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CALORIC EQUATIONS OF STATE OF STRUCTURAL MATERIALS

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Two versions of Mie-Gruneisen-type caloric equation of state (EOS) model are proposed. Constructed are EOS for about 150 structural materials (metals, alloys, rocks, minerals, polymers, composites and other materials). The carried out comparison of the calculated by EOS thermodynamic properties with numerous high-pressure data testified their reliable description. The presence of correct theoretical asymptotes guaranties the reliable thermodynamic description in the phase diagram regions unaccessable to experimental test. These allow a wide use of the EOS in carrying out computer simulation.

INTRODUCTION

The computer simulation of nonsteady high-energy processes requires reliable EOS for used materials [1]. Wide-range analytic EOS provide for an effective implementation and usage in gasdynamic codes. We reported two caloric EOS models and results of EOS construction for some structural materials in comparison with shock-wave data.

EOS FOR METALS, ALLOYS, ROCKS

The knowledge of pressure, density, energy and isentropic sound velocity is quite enough for the solution of typical problems in high-energy density physics, such as high-velocity impact, for example. EOS in the caloric form $p=p(V,E)$ closing the equation-of-motion system can be used for these purposes.

EOS Model

The pressure is comfortably calculated by means of the most simple but realistic Mie-Gruneisen EOS, which is ordinarily used for describing material properties in the condensed phase at relatively low temperatures [2]. A generalization of the EOS has been carried out in the model developed, which allows us to extend the thermodynamic description for the gaslike region and the case of arbitrary energies.

The caloric EOS is represented in generalized form by

$$p(V,E) = p_c(V) + \frac{\Gamma(V,E)}{V}\left[E - E_c(V)\right], \qquad (1)$$

where $E_c(V)$, $p_c=-dE_c/dV$ are the elastic components of the energy and pressure at T=0 K.

The elastic energy is given in compression region $\sigma_c \geq 1$ ($\sigma_c=V_{0c}/V$, V_{0c} - specific volume at p=0) in form

$$E_c(V)=3V_{0c}\sum_{i=1}^{5}\frac{a_i}{i}\left(\sigma_c^{i/3}-1\right), \qquad (2)$$

providing for $E_c(V_{0c})=0$ condition, correct tabular values (with heat component) of bulk compression modulus and its pressure derivative, as well as the accordance with first-principle theories up to 100-fold compressions [3].

In the rarefaction region ($\sigma_c<1$) the elastic energy is represented by a polynomial of the form

$$E_c(V)=\frac{B_{0c}V_{0c}}{m-n}\left[\frac{\sigma_c^m}{m}-\frac{\sigma_c^n}{n}\right]+E_{sub}, \qquad (3)$$

which leads to the tabular values [4] of the cohesion energy $E_c(V\to\infty)=E_{sub}$ and satisfies the condition $p_c(V_{0c})=0$.

The volume-energy depending Gruneisen coefficient is given in the form

$$\Gamma(V,E)=\gamma_i+\frac{\gamma_c(V)-\gamma_i}{1+\sigma_c^{-2/3}\left[E-E_c(V)\right]/E_a}, \qquad (4)$$

where the expression for $\gamma_c(V)$ corresponds to the case of low heat energies (temperatures), while the value γ_i characterizes a region of hot dense plasma.

The "anharmonic" energy E_a defines the heat energy of transition from one limit case to the other and is found by dynamic experimental data at high pressures. The typical 3-D $\Gamma(V,E)$ plot is shown on Figure 1.

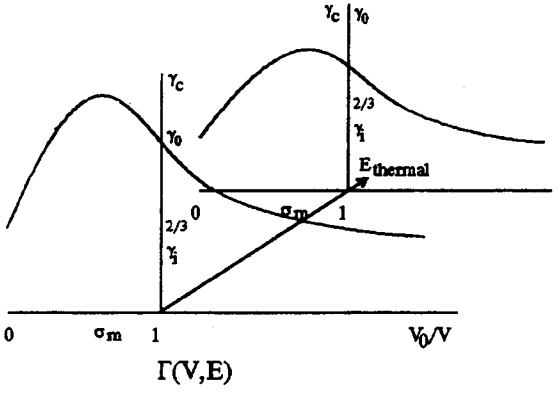


Figure 1. 3-D generalized Gruneisen gamma

In Formula (4) the expression for γ_c is defined by differential equation [5] in region $\sigma_c \geq 1$, while in the rarefaction region $\sigma_c < 1$ by simple approximating relationship [3]

$$\gamma_c(V) = \begin{cases} \dfrac{t}{2} + \dfrac{1}{3} - \dfrac{\sigma}{2} \dfrac{\left(p_c \sigma^{-t}\right)_{\sigma\sigma}}{\left(p_c \sigma^{-t}\right)_{\sigma}}, & \sigma_c \geq 1 \quad (5a) \\ \dfrac{2}{3} + \gamma_m \sigma^q \left[\dfrac{1}{q} - \left(\dfrac{\sigma}{\sigma_m} \right)^r \dfrac{1}{r+q} \right], & \sigma_c < 1 \quad (5b) \end{cases}$$

in which the corresponding matching conditions at $\sigma_c = 1$ are provided for γ_c and $d\gamma_c/d\sigma_c$.

Note that EOS model (1)-(5) have correct asymptotes for cases of low and high densities at low (ideal gas) and high (plasma) thermal energies.

The total number of EOS constructed on the base of the model (1)-(5) is about fifty. Typical results for some materials are presented below.

EOS for Metals

Molibdenum EOS is of practical significance as this metal is of wide use at high temperatures. Molibdenum was also served as standard material on carrying out nuclear-impedance measurements [6,7]. The comparison of calculated Hugoniot with high-pressure shock-wave data (points) is presented for molibdenum, tungsten, berillium and aluminum on Figure 2 as shock velocity-mass velocity plot.

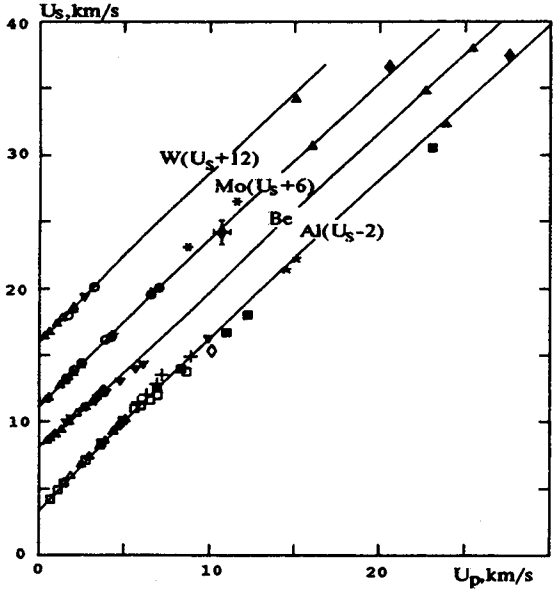
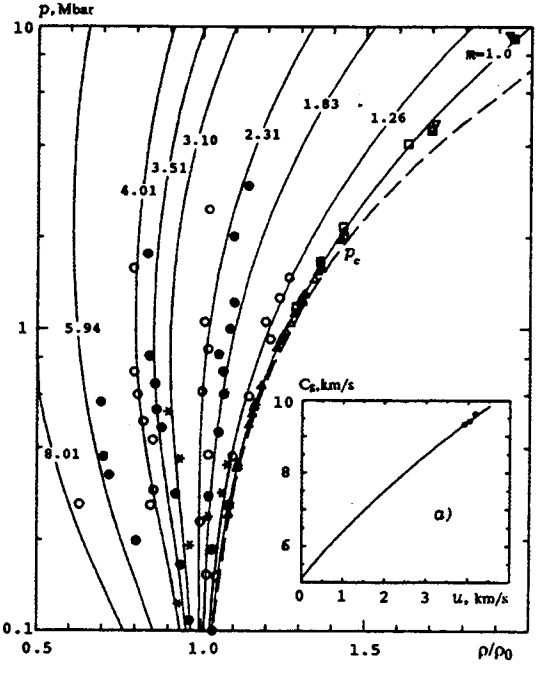
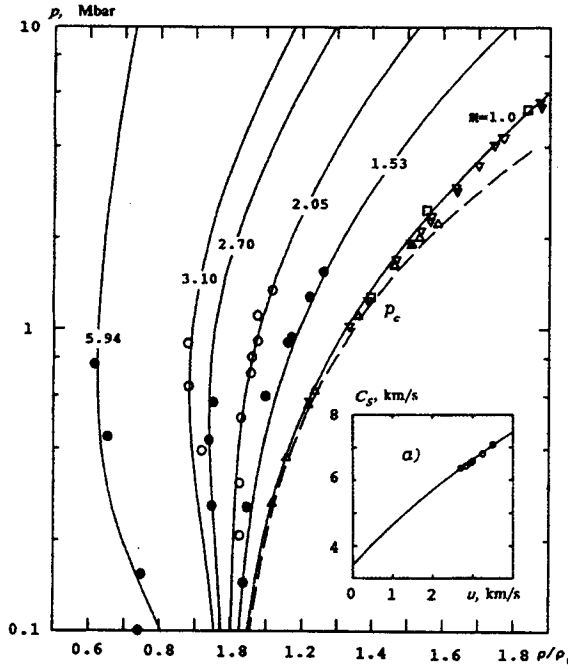


Figure 2. Hugoniots at extreme pressures





Figures 3,4. Pressure-density plots for Mo (upper) and Ta. $m=V_{00}/V_0$ - porous Hugoniots; p_c - cold pressure, points - experiment.
a) sound velocity in shocked metal

Figure 2 demonstrates that the EOS constructed describe with the good accuracy high-pressure data on principal Hugoniot. The comparison for porous Hugoniots is presented on Figure 3. It is shown that molibdenum EOS provides for the reliable description of regions with lower densities with respect to principal Hugoniot.

The same conclusion can be made for case of tantalum. Its EOS also describes with good accuracy and reliability all available shock-wave data (see Figure 4).

EOS for Minerals and Rocks

The knowledge of thermodynamics for rocks and minerals in broad range of the phase diagram is of practical significance, for example, to calculate the large asteroid impact with Earth.

Due to very high value of impact velocity for this process EOS for high-pressure phase for quartz, namely stishovite, was developed.

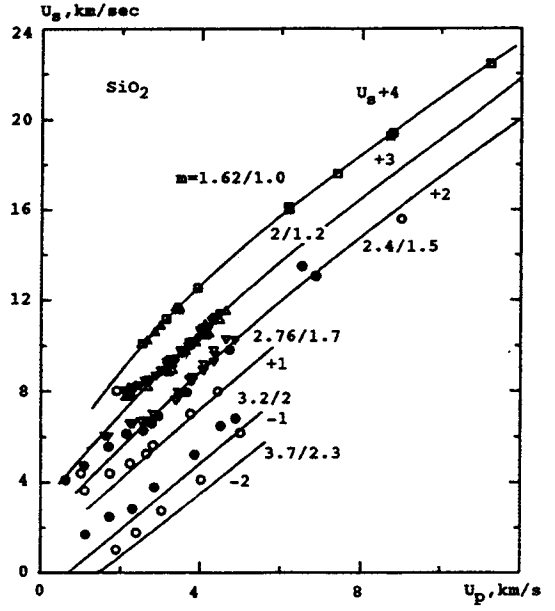


Figure 5. Shock velocity-mass velocity plot for quartz. m=ms/mq - porous Hugoniots (ms - stishovite porosity, mq - quartz porosity), points - experimental data.

As shown of Figure 5, calculated by EOS Hugoniots are in good agreement with numerous shock-wave data which are available for quartz.

EOS FOR CHEMICAL MATERIALS

A more simple form of EOS (1)-(5) is proposed to calculate thermodynamic properties for structural materials, which have complicated physical and chemical composition (polymers, plastics, composites, etc.)

EOS Model

Such materials are characterized by a highly limited set of static and dynamic data. This puts essential restrictions on the number of free parameters of the potential. This is the reason that the elastic energy is given by Formula (3) over the whole density region (note that in this case E_{sub} means the destruction energy). The volume dependence of the Gruneisen coefficient has a very simple representation

$$\gamma_c(V) = \frac{2}{3} + \left(\gamma_0 - \frac{2}{3}\right)\frac{1+\sigma_m^2}{\sigma^2+\sigma_m^2}\sigma, \qquad (6)$$

satisfying the condition $\gamma_c(V_0) = \gamma_0$ and asymptotics of γ_c=2/3 in limiting cases of low and high compressions. The only fitting parameter σ_m in Formula (6) is found by the conditions of the best description of the dynamic experimental data.

EOS for Polymers

EOS for about one hundred structural materials were constructed on the base of the model (1),(3),(4),(6). Presented here are results obtained for teflon and PMMA (polymethilmetaclrylate).

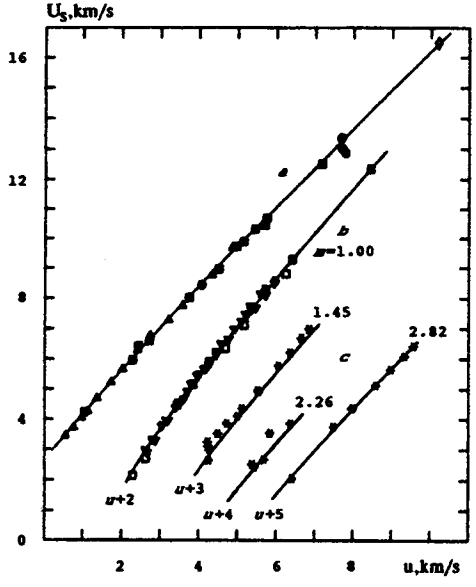


Figure 6. Principal Hugoniots for PMMA (a), teflon (b) and porous Hugoniots for teflon (c). Solid lines - EOS, points - experiment.

Shown of Figure 6 are Hugoniots of PMMA and teflon as shock velocity-particle velocity dependencies. Developed EOS describe with high accuracy both principal- and porous-Hugoniot data over whole range of dynamical characteristics. This testifies the reliability of the EOS on descibing states with lower, with respect to principal Hugoniot, density.

The analogous conclusion can be made by the analysis of Figure 7, presented on which is the comparison with EOS and experimental data on double shock compression and release expansion of teflon. Note that states in teflon release isentrope respond to final density of the order of $0.1\rho_0$.

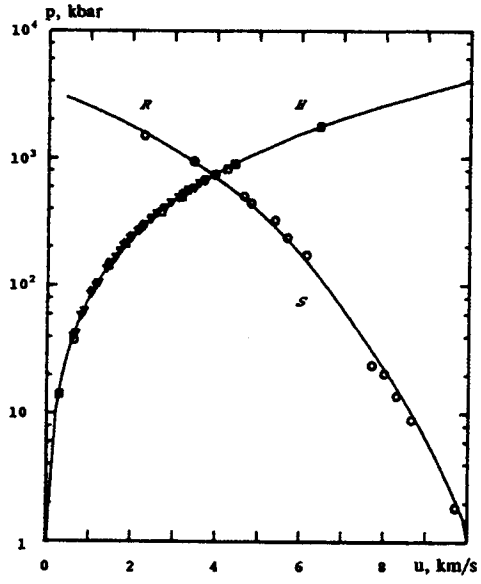


Figure 7. Principal Hugoniot (H), double shock (R) and release isentrope waves (S) for teflon. Solid lines - EOS, points - experiment

CONCLUSIONS

Simple caloric models are developed and EOS for about 150 structural materials (metals, alloys, steels, minerals, rocks, polymers, composites and others) are constructed, describing theoretical and experimental high-pressure data. Developed EOS were implemented in gasdynamic codes.

REFERENCES

[1] A. V. Bushman, G. I. Kanel, A. L. Ni, and V. E. Fortov, *Intense Loading of Condensed Matter*, London: Taylor&Francis, 1993.

[2] A. V. Busman and V. E. Fortov, Sov. Phys. Usp., 26, 465 (1983).

[3]. I. V. Lomonosov, A. V. Bushman, V. E. Fortov, Equations of state for metals at high energy densities, this proceedings.

[4] R. Hultrgen, P. D. Desay, D. T. Hawkins, M. Gleiser, K. K. Kelley and D. D. Wagman, *Selected Values of the Thermodynamic Properties of Elements*, Metals Park, Ohio: American Society for Metals, 1973.

[5] V. Ya. Vashenko and V. N. Zubarev, *Sov. Phys.-Solid State*, 5, 653 (1963).

[6] C. E. Ragan, *Phys. Rev. Ser. A.*, 25, 3360 (1982).

[7] C. E. Ragan, *Phys. Rev. Ser. A.*, 29, 1391 (1984).

[8]. A. V. Bushman, M. V. Zhernolketov, I. V. Lomonosov, Yu. N. Sutulov, V. E. Fortov, and K. V. Khishchenko, *Dokl. Ross. Akad. Nauk*, 329(5), 581 (1993) [in Russian].