Equation of state for vanadium at high pressures

K V Khishchenko¹,²,³
¹ Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13
² Bldg 2, Moscow 125412, Russia
³ Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
⁴ South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia

E-mail: konst@ihed.ras.ru

Abstract. An equation of state for vanadium is proposed over a wide range of densities and pressures in the form of an analytic function of pressure on the specific volume and internal energy. The calculated cold curve and shock adiabat are compared with the available data from static and dynamic compression experiments. The developed equation of state can be used to simulate physical processes in vanadium under conditions of high energy density.

1. Introduction

The equations of state (EOSs) of materials are of interest for fundamental and applied physics of high energy densities [1–9], in particular, since they are necessary in the numerical simulation of various processes occurring under such extreme conditions as in high-speed collisions of bodies [10–14], in the interaction of intense laser [15–21] and corpuscular [22–25] beams with solids, at electrical explosion of conductors [26–31]. The EOS closes the system of equations of hydrodynamics and serves as the basis for a solution that qualitatively and quantitatively corresponds to the behavior of materials in the problem under consideration.

Vanadium is widely used as a component of structural alloys [32] because of its high tensile strength, and is also a promising refractory material for thermonuclear reactors [33], where high resistance to damage caused by neutron irradiation is required.

In this work, the EOS for vanadium is constructed within the framework of a semiempirical approach, in which the function of pressure (P) on the specific volume (V) and internal energy (E) is taken from theoretical consideration, and the coefficients in this function are determined using experimental data. The calculation results are presented in comparison with the data of static and dynamic experiments with this metal.

2. EOS model

The EOS is taken in the form of a single analytic function for the entire region, which is achieved both when the condensed matter is compressed and when it expands to almost gaseous densities, as follows [34–36]:

\[ P(V, E) = P_c(V) + \frac{\Gamma(V, E)}{V}[E - E_c(V)], \]

where \( E_c \) is the internal energy at zero absolute temperature, \( T = 0 \); \( P_c \) is the corresponding pressure at \( T = 0 \), \( P_c = -dE_c/dV \).
The cold energy is given by a polynomial,
\[ E_c(V) = \frac{B_0cV_0c}{m-n} \left( \frac{\sigma_m^n}{m} - \frac{\sigma_n^n}{n} \right) + E_{\text{sub}}, \]
where \( \sigma_c = \frac{V_0c}{V} \); \( V_0c \) and \( B_0c \) are the specific volume and the bulk modulus at \( T = 0 \) and \( P = 0 \); \( E_{\text{sub}} = \frac{B_0cV_0c}{mn} \); \( m \) and \( n \) are parameters.

The thermal contribution to the EOS is determined by the second term on the right-hand side of equation (1) with the coefficient \( \Gamma \) depending on the volume and internal energy:
\[ \Gamma(V, E) = \gamma_i + \gamma_c(V) - \frac{\gamma_i}{1 + \sigma^{-2/3} [E - E_c(V)]/E_a}, \]
where \( \sigma = \frac{V_0}{V} \); \( V_0 \) is the specific volume under normal conditions, \( E = E_0 \) and \( P = P_0 \); \( \gamma_c \) is the Grüneisen coefficient \( \gamma = V(\partial P/\partial E)_V \) in the case \( T = 0 \); \( \gamma_i \) is the constant value of the Grüneisen coefficient in the case of high thermal energies, \( E - E_c \gg E_a \sigma^{2/3} \); \( E_a \) is a parameter. The coefficient \( \gamma_c \) is given by the volume function
\[ \gamma_c(V) = 2/3 + (\gamma_{0c} - 2/3) \frac{\sigma_m^2 + \ln^2(\sigma_m)}{\sigma_m^2 + \ln^2(\sigma/\sigma_m)}, \]
where the value of \( \gamma_{0c} \) corresponds to \( \sigma = 1 \); \( \sigma_m \) and \( \sigma_n \) are parameters.

3. EOS for vanadium

Under normal pressure \( P = P_0 \), vanadium has a body-centered cubic (bcc) structure and melts at a temperature of \( T = 2193 \) K [37].

At room temperature under conditions of quasi-hydrostatic compression, vanadium has been studied up to 224 GPa [38–41]. According to [39], the bcc structure remains stable up to the maximum pressure reached. According to other data [40], bcc vanadium transforms into a rhombohedral structure at 63 and 69 GPa under conditions of quasi-hydrostatic and non-hydrostatic compression, respectively. The appearance of the rhombohedral structure under non-hydrostatic action was also observed at lower pressures of 30 GPa at room temperature and 37 GPa at 425 K [41]. In [42], when vanadium was compressed at room temperature, the appearance of the rhombohedral phase was observed at 53 GPa; at higher pressures when vanadium was heated, the rhombohedral phase was observed only up to a certain temperature: up to 1560 K at 64 GPa and up to 1700 K at 120 GPa. At higher temperatures, only the bcc phase of vanadium was observed in experiments [42] up to 120 GPa.

Shock compressibility of vanadium has been studied using conventional explosive systems up to pressures of 130 GPa [43–45]. The use of special explosive systems [44] and two-stage light-gas guns [46, 47] made it possible to expand the range of studies of vanadium in shock waves to 340 GPa. The shock compressibility of vanadium at relatively low pressures up to 10 GPa was studied using a single-stage gas gun [48].

In measurements with the acceleration of an aluminum flyer by magnetic pressure [49], the highest pressure in shock-compressed vanadium was obtained, about 870 GPa.

The results of the present calculation of the shock adiabat of vanadium are shown in figures 1 and 2 in comparison with available shock-wave data [44–49]. An analysis of the comparison of these results and data shows that the obtained EOS adequately describes the thermodynamic properties of the metal in the entire investigated range of shock and particle velocities (\( U_s \) and \( U_p \), respectively), pressures and densities, except for the point at the highest pressure reached in experiment [49].
Figure 1. Principal shock adiabat of vanadium (i.e., the initial density of samples $\rho_{00}$ is equal to the normal density $\rho_0 = 1/V_0$): (a) shock velocity and (b) pressure as functions of particle velocity; lines—the result of the present work; markers—experimental data (H1—[44]; H2—[45]; H3—[48]; H4—[46]; H5—[47]; H6—[49]).
Figure 2. Cold curve ($P_c$) and principal shock adiabat (H) of vanadium within (a) narrower and (b) wider ranges of densities and pressures: lines—the result of this work; markers—data from experiments on shock loading ($H_1$—[44]; $H_2$—[45]; $H_3$—[48]; $H_4$—[46]; $H_5$—[47]; $H_6$—[49]) and static compression at room temperature ($T_0$—[38]; $T_1$—[39]; $T_2$ and $T_3$—[40], quasi-hydrostatic, bcc and rhombohedral, respectively; $T_4$ and $T_5$—[40], non-hydrostatic, bcc and rhombohedral, respectively; $T_6$—[41]; $T_7$—[50]; $T_8$ and $T_9$—[42], bcc and rhombohedral, respectively).
As one can see in figure 2, the calculated cold curve is in a good agreement with data from quasi-hydrostatic experiments [38–41] for both bcc and rhombohedral structures. Data from non-hydrostatic experiments [40, 41] lie at higher pressures than data from quasi-hydrostatic [40, 41] and even shock-wave [44–48] experiments at the same compression ratios. Note that data from static experiments [42, 50] also appear at higher pressures than shock-wave data [44, 45, 47, 48] at the same densities, which is hardly possible under hydrostatic conditions.

The obtained coefficients of the EOS (1)–(4) for vanadium are as follows:

\( V_0 = 0.16447 \text{ cm}^3/\text{g}, \)  
\( V_0c = 0.16371 \text{ cm}^3/\text{g}, \)  
\( B_0c = 154.875 \text{ GPa}, \)  
\( m = 1, \)  
\( n = 0.99, \sigma_m = 0.8, \sigma_n = 0.5, \gamma_{0c} = 1.5, \gamma_i = 0.45 \) and \( E_a = 200 \text{ kJ/g}. \)

4. Conclusion

So, the EOS for vanadium has been constructed in the form of pressure dependence on specific volume and internal energy. This EOS is in good agreement with the available data from static and dynamic experiments. It can be effectively used to simulate various processes in this metal at high pressures.

Acknowledgments

The work is supported by the Russian Science Foundation (grant No. 19-19-00713).

References

[1] Bushman A V, Fortov V E, Kanel’ G I and Ni A L 1993 *Intense Dynamic Loading of Condensed Matter* (Washington: Taylor & Francis)
[2] Bushman A V, Fortov V E and Lomonosov I V 1993 *J. Non-Cryst. Solids* 156–158 631–8
[3] Fortov V 2016 *Thermodynamics and Equations of State for Matter: From Ideal Gas to Quark–Gluon Plasma* (Singapore: World Scientific Publishing)
[4] Molodets A M, Golyshin A A and Shakhray D V 2016 *J. Phys.: Conf. Ser.* 774 012008
[5] Lomonosov I V and Fortova S V 2017 *High Temp.* 55 585–610
[6] Maevskii K K 2019 *Math. Montis.* 45 52–9
[7] Lineva V I, Sineva M A, Morozov I V and Belov G V 2020 *High Temp.* 58 44–9
[8] Gilev S D 2020 *High Temp.* 58 166–72
[9] Bodryakov V Yu 2020 *High Temp.* 58 213–7
[10] Fortov V E, Kim V V, Lomonosov I V, Matveichev A V and Ostrik A V 2006 *Int. J. Impact Eng.* 33 244–53
[11] Povarnitsyn M E, Khishchenko K V and Levashov P R 2006 *Int. J. Impact Eng.* 33 625–33
[12] Popova T V, Mayer A E and Khishchenko K V 2018 *J. Appl. Phys.* 123 235902
[13] Kanel’ G I 2020 *High Temp.* 58 550–65
[14] Khishchenko K V and Mayer A E 2021 *Int. J. Mech. Sci.* 189 105971
[15] Povarnitsyn M E, Itina T E, Khishchenko K V and Levashov P R 2011 *Appl. Surf. Sci.* 257 5168–71
[16] Povarnitsyn M E, Andreev N E, Levashov P R, Khishchenko K V, Kim D A, Novikov V G and Rosmej O N 2013 *Laser Part. Beams* 31 663–71
[17] Ihitsky D K, Khokhlov V A, Inogamov N A, Zhakhovskiy V V, Petrov Yu V, Khishchenko K V, Migdal K P and Ansimov S I 2014 *J. Phys.: Conf. Ser.* 500 032021
[18] Krasyuk I K, Pashinin P P, Semenov A Yu, Khishchenko K V and Fortov V E 2016 *Laser Phys.* 26 094001
[19] Gus’kov S Yu, Krasyuk I K, Semenov A Yu, Stuchebryukhov I A and Khishchenko K V 2019 *JETP Lett.* 109 516–20
[20] Mazhukin V I, Shapranov A V and Mazhukin A V 2019 *Math. Montis.* 44 110–21
[21] Inogamov N A, Petrov Yu V, Khokhlov V A and Zhakhovskii V V 2020 *High Temp.* 58 632–46
[22] Charakhch’yan A A and Khishchenko K V 2015 *Laser Part. Beams* 33 65–80
[23] Guyusov S F, Rotstein V P, Mayer A E, Rostov V V, Gunin A V, Khishchenko K V and Levashov P R 2016 *Int. J. Fract.* 199 59–70
[24] Frolova A A, Khishchenko K V and Charakhch’yan A A 2019 *Phys. Plasmas* 26 034501
[25] Schoenfield K et al 2020 *Phys. Plasmas* 27 043103
[26] Roussikh A G, Bakht R R, Chaikovsky S A, Fedunin A V, Khishchenko K V, Labetsky A Yu, Levashov P R, Shishlov A V and Tkachenko S I 2006 *IEEE Trans. Plasma Sci.* 34 2323–8
[27] Rososhek A, Efimov S, Nitishinski M, Yanuka D, Tewari S V, Gurovich V Tz, Khishchenko K and Krasik Ya E 2017 *Phys. Plasmas* 24 122705
[28] Senchenko V N and Belikov R S 2019 *J. Phys.: Conf. Ser.* **1147** 012011
[29] Kondratyev A M, Korobenko V N and Rakhel A D 2018 *J. Exp. Theor. Phys.* **127** 1074–86
[30] Kostanovskii A V and Kostanovskaya M E 2020 *Meas. Tech.* **63** 204–9
[31] Savvatimsky A I, Omufiev S V, Valyano G E, Kireeva A N and Patrikeev Yu B 2020 *High Temp.* **58** 144–7
[32] Chandler H 1998 *Metallurgy for the Non-Metallurgist* (Materials Park, OH: ASM International)
[33] Matsui H, Fukumoto K, Smith D L, Ching H M, van Witzenburg W and Votinov S N 1996 *J. Nucl. Mater.* **233–237** 92–9
[34] Khishchenko K V, Zhernokletov M V, Lomonosov I V and Sutulov Yu N 2005 *Tech. Phys.* **50** 197–201
[35] Khishchenko K V 2020 *Math. Montis.* **47** 119–23
[36] Khishchenko K V 2020 *J. Phys.: Conf. Ser.* **1556** 012041
[37] Tonkov E Yu 1979 *Phase Diagrams of Elements at High Pressures* (Moscow: Nauka)
[38] Ming L and Manghmani M H 1978 *J. Appl. Phys.* **49** 208–12
[39] Nakamoto Y, Takemura K, Ishizuka M, Shimizu K and Kikegawa T 2005 Equation of state for vanadium under hydrostatic conditions *Proc. of the Joint 20th AIRAPT–43rd EHPRG Conf. on Science and Technology of High Pressure: Karlsruhe, June 27th–July 1st, 2005* (Karlsruhe: Karlsruhe Forschungszentrum) p P120
[40] Ding Y, Ahuja R, Shu J, Chow P, Luo W and Mao H K 2007 *Phys. Rev. Lett.* **98** 085502
[41] Jenei Zs, Liermann H P, Cynn H, Klepeis J H P, Baer B J and Evans W J 2011 *Phys. Rev. B* **83** 054101
[42] Errandonea D, MacLeod S G, Burakovksy L, Santamaria-Perez D, Proctor J E, Cynn H and Mezouar M 2019 *Phys. Rev. B* **100** 094111
[43] McQueen R G and Marsh S P 1960 *J. Appl. Phys.* **31** 1253–69
[44] Al’tshuler L V, Bakanova A A and Dudoladov I P 1968 *Sov. Phys. JETP* **26** 1115–20
[45] Marsh S P (ed) 1980 *LASL Shock Hugoniot Data* (Berkeley, CA: University of California Press)
[46] Gathers G R 1986 *J. Appl. Phys.* **59** 3291–3
[47] Yu Y Y, Tan Y, Dai C D, Li X M, Li Y H and Tan H 2014 *Acta Phys. Sin.* **63** 026202
[48] Chhabildas L C and Hills C R 1986 Dynamic shock studies of vanadium *Metallurgical Applications of Shock-Wave and High-Strain-Rate Phenomena* ed Murr L E, Straudhammer K P and Meyers M A (New York: Marcel Dekker, Inc.) pp 429–48
[49] Weck P F, Kalita P E, Ao T, Crockett S D, Root S and Cochrane K R 2020 *Phys. Rev. B* **102** 184109
[50] Crichton W A, Guignard J, Bailey E, Dobson D P, Hunt S A and Thomson A R 2016 *High Pressure Res.* **36** 16–22