(\partial P/\partial E)_V$ at the case of $T = 0$; γ_i is the value of the Grüneisen coefficient at the case of high thermal energies, $E - E_c \gg E_a\sigma^{2/3}$; E_a is a parameter.

The coefficient γ_c is represented by the volume function

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

where the value of γ_{0c} corresponds to the normal volume V_0; σ_m and σ_n are parameters.

The cold energy is represented by a polynomial

$$E_c(V) = \frac{B_{0c}V_{0c}}{m-n}\left(\frac{\sigma_c^m}{m} - \frac{\sigma_c^n}{n}\right) + E_{sub}. \tag{4}$$

Here, $\sigma_c = V_{0c}/V$; V_{0c} and B_{0c} are the specific volume and the bulk modulus at $T = 0$ and $P = 0$; $E_{sub} = B_{0c}V_{0c}/(mn)$; m and n are parameters.

3 EOS FOR NIOBIUM

Under normal pressure, the solid phase of niobium has a body-centered cubic (bcc) structure; it melts at $T = 2740$ K [14]. At quasi-hydrostatic compression at room temperature, niobium was studied up to 134 GPa [15]; no transformations of the bcc phase were observed.

At shock compression, niobium was studied up to 180 GPa with traditional explosive systems [16–19]. Pressure up to 400 GPa in niobium was recorded in experiments with special explosive systems [17].

Figures 1–3 display the results of the calculation of the principal Hugoniot curve of niobium over entire range of measured shock and particle velocities, pressures and compression ratios [16–19]. The shock adiabat of the material is calculated using the energy conservation law at the shock front [20],

$$E = E_0 + \frac{1}{2}(P_0 + P)(V_0 - V), \tag{5}$$

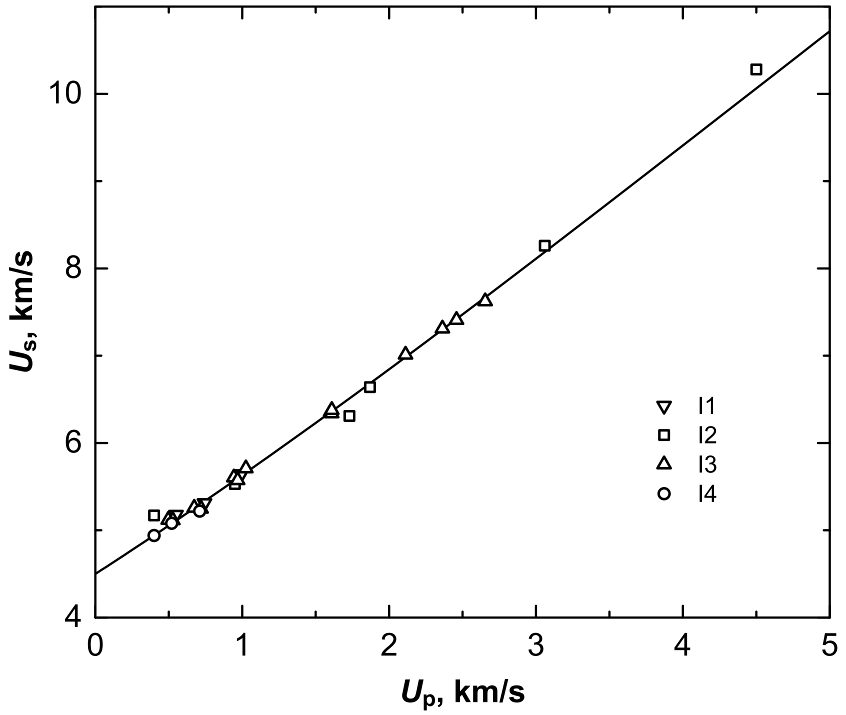

Figure 1: The principal Hugoniot adiabat of niobium: curve corresponds to the present calculations; markers—experimental data (I1—[16]; I2—[17]; I3—[18]; I4—[19]).

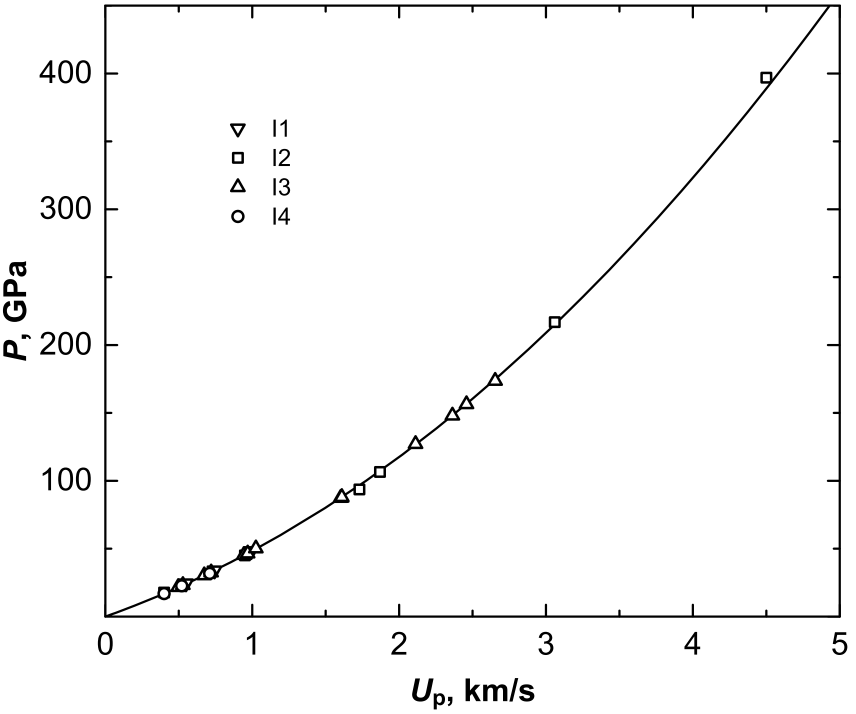

Figure 2: The principal Hugoniot adiabat of niobium: the notation is similar to figure 1.

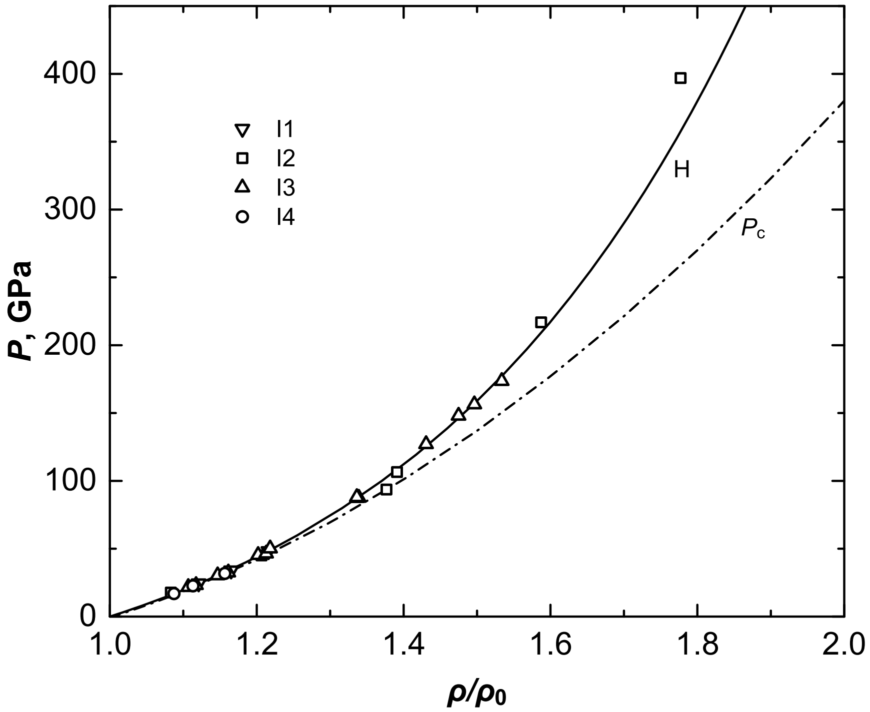

Figure 3: The cold curve (P_c) and the principal Hugoniot adiabat (H) of niobium: curves correspond to the present calculations; marker designations are similar to those used in figure 1.

along with the EOS (1)–(4). The velocities of the shock front (U_s) and particles behind it (U_p) are calculated with the use of the mass and momentum conservation laws [20]:

$$U_s = V_0 \sqrt{(P - P_0)/(V_0 - V)}, \tag{6}$$

$$U_p = \sqrt{(P - P_0)(V_0 - V)}. \tag{7}$$

Comparison of the calculated adiabat with experimental data [16–19] is illustrated in figures 1–3. One can see that the EOS (1)–(4) adequately describes thermodynamic properties of niobium in the region studied in shock waves.

The coefficients of the EOS (1)–(4) for niobium are as follows: $V_0 = 0.11646$ cm^3/g, $V_{0c} = 0.116$ cm^3/g, $B_{0c} = 174.449$ GPa, $m = 0.66$, $n = 0.68$, $\sigma_m = 0.9$, $\sigma_n = 1.2$, $\gamma_{0c} = 1.6$, $\gamma_i = 0.45$ and $E_a = 60$ kJ/g.

4 CONCLUSIONS

Thus, EOS for niobium is developed, which is consistent with data from experiments with shock waves at high pressures. The EOS has a form suitable for use in the numerical simulation of adiabatic processes in a wide range of densities and internal energies.

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