MATHEMATICA MONTISNIGRI
Vol XL (2017)

EQUATION OF STATE OF SODIUM FOR MODELING OF SHOCK-WAVE PROCESSES AT HIGH PRESSURES

K. V. KHISHCHENKO[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences
Izhorskaya 13 Bldg 2, 125412 Moscow, Russia
e-mail: konst@ihed.ras.ru

[2] Moscow Institute of Physics and Technology
Institutskiy Pereulok 9, 141700 Dolgoprudny, Moscow Region, Russia

Summary. A simple model of equation of state, which represents the relationship of pressure with density and internal energy in the form of an analytic function, is used for sodium in bcc-solid and liquid phases. Thermodynamic characteristics along the principal Hugoniot adiabat are calculated for the metal and compared with available data from shock-wave experiments. The calculation results are in a good agreement with the data over whole investigated region. The equation of state can be used effectively at numerical modeling of shock-wave processes in sodium at high pressures.

1 INTRODUCTION

An equation of state (EOS) of a medium is indispensable for numerical modeling of physical processes under intense pulsed influences on materials [1–3]. For example, at high-velocity impact of bodies [4–12], interaction of intense laser [13–24] and particle beams [25–30] with matter, electrical explosion of conductors under action of high power current pulses [31–37] etc. Accuracy of thermodynamic description of properties of the medium over wide range of pressures and densities determine the adequacy of results of the modeling [38].

It is traditional to use semiempirical approach for construction of wide-range EOS models [1, 39–41]. At that, a functional form of a thermodynamic potential is chosen with taking into account theoretical considerations, while numerical coefficients in the function are determined using experimental data.

This work is devoted to description of thermodynamic properties of sodium at high pressures. The metal is used as a coolant in power plants, especially in fast neutron reactors. In particular, EOS for sodium is interesting for numerical modeling of different working regimes of such reactors under conditions of intense mechanical and thermal influences.

In the work, a semiempirical EOS in a form of simple analytic function $P = P(V,E)$ [42–44] is presented for Na, which is in contrast with more complex EOSs for the metal [45–51]. Here, P is the pressure, $V = \rho^{-1}$ is the specific volume, ρ is the density, E is the specific internal energy. The quality of proposed EOS is evaluated by a comparison of calculated kinematic and

2010 Mathematics Subject Classification: 74A15, 74J40, 76L05, 80A10, 82D35.
Key words and phrases: equation of state, analytic function, sodium, shock wave, high pressure.

dynamic parameters along the principal Hugoniot adiabat with available data from shock-wave experiments.

2 EOS MODEL

The EOS model is formulated in the general form as

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

where $E_{\rm c}$ and $P_{\rm c} = -{\rm d}E_{\rm c}/{\rm d}V$ are the cold components of internal energy and pressure at $T = 0$; Γ is a coefficient determining the contribution of thermal components of the EOS.

The cold energy is given by a polynomial [42–44, 52–54]

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

Here, $\sigma_{\rm c} = V_{0{\rm c}}/V$; $V_{0{\rm c}}$ and $B_{0{\rm c}}$ are the specific volume and bulk modulus at $P = 0$ and $T = 0$. The quantity $E_{\rm sub}$ has meaning of the sublimation energy and is determined by a condition

$$E_{\rm c}(V_{0{\rm c}}) = 0, \tag{3}$$

which gives

$$E_{\rm sub} = \frac{B_{0{\rm c}}V_{0{\rm c}}}{mn}. \tag{4}$$

Parameters m and n are determined with the use of shock-wave data for solid samples.

The dependence of the coefficient Γ upon the volume and internal energy is defined analogously to caloric models [42–44, 55–57] in the following form:

$$\Gamma(V,E) = \gamma_{\rm i} + \frac{\gamma_{\rm c}(V) - \gamma_{\rm i}}{1 + \sigma^{-2/3}\left[E - E_{\rm c}(V)\right]/E_{\rm a}}, \tag{5}$$

where

$$\gamma_{\rm c}(V) = 2/3 + (\gamma_{0{\rm c}} - 2/3)\,\frac{\sigma_{\rm n}^2 + \ln^2\sigma_{\rm m}}{\sigma_{\rm n}^2 + \ln^2(\sigma/\sigma_{\rm m})}, \tag{6}$$

$\sigma = V_0/V$; V_0 is the specific volume under normal conditions; $\gamma_{\rm c}(V)$ corresponds to the case of low thermal energies, and $\gamma_{\rm i}$ characterizes the region of highly-heated matter. The value of $E_{\rm a}$, which defines the thermal energy of the transition of Γ from one limiting case to the other, is determined from the results of shock-wave experiments at high pressures. From (1), (5) and (6), a relation of the parameter $\gamma_{0{\rm c}}$ with values of the Grüneisen coefficient $\gamma = V(\partial P/\partial E)_V$, the

internal energy and the specific volume under normal conditions (γ_0, E_0 and V_0, respectively) can be obtained:

$$\gamma_{0c} = \gamma_i + (\gamma_0 - \gamma_i)\left[1 + \frac{E_0 - E_c(V_0)}{E_a}\right]^2. \tag{7}$$

The interpolational function (6) ensures validity of the condition $\gamma(V_0, E_0) = \gamma_0$, and gives the asymptotic value $\gamma_c = 2/3$ in the limiting cases of low and high compression ratios σ. The parameters σ_n and σ_m are determined from the requirement of optimum fit to experimental data on shock compressibility of a substance in question.

3 EOS FOR SODIUM

Sodium under atmospheric pressure has a body-centered cubic (bcc) structure ($T > 6$ K) [58]. It melts at 371 K. Under static compression at room temperature, the bcc phase transforms at pressure 65 GPa to the phase with a face-centered cubic (fcc) structure. At further increase of pressure at room temperature, more crystalline phases of sodium are observed [59–61].

Shock compressibility of sodium is investigated with the use of traditional explosive systems up to 0.1 TPa [62–64]. Shock compression leads to increase of temperature and melting of the bcc phase [49].

In this work, the unified EOS for bcc-solid and liquid phases of sodium is constructed. The EOS coefficients obtained within the framework of the model are as follows: $V_0 = 1.0331$ cm^3/g, $V_{0c} = 0.99306$ cm^3/g, $B_{0c} = 6.817$ GPa, $m = 1$, $n = 0.96$, $\sigma_m = 1.2$, $\sigma_n = 1.5$, $\gamma_{0c} = 0.9$, $\gamma_i = 0.45$ and $E_a = 45$ kJ/g.

Calculated principal Hugoniot adiabat of sodium is presented in figures 1–3 in comparison with data from experiments [62–64]. Calculation of the Hugoniot adiabat is performed by solving the equation of energy conservation in the shock-wave front [1]:

$$E = E_0 + \frac{1}{2}(P_0 + P)(V_0 - V), \tag{8}$$

where the left-hand side is closed by the EOS function $E = E(P,V)$. Equation (8) and the EOS determine the specific volume as a function of pressure along the Hugoniot adiabat for samples of initial density $\rho_0 = {V_0}^{-1}$. Then the shock (U_s) and particle (U_p) velocities are calculated using the equations of conservation of mass and momentum in the shock-wave front [1]:

$$U_s = V_0\sqrt{(P - P_0)/(V_0 - V)}, \qquad U_p = \sqrt{(P - P_0)(V_0 - V)}. \tag{9}$$

Analysis of the comparison results in figures 1–3 shows that the obtained EOS provides for a reliable description of thermodynamic properties of the metal over a whole investigated range of shock and particle velocities, pressures and compression ratios.

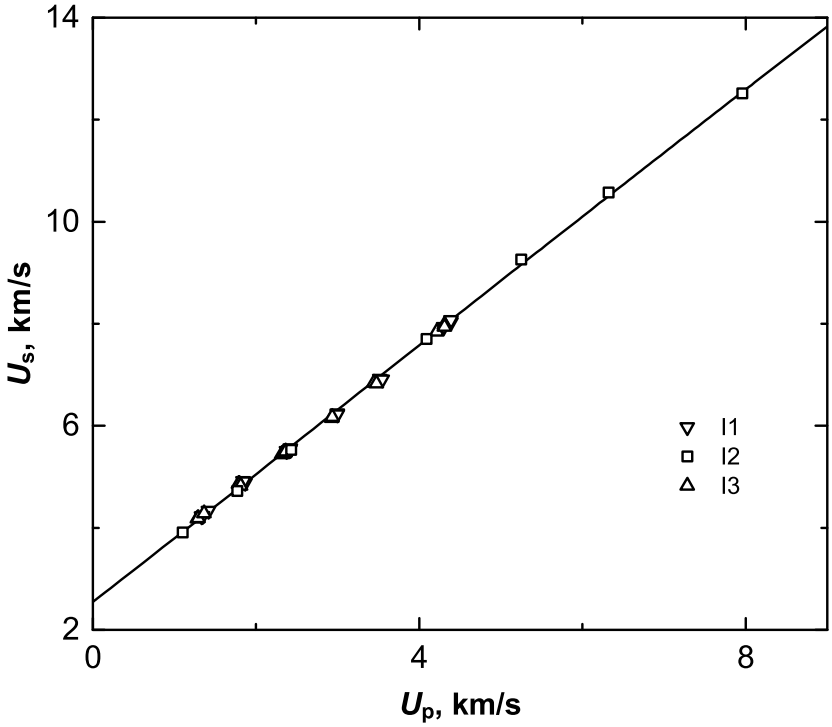

Figure 1: The principal Hugoniot adiabat of sodium: curve corresponds to the present calculations; markers—experimental data (I1—[62], I2—[63], I3—[64]).

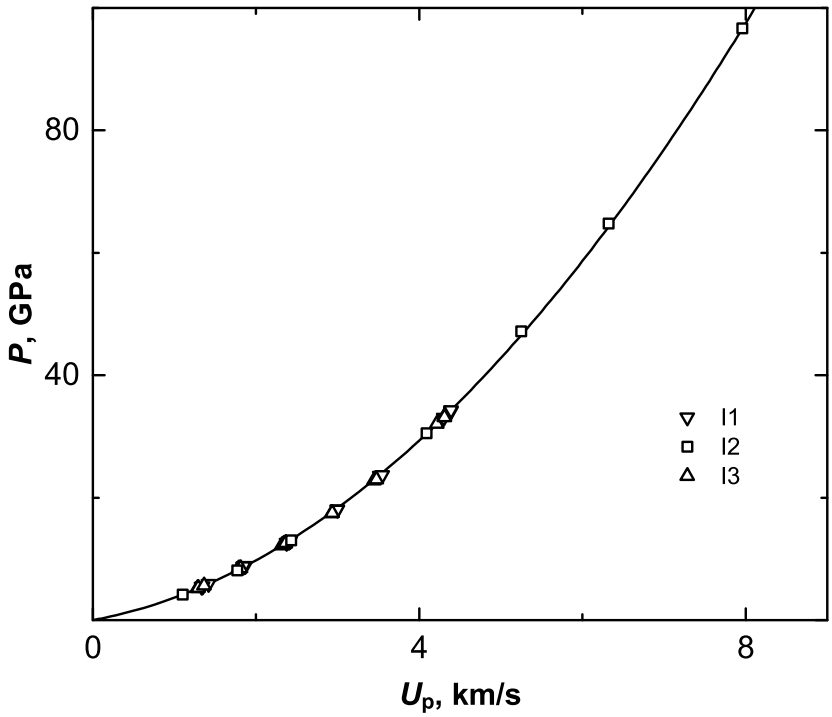

Figure 2: The principal Hugoniot adiabat of sodium: notations are analogous to figure 1.

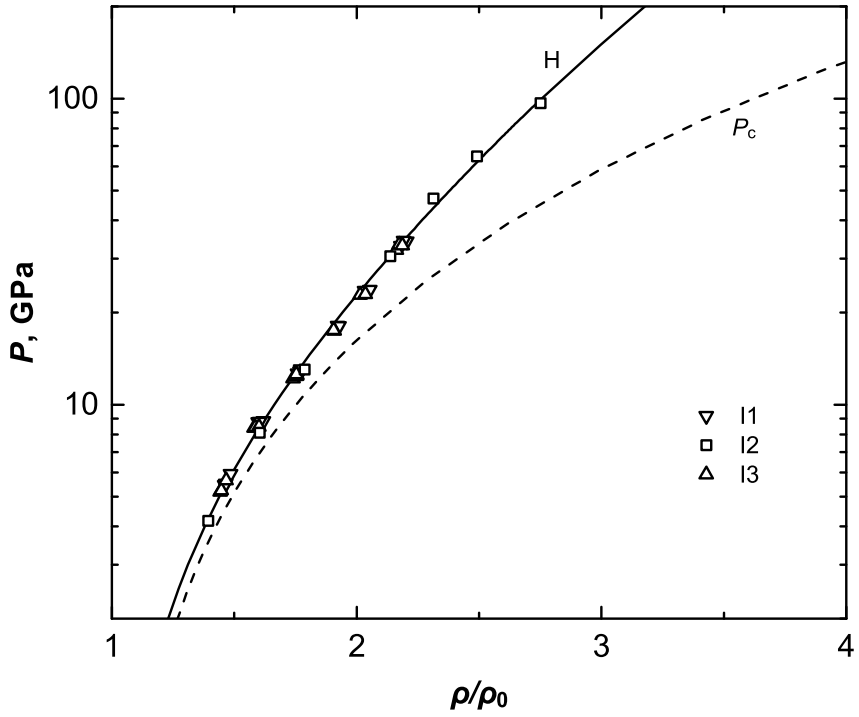

Figure 3: The cold curve (P_c) and the principal Hugoniot adiabat (H) of sodium: curves correspond to the present calculations; markers—experimental data (I1—[62], I2—[63], I3—[64]).

4 CONCLUSIONS

The EOS, which has the form of an analytic function, is proposed for sodium in bcc-solid and liquid phases. This EOS agrees well with available data from dynamic experiments; it can be used effectively at numerical modeling of shock-wave processes in the metal at high pressures.

Acknowledgments: The work is supported by the Russian Science Foundation (grant No. 14-50-00124).

The paper is based on the proceedings of the XXXII International Conference on Interaction of Intense Energy Fluxes with Matter, which was held in Elbrus settlement, in the Kabardino-Balkar Republic of the Russian Federation, from March 1 to 6, 2017.

REFERENCES

[1] Ya. B. Zel'dovich and Yu. P. Raizer, *Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena*, New York: Academic Press, (1967).

[2] A. V. Bushman, V. E. Fortov, G. I. Kanel', and A. L. Ni, *Intense Dynamic Loading of Condensed Matter*, Washington: Taylor & Francis, (1993).

[3] V. Fortov, *Thermodynamics and Equations of State for Matter: From Ideal Gas to Quark–Gluon Plasma*, Singapore: World Scientific Publishing, (2016).

[4] V. E. Fortov, V. V. Kim, I. V. Lomonosov, A. V. Matveichev, and A. V. Ostrik, "Numerical modeling of hypervelocity impacts", *Int. J. Impact Eng.* **33**(1–12), 244–253 (2006).

[5] M. E. Povarnitsyn, K. V. Khishchenko, and P. R. Levashov, "Hypervelocity impact modeling with different equations of state", *Int. J. Impact Eng.* **33**(1–12), 625–633 (2006).
[6] V. V. Milyavskii, V. E. Fortov, A. A. Frolova, K. V. Khishchenko, A. A. Charakhch'yan, and L. Shurshalov, "Calculation of shock compression of porous media in conical solid-state targets with an outlet hole", *Comput. Math. Math. Phys.* **46**(5), 873–890 (2006).
[7] V. V. Milyavskii, V. E. Fortov, A. A. Frolova, K. V. Khishchenko, A. A. Charakhch'yan, and L. Shurshalov, "On the mechanism of pressure increase with increasing porosity of the media compressed in conical and cylindrical targets", *Comput. Math. Math. Phys.* **50**(12), 2082–2094 (2010).
[8] L. V. Shurshalov, A. A. Charakhch'yan, and K. V. Khishchenko, "Numerous experiment on impact compression of a mixture of graphite and water", *Combust., Explos. Shock Waves* **53**(4), 471–478 (2017).
[9] A. E. Mayer, K. V. Khishchenko, P. R. Levashov, and P. N. Mayer, "Modeling of plasticity and fracture of metals at shock loading", *J. Appl. Phys.* **113**(19), 193508 (2013).
[10] E. I. Kraus and I. I. Shabalin, "The tool for high-velocity interaction and damage of solids", *Mathematica Montisnigri* **39**, 18–29 (2017).
[11] A. E. Mayer and A. A. Ebel, "Shock-induced compaction of nanoparticle layers into nanostructured coating", *J. Appl. Phys.* **122**(16), 165901 (2017).
[12] A. L. Coleman, R. Briggs, M. G. Gorman, S. Ali, A. Lazicki, D. C. Swift, P. G. Stubley, E. McBride, G. Collins, J. S. Wark, and M. I. McMahon, "Implementation of hydrodynamic simulation code in shock experiment design for alkali metals", *J. Phys.: Conf. Ser.* **950**, 042037 (2017).
[13] M. Povarnitsyn, K. Khishchenko, P. Levashov, A. Zakharenkov, J. Hermann, S. De Falco, and T. Itina, "Simulation of ultrashort double pulse laser ablation of metals", *J. Optoelectron. Adv. Mater.* **12**(3), 674–676 (2010).
[14] M. E. Povarnitsyn, N. E. Andreev, P. R. Levashov, K. V. Khishchenko, and O. N. Rosmej, "Dynamics of thin metal foils irradiated by moderate-contrast high-intensity laser beams", *Phys. Plasmas* **19**(2), 023110 (2012).
[15] S. A. Abrosimov, A. P. Bazhulin, V. V. Voronov, A. A. Geras'kin, I. K. Krasyuk, P. Pashinin, A. Semenov, I. A. Stuchebryukhov, K. V. Khishchenko, and V. E. Fortov, "Specific features of the behaviour of targets under negative pressures created by a picosecond laser pulse", *Quantum Electron.* **43**(3), 246–251 (2013).
[16] N. A. Inogamov, V. V. Zhakhovsky, Y. V. Petrov, V. A. Khokhlov, S. I. Ashitkov, K. V. Khishchenko, K. P. Migdal, D. K. Ilnitsky, Y. N. Emirov, P. S. Komarov, V. V. Shepelev, C. W. Miller, I. I. Oleynik, M. B. Agranat, A. V. Andriyash, S. I. Anisimov, and V. E. Fortov, "Electron-ion relaxation, phase transitions, and surface nano-structuring produced by ultrashort laser pulses in metals", *Contrib. Plasma Phys.* **53**(10), 796–810 (2013).
[17] P. V. Breslavskiy, A. V. Mazhukin, and O. N. Koroleva, "Simulation of the dynamics of plasma expansion, the formation and interaction of shock and heat waves in the gas at the nanosecond laser irradiation", *Mathematica Montisnigri* **33**, 5–24 (2015).
[18] A. A. Samokhin, V. I. Mazhukin, A. V. Shapranov, M. M. Demin, and P. A. Pivovarov, "Continual and molecular-dynamic modeling of phase transitions during laser ablation", *Mathematica Montisnigri* **33**, 25–42 (2015).
[19] N. E. Andreev, M. E. Povarnitsyn, M. E. Veysman, A. Ya. Faenov, P. R. Levashov, K. Khishchenko, T. A. Pikuz, A. I. Magunov, O. N. Rosmej, A. Blazevic, A. Pelka, G. Schaumann, M. Schollmeier, and M. Roth, "Interaction of annular-focused laser beams with solid targets", *Laser Part. Beams* **33**(3), 541–550 (2015).
[20] A. A. Samokhin and P. A. Pivovarov, "On spinodal manifestation during fast heating and evaporation of thin liquid film", *Mathematica Montisnigri* **33**, 125–128 (2015).
[21] I. K. Krasyuk, P. P. Pashinin, A. Yu. Semenov, K. V. Khishchenko, and V. E. Fortov, "Study of extreme states of matter at high energy densities and high strain rates with powerful lasers", *Laser Phys.* **26**(9), 094001 (2016).
[22] V. I. Mazhukin, A. V. Shapranov, A. V. Mazhukin, and O. N. Koroleva, "Mathematical formulation of a kinetic version of Stefan problem for heterogeneous melting/crystallization of metals", *Mathematica Montisnigri* **36**, 58–77 (2016).

[23] A. E. Zubko and A. A. Samokhin, "Modeling of thermoacoustic and evaporation pressure signals in absorbing liquids irradiated with nanosecond laser pulses", *Mathematica Montisnigri* **36**, 78–85 (2016).
[24] A. A. Samokhin, S. I. Kudryashov, A. E. Zubko, and A. V. Sidorin, "Modelling of nanosecond laser ablation. Continual approach", *Mathematica Montisnigri* **37**, 76–90 (2016).
[25] A. A. Charakhch'yan and K. V. Khishchenko, "Plane thermonuclear detonation waves initiated by proton beams and quasi-one-dimensional model of fast ignition", *Laser Part. Beams* **33**(1), 65–80 (2015).
[26] K. V. Khishchenko and A. A. Charakhch'yan, "Collision of plane thermonuclear detonation waves in a preliminarily compressed DT mixture", *Plasma Phys. Rep.* **41**(3), 220–230 (2015).
[27] A. E. Mayer and P. N. Mayer, "Continuum model of tensile fracture of metal melts and its application to a problem of high-current electron irradiation of metals", *J. Appl. Phys.* **118**(3), 035903 (2015).
[28] S. F. Gnyusov, V. P. Rotshtein, A. E. Mayer, V. V. Rostov, A. V. Gunin, K. Khishchenko, and P. Levashov, "Simulation and experimental investigation of the spall fracture of 304L stainless steel irradiated by a nanosecond relativistic high-current electron beam", *Int. J. Fract.* **199**(1), 59–70 (2016).
[29] A. A. Frolova, K. V. Khishchenko, and A. A. Charakhch'yan, "Track method for the calculation of plasma heating by charged thermonuclear reaction products for axisymmetric flows", *Comput. Math. Math. Phys.* **56**(3), 437–449 (2016).
[30] M. E. Zhukovsky, M. B. Markov, S. V. Podolyako, I. A. Tarakanov, R. V. Uskov, A. M. Chlenov, and V. F. Zinchenko, "Researching the spectrum of bremsstrahlung generated by the RIUS-5 electron accelerator", *Mathematica Montisnigri* **35**, 54–67 (2016).
[31] S. I. Tkachenko, K. V. Khishchenko, V. S. Vorob'ev, P. R. Levashov, I. V. Lomonosov, and V. E. Fortov, "Metastable states of liquid metal under conditions of electric explosion", *High Temp.* **39**(5), 674–687 (2001).
[32] V. I. Oreshkin, R. B. Baksht, A. Yu. Labetsky, A. G. Rousskikh, A. Shishlov, P. Levashov, K. Khishchenko, and I. V. Glazyrin, "Study of metal conductivity near the critical point using a microwire electrical explosion in water", *Tech. Phys.* **49**(7), 843–848 (2004).
[33] A. G. Rousskikh, R. B. Baksht, S. A. Chaikovsky, A. V. Fedunin, K. V. Khishchenko, A. Yu. Labetsky, P. R. Levashov, A. V. Shishlov, and S. I. Tkachenko, "The effects of preheating of a fine tungsten wire and the polarity of a high-voltage electrode on the energy characteristics of an electrically exploded wire in vacuum", *IEEE Trans. Plasma Sci.* **34**(5), 2232–2238 (2006).
[34] S. I. Tkachenko, P. R. Levashov, and K. V. Khishchenko, "Analysis of electrical conductivity measurements in strongly coupled tungsten and aluminum plasmas", *Czech. J. Phys.* **56**, B419–B424 (2006).
[35] E. V. Grabovskii, P. R. Levashov, G. M. Oleinik, C. L. Olson, P. V. Sasorov, V. P. Smirnov, S. I. Tkachenko, and K. V. Khishchenko, "Formation and dynamics of plasma layers formed on the foil surface under the action of a high-current pulse", *Plasma Phys. Rep.* **32**(9), 718–728 (2006).
[36] V. I. Oreshkin, K. V. Khishchenko, P. R. Levashov, A. G. Rousskikh, and S. A. Chaikovskii, "Strata formation at fast electrical explosion of cylindrical conductors", *High Temp.* **50**(5), 584–595 (2012).
[37] S. I. Tkachenko, V. A. Gasilov, A. Yu. Krukovskiy, O. G. Olkhovskaya, and I. P. Tsygvintsev, "Computational model and numerical analysis of a thin aluminum wire electric explosion", *Mathematica Montisnigri* **28**, 39–61 (2013).
[38] S. I. Tkachenko, P. R. Levashov, and K. V. Khishchenko, "The influence of an equation of state on the interpretation of electrical conductivity measurements in strongly coupled tungsten plasma", *J. Phys. A: Math. Gen.* **39**(23), 7597–7603 (2006).
[39] A. V. Bushman and V. E. Fortov, "Model equations of state", *Sov. Phys. Usp.* **26**(6), 465–496 (1983).
[40] V. E. Fortov and I. V. Lomonosov, "Ya. B. Zeldovich and equation of state problems for matter under extreme conditions", *Phys. Usp.* **57**(3), 219–233 (2014).
[41] I. V. Lomonosov and S. V. Fortova, "Wide-range semiempirical equations of state of matter for numerical simulation on high-energy processes", *High Temp.* **55**(4), 585–610 (2017).
[42] I. V. Lomonosov, V. E. Fortov, and K. V. Khishchenko, "Model of wide-range equations of polymer materials state under high-energy densities", *Khim. Fiz.* **14**(1), 47–52 (1995).

[43] K. V. Khishchenko, I. V. Lomonosov, and V. E. Fortov, "Equations of state for organic compounds over wide range of densities and pressures", *AIP Conf. Proc.* **370**, 125–128 (1996).
[44] A. V. Bushman, M. V. Zhernokletov, I. V. Lomonosov, Yu. N. Sutulov, V. E. Fortov, and K. V. Khishchenko, "Experimental study of phenylone and polystyrene under the shock loading conditions and isentropic expansion. Plastics state equation under high densities of energy", *Zh. Eksp. Teor. Fiz.* **109**(5), 1662–1670 (1996).
[45] D. J. Pastine, "P, V, E, T equation of state of metallic sodium in the classical region of temperature", *Phys. Rev. Lett.* **18**(26), 1187–1189 (1967).
[46] D. J. Pastine, "Equation of state for sodium metal", *Phys. Rev.* **166**(3), 703–709 (1968).
[47] M. Ross, "Extension of liquid-metal theory to dense partially ionized plasmas", *Phys. Rev. B* **21**(8), 3140–3151 (1980).
[48] D. A. Young and M. Ross, "Theoretical high-pressure equations of state and phase diagrams of the alkali metals", *Phys. Rev. B* **29**(2), 682–691 (1984).
[49] K. V. Khishchenko, "Equations of state for two alkali metals at high temperatures", *J. Phys.: Conf. Ser.* **98**, 032023 (2008).
[50] D. K. Belashchenko, "Impact compression of alkali metals: Computer-aided simulation", *High Temp.* **51**(5), 626–639 (2013).
[51] S. Zhang, K. P. Driver, F. Soubiran, and B. Militzer, "Equation of state and shock compression of warm dense sodium—A first-principles study", *J. Chem. Phys.* **146**(7), 074505 (2017).
[52] A. V. Bushman, M. V. Zhernokletov, I. V. Lomonosov, Yu. N. Sutulov, V. E. Fortov, and K. V. Khishchenko, "Investigation of plexiglas and teflon under double shock loading and in isentropic release waves. Polymers equation of state at high-energy density", *Dokl. Akad. Nauk* **329**(5), 581–584 (1993).
[53] A. V. Bushman, I. V. Lomonosov, V. E. Fortov, K. V. Khishchenko, M. V. Zhernokletov, and Yu. Sutulov, "Shock compressibility and equation of state of a polyimide", *JETP Lett.* **58**(8), 620–624 (1993).
[54] I. V. Lomonosov, A. V. Bushman, V. E. Fortov, and K. V. Khishenko, "Caloric equations of state of structural materials", in: *High-Pressure Science and Technology—1993* ed. by S. C. Schmidt et al., New York: AIP Press, pp. 133–136 (1994).
[55] K. V. Khishchenko, "The equation of state for magnesium at high pressures", *Tech. Phys. Lett.* **30**(10), 829–831 (2004).
[56] K. V. Khishchenko, "Equation of state for tungsten over a wide range of densities and internal energies", *J. Phys.: Conf. Ser.* **653**, 012081 (2015).
[57] K. V. Khishchenko, "Equation of state for titanium at high energy densities", *J. Phys.: Conf. Ser.* **774**, 012001 (2016).
[58] E. Yu. Tonkov, *Phase Diagrams of Elements at High Pressures*, Moscow: Nauka, (1979).
[59] E. G. Maksimov, M. V. Magnitskaya, and V. E. Fortov, "Non-simple behavior of simple metals at high pressure", *Phys. Usp.* **48**(8), 761–780 (2005).
[60] V. F. Degtyareva, "Simple metals at high pressures: the Fermi sphere–Brillouin zone interaction model", *Phys. Usp.* **49**(4), 369–388 (2006).
[61] O. Degtyareva, "Crystal structure of simple metals at high pressures", *High Pressure Res.* **30**(3), 343–371 (2010).
[62] M. H. Rice, "Pressure-volume relations for the alkali metals from shock-wave measurements", *J. Phys. Chem. Solids* **26**(3), 483–492 (1965).
[63] A. A. Bakanova, I. P. Dudoladov, and R. F. Trunin, "Compression of alkali metals by strong shock waves", *Fiz. Tverd. Tela* **7**(6), 1615–1622 (1965).
[64] S. P. Marsh (ed.), *LASL Shock Hugoniot Data*, Berkeley, CA: University of California Press, (1980).

Received October 10, 2017