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# EQUATION OF STATE FOR MAGNESIUM HYDRIDE UNDER CONDITIONS OF SHOCK LOADING

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**Summary.** An equation of state is proposed for magnesium hydride $MgH_2$ at high pressures. The equation of state has the form of an analytic function of pressure upon specific volume and specific internal energy. Results of calculations of the Hugoniot curve are given in comparison with available data from shock-wave experiments. One can use this equation of state in numerical simulations of hydrodynamic processes in magnesium hydride under shock loading conditions.

## 1 INTRODUCTION

Equation of state (EOS) of matter is a necessary part of hydrodynamic simulations of different non-steady processes [1–4]. For such processes as intense laser–substance interaction [5–16], high-energy particle beams action upon materials [17–21], electrical explosion of conductors by powerful current pulses [22–28], flows of dielectric liquids at high electric fields [29], and high velocity impingement of bodies [30–34], states in a broad region on the phase diagram of a medium can be realized. The EOS, which is involved in simulations, over whole this region influences on the accuracy of simulated results [35, 36].

Hydrides are chemical compounds with properties, which are of interest for the use, e.g., in nuclear technologies [37–39]. Hydrides can appear in metals, when those are used in hydrogenous surroundings [40], and cause the change of properties of the initial materials.

In the present paper, an EOS of magnesium hydride $MgH_2$ is proposed in the form of an analytic function [41–44] of pressure ($P$) upon specific volume ($V$) and specific internal energy ($E$). Results of calculations of thermodynamic characteristics of this substance are compared with available experimental data on shock compressibility of $MgH_2$.

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## 2 EOS MODEL

The chosen EOS model [41–44] is formulated in the framework of quasiharmonic approximation with taking into account anharmonic effects in the general form

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

where $E_{\mathrm{c}}$ is the energy of the substance at zero temperature $T = 0$; $P_{\mathrm{c}} = -\mathrm{d}E_{\mathrm{c}}/\mathrm{d}V$ is the corresponding pressure at $T = 0$; the coefficient $\Gamma$ determines the thermal contribution to the EOS.

The cold energy is taken in the form of polynomial [45–52]

$$E_{\mathrm{c}}(V) = \frac{B_{0\mathrm{c}}V_{0\mathrm{c}}}{m-n}\left(\frac{\sigma_{\mathrm{c}}^{m}}{m} - \frac{\sigma_{\mathrm{c}}^{n}}{n}\right) + E_{\mathrm{sub}}, \tag{2}$$

in which, $\sigma_{\mathrm{c}} = V_{0\mathrm{c}}/V$; $V_{0\mathrm{c}}$ and $B_{0\mathrm{c}}$ are the specific volume and the bulk modulus at $P = 0$ and $T = 0$. The sublimation energy $E_{\mathrm{sub}}$ is determined from the normalizing condition $E_{\mathrm{c}}(V_{0\mathrm{c}}) = 0$ that gives

$$E_{\mathrm{sub}} = \frac{B_{0\mathrm{c}}V_{0\mathrm{c}}}{mn}. \tag{3}$$

Coefficients $m$ and $n$ are determined with the use of shock-wave data.

The ratio of the thermal pressure $P - P_{\mathrm{c}}$ to the thermal energy density $[E - E_{\mathrm{c}}]/V$ is defined as a function of $V$ and $E$ [41–44]:

$$\Gamma(V,E) = \gamma_{\mathrm{i}} + \frac{\gamma_{\mathrm{c}}(V) - \gamma_{\mathrm{i}}}{1 + \sigma^{-2/3}[E - E_{\mathrm{c}}(V)]/E_{\mathrm{a}}}, \tag{4}$$

where $\sigma = V_0/V$; $V_0$ is the specific volume under normal conditions, $P = P_0 = 0.1$ MPa, $E = E_0$; the volume function $\gamma_{\mathrm{c}}(V)$ corresponds to the case of low thermal energies, $E - E_{\mathrm{c}} \ll E_{\mathrm{a}}\sigma^{2/3}$; the constant $\gamma_{\mathrm{i}}$ characterizes the region of highly-heated matter, $E - E_{\mathrm{c}} \gg E_{\mathrm{a}}\sigma^{2/3}$. The value of $E_{\mathrm{a}}$ determines the thermal energy of the transition of $\Gamma$ from one limiting case to the other; it is generally found from the results of experiments with strong shock waves. The Grüneisen coefficient $\gamma = V(\partial P/\partial E)_V$ at $T = 0$ is taken as follows:

$$\gamma_{\mathrm{c}}(V) = 2/3 + (\gamma_{0\mathrm{c}} - 2/3)\frac{\sigma_{\mathrm{n}}^2 + \ln^2\sigma_{\mathrm{m}}}{\sigma_{\mathrm{n}}^2 + \ln^2(\sigma/\sigma_{\mathrm{m}})}, \quad \gamma_{0\mathrm{c}} = \gamma_{\mathrm{i}} + (\gamma_0 - \gamma_{\mathrm{i}})\left[1 + \frac{E_0 - E_{\mathrm{c}}(V_0)}{E_{\mathrm{a}}}\right]^2. \tag{5}$$

This form guarantees the value of the Grüneisen coefficient under normal conditions, $\gamma(V_0, E_0) = \gamma_0$, and gives the asymptotic value $\gamma_{\mathrm{c}} = 2/3$ in the limiting cases of low and high compression ratios $\sigma$. The parameters $\sigma_{\mathrm{n}}$ and $\sigma_{\mathrm{m}}$ in (5) are determined from the requirement of a good agreement with shock-wave data for a substance in question.

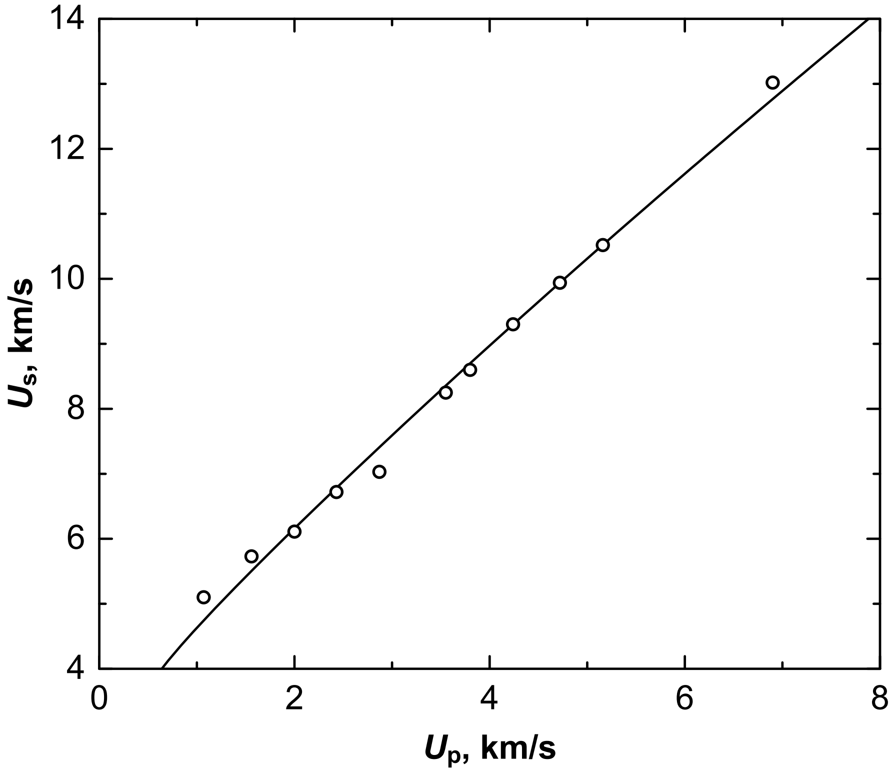

Figure 1: Hugoniot adiabat of magnesium hydride samples with initial density $\rho_{00} = 1.37$ g/cm$^3$: line corresponds to the present EOS calculations; markers—experimental data [57].

## 3 PROPERTIES OF MAGNESIUM HYDRIDE

Magnesium hydride $MgH_2$ under atmospheric pressure has a tetragonal structure [53]. Treatment at pressures 2.5–8 GPa and temperatures up to 1173 K induces the formation of orthorhombic [54, 55] and cubic [55] structures of $MgH_2$. At that, the cubic structure transforms to the orthorhombic one when releasing pressure [55]. Under compression at room temperature, the orthorhombic phase appears from 0.9 to 4 GPa and coexist with the tetragonal phase up to 9 GPa [56]. At pressures 9 and 17 GPa at room temperature, transformations to two more phases with orthorhombic structures have been observed [56].

Shock compressibility of $MgH_2$ is investigated using traditional planar explosive systems up to pressure about 120 GPa [57].

In the framework of expressions (1)–(5), shock-wave data [57] have been generalized in the form of an EOS for a whole investigated range of pressures. The EOS coefficients are obtained as follows: $V_0 = 0.70423$ cm$^3$/g, $V_{0c} = 0.69451$ cm$^3$/g, $B_{0c} = 18.0276$ GPa, $m = 1$, $n = 1.79$, $\sigma_m = 0.8$, $\sigma_n = 1$, $\gamma_{0c} = 1.45$, $\gamma_i = 0.45$ and $E_a = 20$ kJ/g.

Calculated Hugoniot curve of $MgH_2$ samples with initial density $\rho_{00} = 1.37$ g/cm$^3$ is compared with data from shock-wave experiments [57] in figures 1–3.

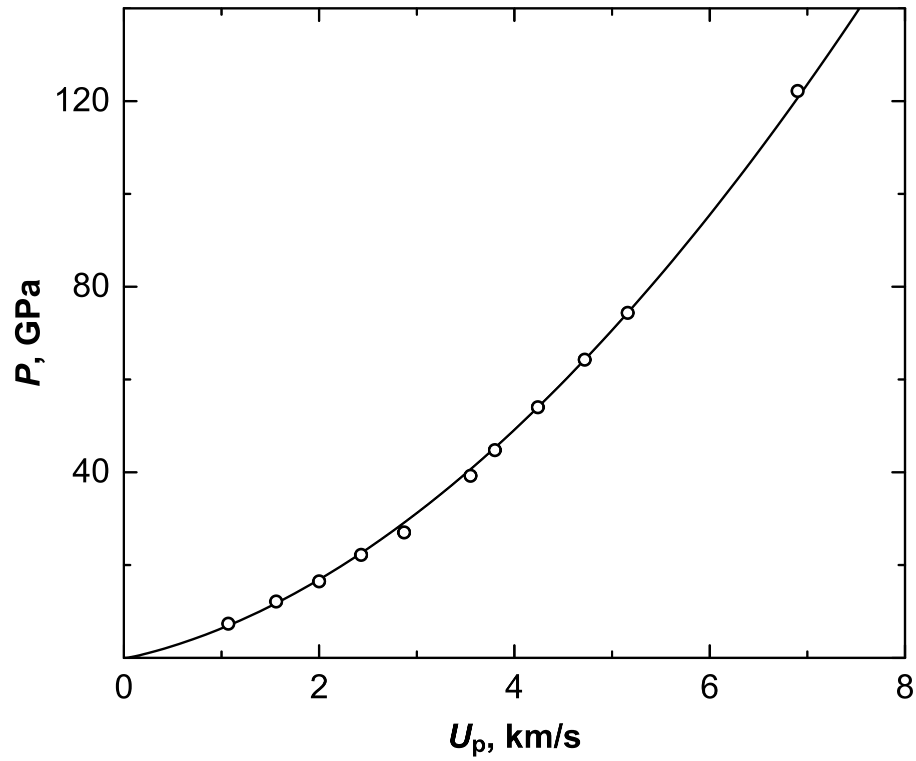

Figure 2: Hugoniot adiabat of $MgH_2$ samples with $\rho_{00} = 1.37$ g/cm$^3$: notations are analogous to figure 1.

This Hugoniot calculation is based on the energy conservation relation for the shock front [1]:

$$E = E_0 + \frac{1}{2}(P_0 + P)(V_{00} - V), \tag{6}$$

where parameters of shock-compressed state are related by the EOS function $E = E(P, V)$; $V_{00} = \rho_{00}{}^{-1}$ is the initial specific volume of samples, which is greater than $V_0$ because of initial porosity. Equation (6) gives the specific volume of shock-compressed material as a function of pressure. Kinematic parameters of a shock-wave flow, which are the shock ($U_s$) and particle ($U_p$) velocities, follow from the mass and momentum conservation relations for the shock front [1]:

$$U_s = V_0\sqrt{(P - P_0)/(V_{00} - V)}, \quad U_p = \sqrt{(P - P_0)(V_{00} - V)}. \tag{7}$$

An analysis of diagrams in figures 1–3 lets one to infer that the EOS provides for a good overall agreement with shock-wave data. However, an alternative description of these data is possible, where one can represent the Hugoniot consisting of two parts with a break between them (see, e.g., a variant of such representation in [57]).

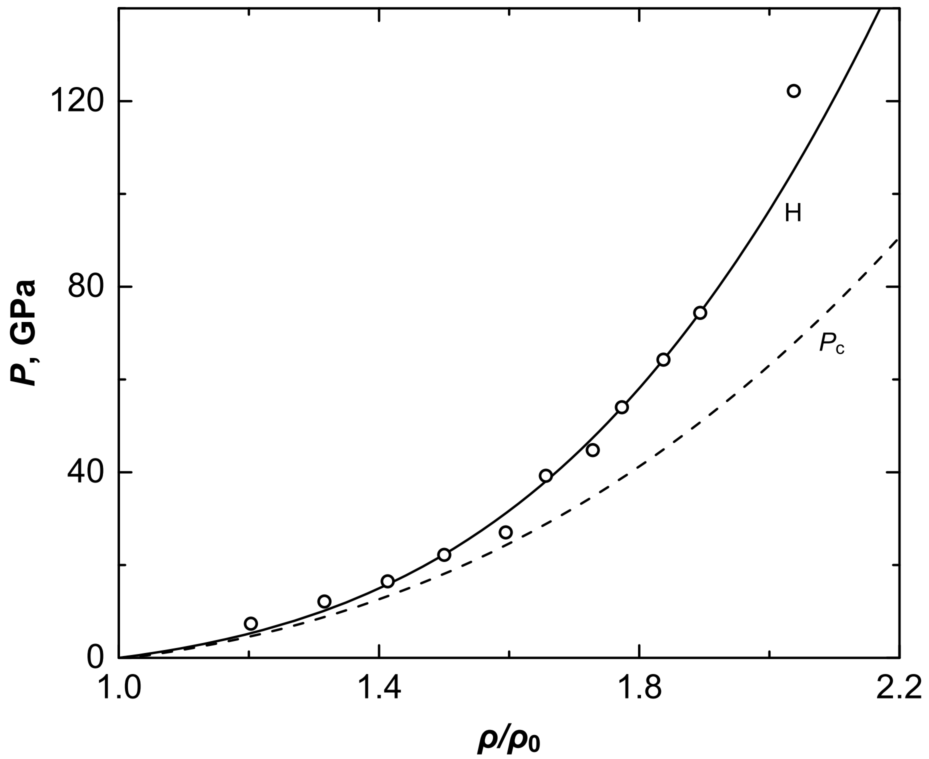

Figure 3: The cold curve ($P_c$) and the Hugoniot adiabat of samples with initial density $\rho_{00} = 1.37$ g/cm$^3$ (H) for $MgH_2$: lines correspond to the present EOS calculations; markers—experimental data [57].

## 4 CONCLUSIONS

Thus, the EOS of magnesium hydride $MgH_2$ is proposed in the form of an analytic function $P = P(E,V)$. This EOS describes thermodynamic properties of the compound over whole region investigated in shock-wave experiments. One can use the EOS in numerical simulations of processes in this material at high energy densities.

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