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THERMODYNAMIC PARAMETERS OF MIXTURES WITH SILICON NITRIDE UNDER SHOCK-WAVE LOADING

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Summary. The results of numerical experiments on modeling thermodynamic parameters such as value of pressure, compression and temperature for shock wave loading of pure silicon nitride Si_3N_4 and mixtures based on it are presented. The model TEC (thermodynamic equilibrium components) and its modification model TEC2 allow to describe thermodynamic parameters of Si_3N_4 with different value of porosity, in a wide range of pressure from 5 to 3000 GPa using model relation and the experimental data of Si_3N_4. The developed model is used to take into account the Si_3N_4 phase transition under shock-wave action. The results of calculations are compared with the data obtained on the basis of experiments for pure Si_3N_4 value of porosity 1 and 1.037; for mixture of Si_3N_4 and periclase MgO value of porosity 1.12. The value of pressure and compression for shock wave loading of nonporous mixture of aluminum nitride AlN and Si_3N_4 are calculated.

1 INTRODUCTION

In this paper, thermodynamically equilibrium model TEC [1, 2] is adapted to shock wave loading of a mixture of powders, including nitrides, when one or more components of the mixture undergo phase transformation. The researches of the behavior of porous mixtures of powder materials under shock-wave loading are of interest for many problems of modern science and technology [3–8]. Given the large variety of mixtures, it is desirable to use the equation of state (EoS) only components of the mixture. The construction of EoSs have been carried out for many years, but given the complexity and diversity of the materials, work in this direction continues [9–17]. The developed models well describe the behavior of pure substances, but are difficult to use in researching of mixtures. It is necessary to take into account the interaction of components for researching shock-wave loading of mixtures. It is preferable to use a simple equation in this case. The construction of simple EoSs is of particular interest in the modeling of thermodynamic parameters of mixtures [18–25]. In the developed model, the fairly simple EoS is used; it gives good correspondence to the experiment in wide range of pressures, both for solid and porous pure materials.

Interest in the investigation of compressibility of such mixtures is associated as with the possibility of creating materials that have the required properties and the properties of the materials themselves. The synthesis of materials, including multicomponent materials, under in-

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tense shock-wave action is an effective way to create new functional and structural materials, in particular different types of ceramics with desired properties on the basis of nitride mixtures. The active researches of the properties and methods of obtaining such materials are carried out [26–32]. Mixtures of different compositions, including Si_3N_4 as a component, are considered in [33–36]. The researchers of Si_3N_4 and mixtures based on it are the purpose of this work.

In phase transition region, thermodynamic characteristics of materials were determined from the assumption that material in this region is a mixture of low-pressure phase and high-pressure phase [37–40]. The results of modeling for this method with the phase transition are given in [41–44] for nitrides and a number of other materials. The beginning of phase transition process is determined by the condition that pressure reaches the critical value obtained on the basis of experiments.

2 CALCULATION MODEL

The numerical simulation of thermodynamic parameters of shock-wave loading of both pure materials and mixtures is based on the assumption that all components of the mixture, including gas in pores, under shock-wave loading are in thermodynamic equilibrium model TEC [1,2,45, 46], it takes into account the interaction of components and uses the author's EoS. The thermal EoS for the condensed component with current density ρ and initial density ρ_0 is as follows:

$$P(\rho,T) = \rho_0 c_0^2/n((\rho/\rho_0)^n - 1) + \Gamma\rho c_V(T - T_0). \quad (1)$$

Here c_0 is the value of sound speed of under normal conditions, T_0 is initial temperature, c_V is specific heat capacity in this case constant. The value n is determined by the derivative of the volume elasticity modulus under initial conditions.

The function Γ reflects the contribution of the thermal components in the model [1,2,45,46]. The conditions of dynamic compatibility at the wave front are written: the mass-flow conservation conditions for each mixture component and the momentum and energy flux conservation conditions for the mixture as a whole. The obtained equations together with EoS for each component are sufficient to find dependencies of type $P(U)$ or $D(U)$ (P, U, and D–pressure, mass and wave velocities), which can be interpreted as shock adiabat of a multicomponent mixture [1, 2]. The model TEC for high-porous samples well describes experimental data up to pressure value of 300 GPa [46].

The presence of experimental data on the dependence of heat capacity c_P on temperature allows to modify the equations that determine the state of the condensed component, increasing the area of reliable description to 3000 GPa. The cold component of the pressure is described also as well as in model TEC by the equation of Tait. Tait equation and its modified versions are one of the most well known empirical state equations. The Tait equation of state for describing

data on the density of sea water up to 50 MPa was originally published by Peter Guthrie Tait in 1888 [47]. The pressure form of the Tate equation of state is identical to that of the Murnaghan equation of state. Thermal components of pressure and specific energy P_T and E_T are considered in the following form:

$$P(\rho,\tau)_T = c_{V0}\rho T_0(\tau-1)k\frac{1+a_1\tau}{1+a_2\tau}, \tag{2}$$

$$E(\rho,\tau)_T = F(\tau) - c_{V0}T_0k\frac{1+2a_2\tau+(a_1-a_2+a_1a_2)\tau^2}{(1+a_2\tau)^2}ln(\rho/\rho_0), \tag{3}$$

$$F(\tau) = c_{V0}T_0\left[(\tau-1)\left(\lambda-\frac{b_1}{b_2}\right)-\frac{1}{b_2}\left(1-\frac{b_1}{b_2}\right)ln\left(\frac{1+b_2\tau}{1+b_2}\right)\right]. \tag{4}$$

In this case, $\tau = T/T_0$ is the relative temperature, c_{V0} is specific heat capacity under initial conditions Parameters are obtained according to the experimental data. For determining parameters k, a_1, and a_2, we can use function Γ. The values of λ, b_1, and b_2 are determined from the correspondence to experimental data for $c_P(T)$. The model with this EoS is defined as model TEC2 [48].

3 MODELING RESULTS

The results of modeling the thermodynamic parameters for Si_3N_4 density $\rho_0 = 3.184$ g/cm^3 and $\rho_0 = 3.07$ g/cm^3 and the data obtained by experiments from [26, 28] are shown in figures 1 and 2. The beginning of the phase transition for silicon nitride is determined at pressure of 30 GPa. The calculations for the silicon nitride was considered transition phase β-Si_3N_4 in the high-density phase of c-Si_3N_4. The calculated lines and data obtained from the experiment are shown in figure 2 with density shift for $m = 1.037$ (porosity m is ratio of density of solid substance to the density of sample). It was shown earlier that the model describes the decrease in the wave velocity with the growth of mass velocity [49] in the phase transition region, and the temperature dependences of nitrides under shock wave loading [46]. The results allow modeling of thermodynamic parameters of the mixture, which contains nitrides as components, using the model parameters for pure nitrides [41].

Figure 3 illustrates the results obtained for nonporous mixture of AlN and Si_3N_4 with equal volume fractions and an initial density $\rho_0 = 3.335$ g/cm^3. For comparison, the data obtained on the basis of experiments for AlN and Si_3N_4 are presented. It is assumed that the phase transition of the components of the mixture begins under the same conditions as for pure substances. The beginning of the phase transition for AlN is determined at pressure of 20 GPa, as well as for Si_3N_4—at 30 GPa. The beginning of the phase transition is assumed in the pressure range 33–36 GPa for a mixture of Si_3N_4 and potassium bromide KBr in a ratio of 10/90 by weight in [50]. The phase transition from β-Si_3N_4 tin c-Si_3N_4 is discovered above 36 GPa [28].

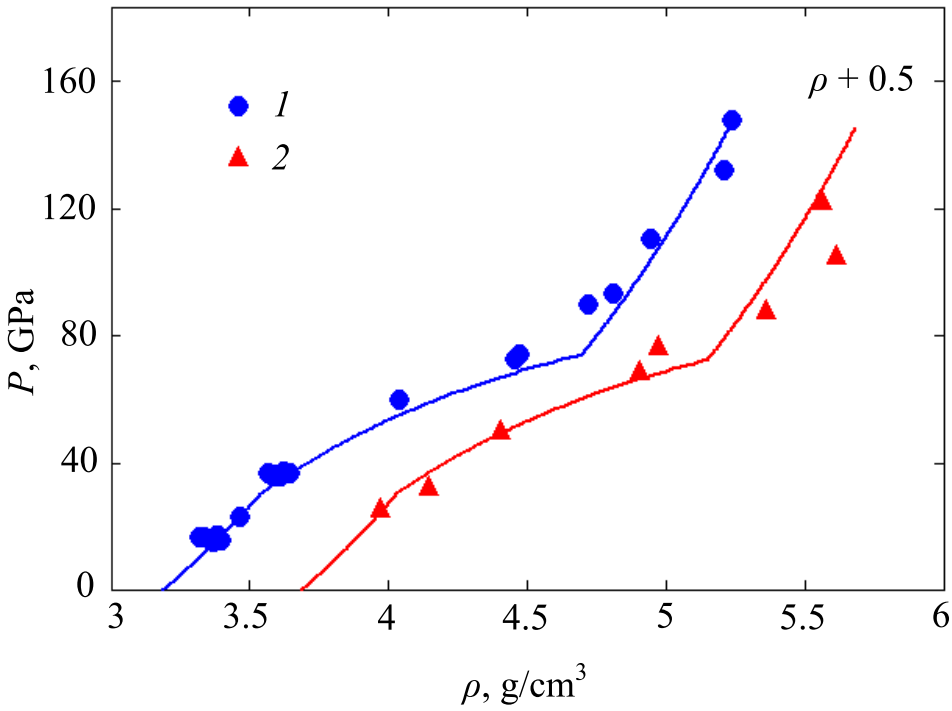

Figure 1: Shock adiabat of Si_3N_4. Calculation by model TEC at $m = 1$ (*1*) and 1.037 (*2*). Experimental data: *1*—[28]; *2*—[26].

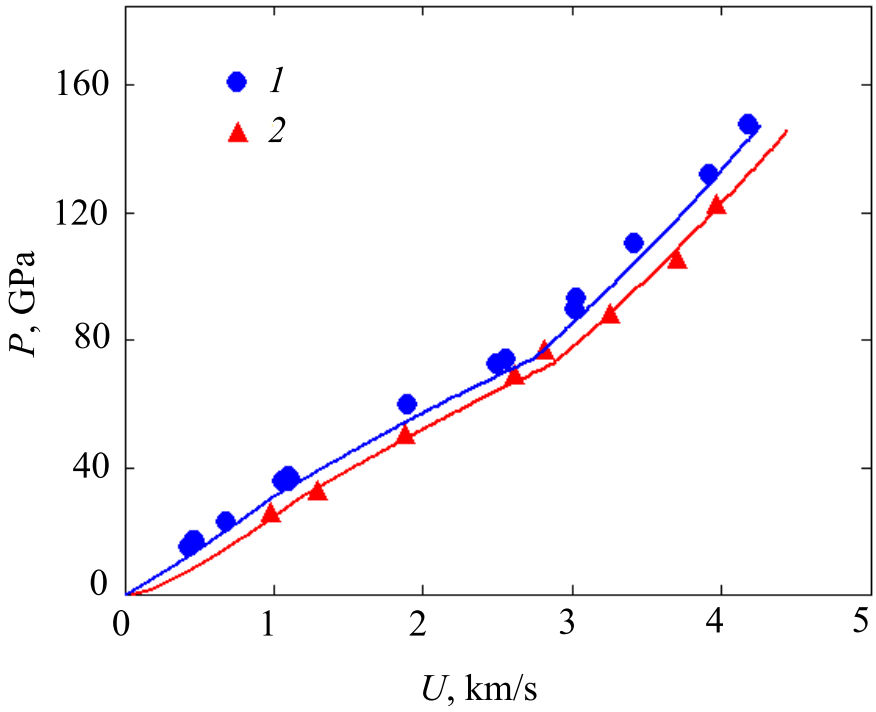

Figure 2: Shock adiabats of Si_3N_4. Symbols are as in figure 1.

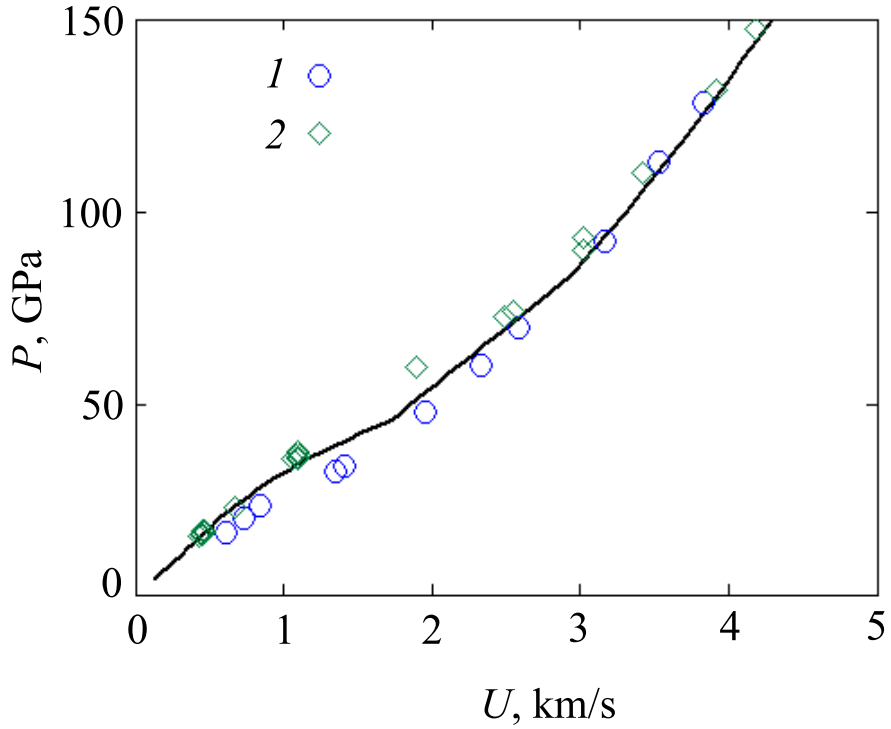

Figure 3: Shock adiabats of AlN and Si_3N_4 mixture. Experimental data: *1*—AlN [26]; *2*—Si_3N_4 [28].

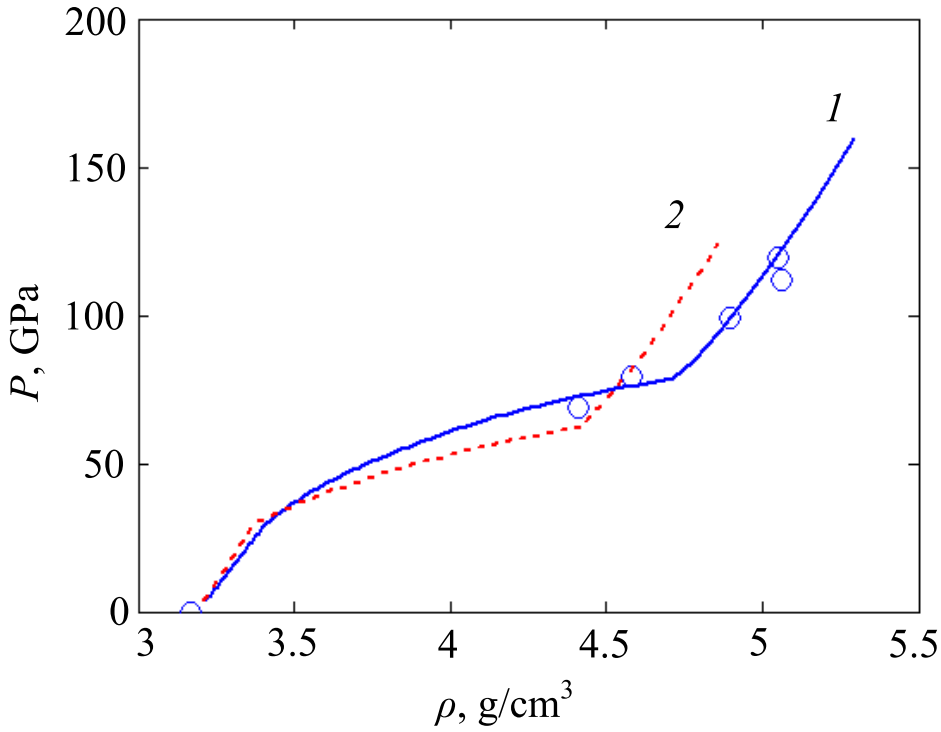

Figure 4: Shock adiabats in pressure–density coordinates for Si_3N_4 and MgO mixture with $m = 1.012$ (*1*) and 1.25 (*2*). Experimental data [51].

The parameters of mixtures of Si_3N_4 with oxides were modeled, for which there were data in [51]. Figure 4 shows the calculation of the mixture of Si_3N_4 and periclase MgO. The mixture with mass fractions Si_3N_4(95) MgO(5) and density $\rho_0 = 3.164$ g/cm^3 was modeled. The average porosity value determined from [51] $m = 1.012$. For comparison, the calculation for a higher value $m = 1.25$ is shown. The curve *2* for the mixture with $m = 1.25$ is above curve *1* with $m = 1.012$ before and after the phase transition region, which is typical for more porous materials. The phase transition ends earlier for more porous material, so curve *2* is below curve *1* in the phase transition region, taking into account the higher internal energy at the same density values. The modeling of this mixture is of interest due to the fact that MgO has a high-pressure phase transition [52]. The calculations are preferably performed on TEC2 for mixture with MgO.

4 CONCLUSIONS

Thus, the model allows calculating thermodynamic parameters of mixtures with nitrides under shock wave loading. The model parameters selected on basis of experimental data allow reliably describing the thermodynamic characteristics of silicon nitride and mixtures based on it. The assumption about thermodynamic equilibrium makes it possible to take into account the interaction between components, which becomes essential especially in case of porous media. The main objective of the research is achieved. The numerical experiments on modeling thermodynamic parameters for shock wave loading of pure Si_3N_4 with value of porosity 1 and 1.037 and for two mixtures Si_3N_4 with MgO and Si_3N_4 with AlN are performed. This model makes it possible to determine the compositions and ratios of the components of mixtures in order to obtain the specified characteristics under shock-wave loading of solid and porous heterogeneous materials.

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REFERENCES

[1] S. A. Kinelovskii and K. K. Maevskii, "Model of the behavior of aluminum and aluminum based mixtures under shock-wave loading", *High Temp.*, **52**, 821–829 (2014).
[2] S. A. Kinelovskii and K. K. Maevskii, "Modeling shock loading of multicomponent materials including bismuth", *High Temp.*, **54**, 675–681 (2016).
[3] B. R. Krueger and T. Vreeland, "A Hugoniot theory for solid and powder mixtures", *J. Appl. Phys.*, **69**, 710–716 (1991).
[4] A. A. Golyshev, V. V. Kim, A. N. Emel'yanov, and A. M. Molodets, "Model for calculation shock compression parameters of a platelet gradient mixture", *J. Appl. Mech. Tech. Phys.*, **56**, 618–625 (2015).
[5] V. V. Yakushev, S. Yu. Ananev, A. V. Utkin, A. N. Zhukov, and A. Yu. Dolgoborodov, "Shock compressibility of mixtures of micro- and nano-sized nickel and aluminum powders", *Combust., Explos. Shock Waves*, **54**, 552–557 (2018).

[6] B. Nayak and S. V. G. Menon, "Non-equilibrium theory employing enthalpy-based equation of state for binary solid and porous mixtures", *Shock Waves*, **28**, 141–151 (2018).
[7] S. A. Kinelovskii and K. K. Maevskii, "Model of the behavior of the mixture with different properties of the species under high dynamic loads", *J. Appl. Mech. Tech. Phys.*, **54**, 524–530 (2013).
[8] K. K. Maevskii and S. A. Kinelovskii, "Numerical simulation of thermodynamic parameters of lithium deuteride and its mixtures under shock wave loading", *AIP Conf. Proc.*, **2051**, 020181 (2018).
[9] Ya. B. Zel'dovich and Yu. P. Raizer, *Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena*, New York: Academic Press, (1967).
[10] A. V. Bushman and V. E. Fortov, "Model equations of state", *Sov. Phys.Usp.*, **26**, 465–496 (1983).
[11] A. V. Bushman, V. E. Fortov, G. I. Kanel', and A. L. Ni, *Intense Dynamic Loading of Condensed Matter*, Washington, DC: Taylor and Francis, (1993).
[12] V. Fortov, *Thermodynamics and Equations of State for Matter: From Ideal Gas to Quark–Gluon Plasma*, Singapore: World Scientific, (2016).
[13] 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**, 585–610 (2017).
[14] W. B. Holzapfel, "Equations of state for Cu, Ag, and Au and problems with shock wave reduced isotherms", *High Pressure Res.*, **30**, 372–394 (2010).
[15] S. A. Kinelovskii and K. K. Maevskii, "Simple model for calculating shock adiabats of powder mixtures", *Combust., Explos. Shock Waves*, **47**, 706–714 (2011).
[16] M. A. Kadatskiy and K. V. Khishchenko, "Theoretical investigation of the shock compressibility of copper in the average-atom approximation", *Phys. Plasmas*, **25**, 112701 (2018).
[17] D. V. Minakov, M. A. Paramonov, and P. R. Levashov, "Consistent interpretation of experimental data for expanded liquid tungsten near the liquid–gas coexistence curve", *Phys. Rev. B*, **97**, 024205 (2018).
[18] K. V. Khishchenko, "The equation of state for magnesium at high pressures", *Tech. Phys. Lett.*, **30**, 829–831 (2004).
[19] K. V. Khishchenko, "Equation of state for tungsten over a wide range of densities and internal energies", *J. Phys.: Conf. Ser.*, **653**, 012081 (2015).
[20] R. K. Belkheeva, "Equation of state for a highly porous material", *High Temp.*, **53**, 348–357 (2015).
[21] E. I. Kraus and I. I. Shabalin, "Calculation of elastic modules behind strong shock wave", *J. Phys.: Conf. Ser.*, **774**, 012009 (2015).
[22] K. V. Khishchenko, "Equation of state of sodium for modeling of shock-wave processes at high pressures", *Mathematica Montisnigri*, **40**, 140–147 (2017).
[23] S. D. Gilev, "Few-parameter equation of state of copper", *Combust., Explos. Shock Waves*, **54**, 482–495 (2018).
[24] K. V. Khishchenko, "Equation of state for magnesium hydride under conditions of shock loading", *Mathematica Montisnigri*, **43**, 70–77 (2018).
[25] K. K. Maevskii, "Thermodynamic parameters of lithium deuteride in pressure range 5–1000 gigapascals", *Mathematica Montisnigri*, **41**, 123–130 (2018).
[26] A. A. Bakanova, V. A. Bugaeva, I. P. Dudoladov, and R. F. Trunin, "Udarnaya szhimaemost' nitridov i karbidov metallov", *Izv. Akad. Nauk SSSR, Fiz. Zemli*, **6**, 58–63 (1995).
[27] T. Sekine, H. He, T. Kobayashi, M. Zhang, and F. Xu, "Shock-induced transformation of β-Si_3N_4 to a high-pressure cubic-spinel phase", *Appl. Phys. Lett.*, **76**, 3706–3708 (2000).
[28] H. He, T. Sekine, T. Kobayashi, and H. Hirosaki, "Shock-induced phase transition of β-Si_3N_4 to c-Si_3N_4", *Phys. Rev. B*, **62**, 11412–11417 (2000).
[29] T. Sekine, "Shock synthesis of cubic silicon nitride", *J. Am. Ceram. Soc.*, **85**, 113–116 (2002).
[30] V. V. Yakushev, A. V. Utkin, A. N. Zhukov, D. V. Shakhrai, and V. V. Kim, "Determination of P,T-conditions developed at high-temperature shock compression of silicon nitride in planar recovery ampoules", *High Temp.*, **54**, 197–205 (2016).
[31] N. Nishiyama, R. Ishikawa, H. Ohfuji, H. Marquardt, A. Kurnosov, T. Taniguchi, B. Kim, H. Yoshida, A. Masuno, J. Bednarcik, E. Kulik, Y. Ikuhara, F. Wakai, and T. Irifune, "Transparent polycrystalline cubic silicon nitride", *Sci. Rep.*, **7**, 44755 (2017).

[32] A. Yamakawa, "Shock-yielding properties of Si_3N_4 ceramics: Correlation with the microstructure and static mechanical strength", *J. Ceram. Soc. Jpn.*, **101**, 1358–1362 (1993).
[33] A. S. Yunoshev, "Shock-wave synthesis of cubic silicon nitride", *Combust., Explos. Shock Waves*, **40**, 370–373 (2004).
[34] A. N. Zhukov, S. E. Zakiev, and V. V. Yakushev, "Assessment of the effect of particle size on the rate of temperature alignment in systems used for shock-wave synthesis of diamond, cubic boron nitride, and γ-silicon nitride, based on a simple model", *High Temp.*, **54**, 62–67 (2016).
[35] T. Mashimo, M. Uchino, and A. Nakamura, "Yield properties, phase transition, and equation of state of aluminum nitride (AlN) under shock compression up to 150 GPa", *J. Appl. Phys.*, **86**, 6710–6716 (1999).
[36] L. A. Gömze and L. N. Gömze, "Rheological principles of development hetero-modulus and hetero-viscous complex materials with extreme dynamic strength", *IOP Conf. Ser.: Mater. Sci. Eng.*, **175**, 012001 (2017).
[37] I. V. Lomonosov, V. E. Fortov, A. Frolova, K. Khishchenko, A. Charakhch'yan, and L. Shurshalov, "The simulation of transformation of graphite to diamond under conditions of dynamic compression in a conic target", *High Temp.*, **41**, 447–458 (2003).
[38] A. A. Charakhch'yan, V. V. Milyavskii, and K. V. Khishchenko, "The use of models of mixture for analysis of shock-wave experiments with incomplete phase transformation", *High Temp.*, **47**, 235–242 (2009).
[39] K. V. Khishchenko, A. A. Charakhch'yan, V. Fortov, A. Frolova, V. Milyavskiy, and L. Shurshalov, "Hydrodynamic simulation of converging shock waves in porous conical samples enclosed within solid targets", *J. Appl. Phys.*, **110**, 053501 (2011).
[40] E. Bourasseau, N. Pineau, J. B. Maillet, and V. Dubois, "Calculation of the shock temperature of moderately porous graphites", *Carbon*, **103**, 464–472 (2016).
[41] K. K. Maevskii and S. A. Kinelovskii, "Model of behavior of nitrides and their mixtures under high dynamic loads", *AIP Conf. Proc.*, **1623**, 391–394 (2014).
[42] K. K. Maevskii and S. A. Kinelovskii, "Thermodynamic parameters for mixtures of quartz under shock wave loading in views of the equilibrium model", *AIP Conf. Proc.*, **1683**, 020132 (2015).
[43] K. K. Maevskii, "Numerical investigations of oxides and silicates under shock-wave loading", *J. Phys.: Conf. Ser.*, **894**, 012057 (2017).
[44] K. K. Maevskii and S. A. Kinelovskii, "Thermodynamic parameters for mixtures of quartz under shock wave loading in views of the equilibrium model", *J. Phys.: Conf. Ser.*, **946**, 012113 (2018).
[45] S. A. Kinelovskii and K. K. Maevskii, "Estimation of the thermodynamic parameters of a shock-wave action on high-porosity heterogeneous materials", *Tech. Phys.*, **61**, 1244–1249 (2016).
[46] K. K. Maevskii and S. A. Kinelovskii, "Thermodynamic parameters of mixtures with silicon nitride under shock-wave impact in terms of equilibrium model", *High Temp.*, **56**, 853–858 (2018).
[47] Y. H. Li, "Equation of state of water and sea water", *J. Geophys. Res.*, **72**, 2665–2678 (1967).
[48] K. K. Maevskii and S. A. Kinelovskii, "Numerical simulation of thermodynamic parameters of high-porosity copper", *Tech. Phys.*, **64**, 1090–1095 (2019).
[49] R. F. Trunin, *Issledovaniya e'kstremal'ny'x sostoyanij kondensirovanny'x veshhestv metodom udarny'x voln. Uravneniya Gyugonio*, Sarov: Rossijskij federal'ny'j yaderny'j centr—VNIIEF, (2006).
[50] V. V. Yakushev, A. N. Zhukov, A. V. Utkin, A. I. Rogacheva, and V. A. Kudakina, "Formation of cubic silicon nitride from the low-pressure phase by high-temperature shock compression", *Combust., Explos. Shock Waves*, **51**, 603–610 (2015).
[51] S. P. Marsh (ed.), *LASL Shock Hugoniot Data*, Berkeley: University of California Press, (1980).
[52] K. Miyanishi, Y. Tange, N. Ozaki, T. Kimura, T. Sano, Y. Sakawa, T. Tsuchiya, and R. Kodama, "Laser-shock compression of magnesium oxide in the warm-dense-matter regime", *Phys. Rev. E*, **92**, 023103 (2015).

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