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Modeling behavior of mixed materials under shock wave loading

*K.K. Maevskii**

Lavrentyev Institute of Hydrodynamics SB RAS, Novosibirsk, Russia
**konstantinm@hydro.nsc.ru*

Abstract. The results of numerical experiments on modeling high-energy loading on heterogeneous materials are presented. The model makes it possible to reliably describe thermodynamic parameters of heterogeneous materials in entire field of available experimental data. The values of pressure, compression ratio and temperature can be calculated depending on composition and ratio of components under shock wave loading. The calculation method makes it possible to reliably describe experimental data in field of phase transition under shock wave loading of various materials (graphite, quartz, nitrides and oxides). Thermodynamic parameters of mixtures are simulated taking into account phase transition of one or more components for the first time.
Keywords: shock adiabatic, phase transition, heterogeneous materials, thermodynamic equality.

1. Introduction

Description of thermodynamic parameters of heterogeneous materials under extreme conditions is one of the important tasks of mechanics, which is waiting for its solution. Theoretical and experimental research in this area has been conducted for many years [1, 2]. This work is related to the modeling of thermodynamic parameters under shock wave loading of powdered porous materials, including mixtures with components undergoing a phase transition, which are of great interest [3]. Although the number of research on the calculation of shock adiabats is quite large, the practical results relate mainly to single-component materials. There is a very limited number of works that consider the shock adiabat of powder mixtures.

The method has been developed for calculating behavior of heterogeneous materials under shock wave loading that takes into account three factors: the equation of state of components, the interaction of components of mixture, and possibility of phase transition of one or more components of investigated material [4]. Due to this, thermodynamic parameters of samples are researched in a wide range of pressure and porosity values using thermodynamically equilibrium model. The low-parametric equation of state is using in the model [5]. The parameters of equation of state have been determined for several dozen pure materials that may be used as components of mixtures and alloys.

2. Calculation model

The assumption of thermodynamic equality between the components is used in the calculations. It becomes extremely significant with increasing porosity and pressure values. The equality of both pressures and temperatures of the components is assumed in this case. This approach provides a wider range of reliable descriptions of porosity values. A fairly simple equation of state was constructed for pure substances, which made it possible to simulate shock wave compression to high pressure values, providing a reliable description of thermodynamic parameters (pressure values, compression ratio and temperature) on the other hand. At the same time, the accuracy of the description of pure substances corresponds to the level of wide-range models in the scope of this model. The description of the model, the method of constructing the equation of state, and the procedure for determining the parameters are described in detail in [6, 7]. The model has been tested for a number of materials [8, 9].

The calculations for a mixture of paraffin and tungsten were performed in [1] for three models that describe the results of experiments [10] with varying degrees of accuracy. The results of calculations are shown for SC-criterion (single component) [11], KEA-method (kinetic energy averaging) [12]. These two methods are based on the principle of additivity, which is widely used at relatively low pressures for alloys, but does not take into account the interaction of components. In

the third TE-method (turbulent entropy), an attempt was made to take into account the interaction of components by additionally introducing turbulent entropy [13].

Fig. 1 shows the calculated and experimental dependences of pressure on the specific volume of mixture of paraffin and tungsten with mass fractions of W (66.2%) and paraffin (33.8%). The figure is used from [1], to which the calculated curve of the model is added for comparison.

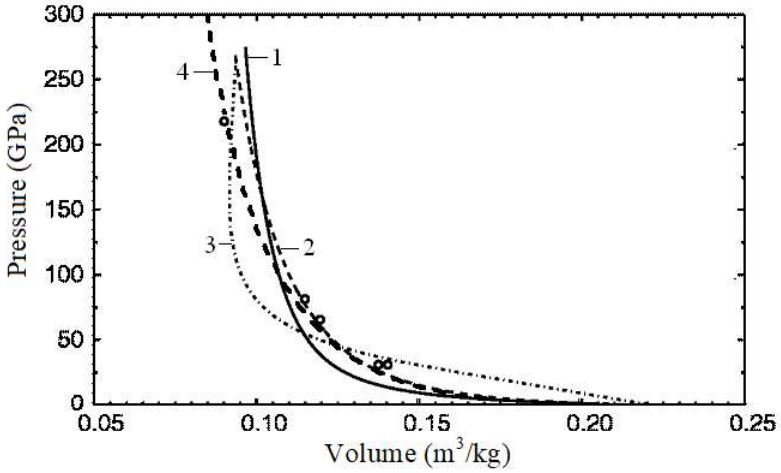

Fig. 1. Calculated lines and experimental data [1] (points).
Calculation: 1 – SC–criterion, 2 – KEA-method, 3 – TE–method, 4 – the model.

The compression ratio is calculated not only for heterogeneous material as a whole, but also for each component individually. It is shown that for a three-component mixture of W, Al and Cu, the change in the compression ratio with increasing pressure may differ for different components not only in value, but also in sign. Fig. 2 and 3 show the results of shock wave compression for double and triple highly porous mixtures $m = 10$. Porosity m is defined as the ratio of the normal density of monolithic substance to the initial density of the sample. The compression ratio of the mixture as a whole and of each component separately along the shock adiabate is shown. The calculation was carried out for the model in the pressure range from 5 to 300 GPa [14].

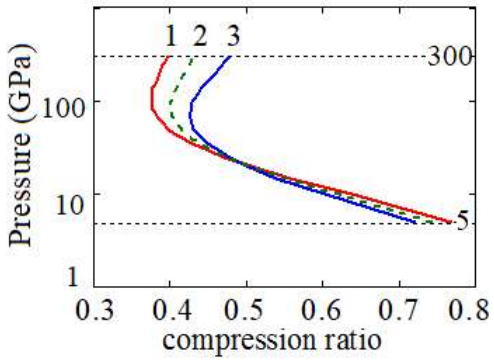

Fig. 2. Pressure versus compression for each component in the mixture and for the mixture as a whole. Calculation: 1– Al, 2 – Cu-Al (50/50), 3 – Cu.

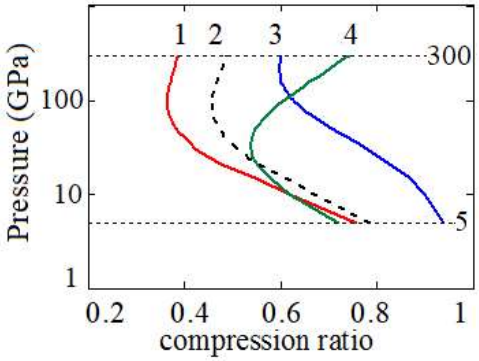

Fig. 3. Pressure versus compression for each component in the mixture and for the mixture as a whole. Calculation: 1– Cu, 2 – Cu-W-Al (50/25/25), 3 – W, 4 – Al.

In research aimed at the synthesis of new composite materials, in particular, the production of high-strength and heat-resistant ceramics based on nitrides, a serious problem arises. These materials, like many others of interest in this field of research, experience a phase transition under shock wave loading, which creates difficulties in calculations. At the moment, existing models

allow us to describe pure substances, for example, quartz, graphite, and some nitrides. But attempts to describe mixtures involving a material undergoing a phase transition under shock wave loading, for example, a mixture of aluminum and quartz, have not been successful. Considering the material in the phase transition region as a mixture, the author's model allows us to solve this problem. Moreover, thermodynamic parameters can be calculated for mixtures with several components with phase transitions. Such investigations have not been conducted before. In this case, it is possible to consider components experiencing several polymorphic phase transitions.

The behavior of mixtures, which, in particular, include quartz, experiencing a phase transition under shock wave loading, is calculated. For the first time, a reliable simulation of a mixture of Al and SiO_2 was performed. Fig. 4 shows the calculation of a mixture of quartz and aluminum with weight fractions (50/50); SiO_2 (50) Al (50) $\rho_0 = 2.684$ g/cm^3, as well as (40/60), (30/70). Here, for comparison, shock adiabats for pure quartz are given, using experimental data from [15]. Taking into account the fact that in the phase transition zone experienced by quartz, the latter is considered as a mixture of a low-pressure phase and a high-pressure phase, this calculation is actually carried out for a three-component mixture according to the number of condensed components.

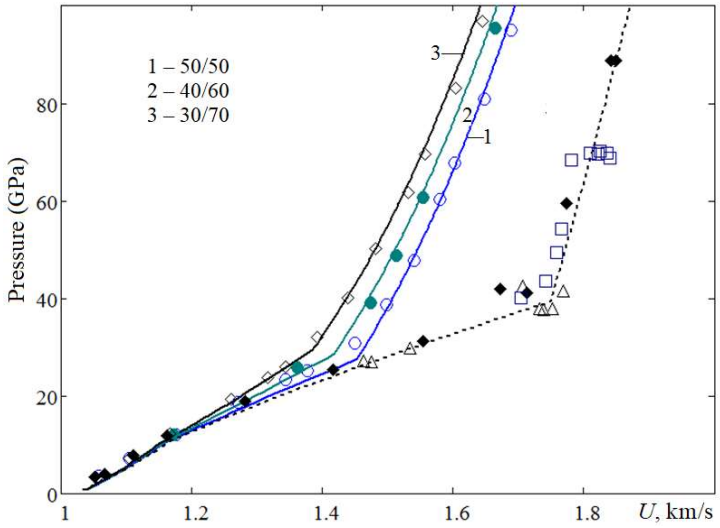

Fig. 4. Shock adiabats of mixture of quartz and aluminum. Experimental data [15].

The recent appearance of data on high-pressure phase transitions of oxides, combined with the capabilities of the author's model, opens up broad prospects for the development of new approach for more accurate description of the internal structure of Earth and other planets, taking into account the high content of oxides in their structure. The region of the high-pressure phase transition MgO has been determined. The results of modeling shock wave loading for periclase and the data obtained on the basis of experiments from [16–18] are shown in Fig. 5 in pressure variables depending on compression. The beginning of the phase transition for periclase is close to the region of change in the density of the Earth at a pressure of 330 GPa [19]. It can be assumed that phase transitions, including periclase, contribute to changes in the density of the Earth's mantle not only in the pressure range of 25 GPa, which was noted earlier in [20], but also at higher pressure values. The value of the density for phase of high-pressure MgO $\rho_0 = 4.050$ g/cm^3 was determined based on decrease in volume by 13% according to experimental data [17]. The curve fracture at pressure value of 380 GPa is defined as the end of the phase transition, that is, the complete transition of the periclase to high pressure phase MgO under shock wave action. A reliable description of the available data has been obtained within the limits of experimental accuracy.

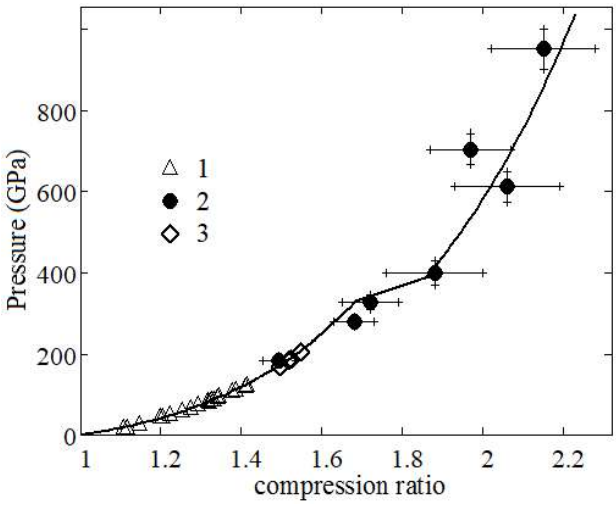

Fig. 5. Shock adiabat MgO. Experimental date 1 [5], 2 [6], 3 [7].

The assumption was verified that enstatite $Mg_2[Si_2O_6]$ [5] and forsterite Mg_2SiO_4 [21] could be considered as mixtures of oxides [22], based on the experimental data in which the dissociation of magnesium silicates under pressure was recorded [23]. Shock-wave loading of mixtures of SiO_2 and MgO oxides in stoichiometric ratio of 1:1 for enstatite is simulated, and a ratio of 1:2 is used for forsterite. The simulation results for forsterite in the pressure range up to 1 TPa and the data [24] are shown in Fig. 6, taking into account the phase transitions of SiO_2 and MgO. For MgO, the phase transition region is defined in the range from 250 to 380 GPa.

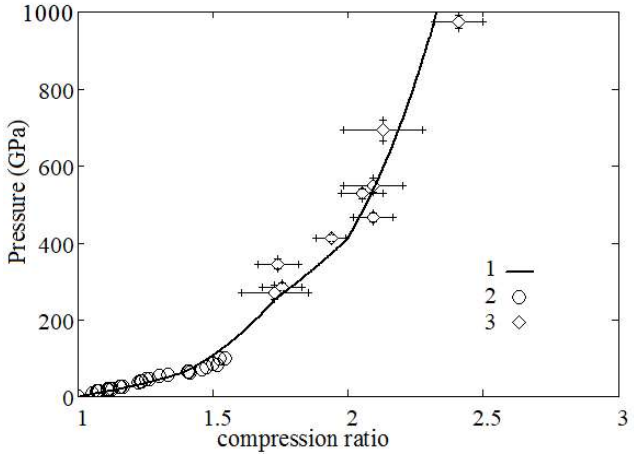

Fig. 6. The shock adiabat of forsterite is $\rho_0 = 3.273$ g/cm^3. Calculation in pressure – compression variables. Calculation – solid curve 1; experimental data: 2 [15], 3 [24].

3. Conclusion

Taking into account the experimentally observed dissociation of magnesium silicates into MgO and SiO_2 oxides [23], it can be assumed that the SiO_2 phase transition to stishovite contributes to a change in the density of the Earth's upper mantle in the area of pressure values of 30 GPa, which corresponds to the SiO_2 phase transition. The jump in the density of the Earth's mantle in the region of 330 GPa according to [19] corresponds to the region of the MgO phase transition. The region of the phase transition of enstatite from the low-pressure phase to the high-pressure phase is determined in the range from 300 to 380 GPa [25]. It is shown that considering magnesium silicates at high dynamic loads as a mixture of components, it is possible to obtain a reliable description of the behavior of the studied material in the pressure range up to 1.4 TPa. The author's model allows

us to reliably describe the phase transitions of all components that make up the researching material. The availability of additional experimental data could help clarify the region of phase transitions of components and clarify the question of the presence of a high-pressure phase transition for SiO_2, which has been discussed for a long time.

Taking into account the reliable description of experimental data on forsterite up to 1000 GPa, which exceeds the pressure value in the center of the Earth by three times [19], it can be assumed that this approach will be useful in calculations for more massive planets. This approach can also be used for other magnesium silicates. The joint results on various silicates will make it possible to predict pressure and temperature profiles, depending on their composition, and will also allow us to assess the contribution of phase transitions of materials to changes in the density of the Earth's mantle.

Acknowledgements

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4. References

[1] E.P. Oren and X. J. Francois, Comparison of methods for calculating the shock hugoniot of mixtures, *Shock Waves*, vol. **20**, 73, 2010, doi: 10.1007/s00193-009-0230-x

[2] R.M. Bolis et al., Decaying shock studies of phase transitions in MgO-SiO_2 systems: Implications for the super-Earths' interiors, *Geophysical Research Letters*, vol. **43**, 9475, 2016, doi: 10.1002/2016GL070466

[3] S.S. Batsanov, Features of solid-phase transformations induced by shock compression, *Russian Chemical Reviews*. vol. **75**, 606, 2006, doi: 10.1070/RC2006v075n07ABEH003613.

[4] K.K. Maevskii and S.A. Kinelovskii, Thermodynamic parameters of mixtures with silicon nitride, *High Temperature*, vol. **56**, 853, 2018, doi: 10.1134/S0018151X18060172

[5] K.K. Maevskii, Numerical simulation of the behavior of enstatite up to 1.4 TPa, *Physics of the Solid State*, vol. **65**, 1025, 2023, doi: 0.21883/PSS.2023.06.56119.38

[6] K.K. Maevskii, Numerical Study of Shock-Wave Loading of the W- and WC-Based Metal Composites, *Technical Physics*, vol. **66**, 749, 2021, doi: 10.1134/S1063784221050145

[7] K.K. Maevskii and S.A Kinelovskii, Model of behavior of nitrides and their mixtures under high dynamic loads, *AIP Conf. Proc*., vol. **1623**, 315, 2014, doi: 10.1063/1.4901487

[8] K.K. Maevskii and S.A Kinelovskii Thermodynamic parameters of mixtures with epoxy as a component under shock wave loading, *Journal of Physics: Conference Series*, vol. **946**, 012113, 2018, doi: 10.1088/1742-6596/946/1/012113

[9] K.K. Maevskii, Simulation of magnesium oxide behavior under high-energy impact, *Combustion, Explosion, and Shock Waves*, vol. **60**, 127, 2024, doi: 10.1134/S0010508224020126

[10] Y.F. Alekseev, L.V. Al'tshuler, and V.P. Krupnikova, Shock compression of two-component paraffin-tungsten mixtures, *Journal of Applied Mechanics and Technical* Physics, vol. **12**, 624, 1971, doi: 10.1007/BF00851875

[11] R. Saurel, O. Le Metayer, J. Massoni, and Gavrilyuk S. Shock jump relations for multiphase mixtures with stiff mechanical relaxation, *Shock Waves*., vol. **16**, 209, 2007, doi: 10.1007/s00193-006-0065-7

[12] S.S. Batsanov, *Effects of explosions on materials: modification and synthesis under high-pressure shock compression*. Berlin: Springer, 1994.

[13] S.L. Gavrilyuk and R. Saurel Rankine–Hugoniot relations for shocks in heterogeneous mixtures, *J. Fluid Mech*., vol. **575**, 495, 2007, doi: 10.1017/S0022112006004496

[14] K.K. Maevskii and S.A Kinelovskii, Modeling of high-porosity copper-based mixtures under shock loading *Journal of Applied Mechanics and Technical Physics*, vol. **60**, 612, 2019, doi: 10.1134/S0021894419040035
[15] P.R. Levashov, K.V. Khishchenko, I.V. Lomonosov, and V.E. Fortov, *Shock compression of condensed matter 2003,* Eds. Furnish M. D., Gupta Y. M., Forbes J. W., Melville−N.Y.: AIP. 2004. http://www.ihed.ras.ru/rusbank
[16] M. van Thiel, *Compendium of Shock Wave Data*. Livermore: Lawrence Livermore Lab., Rep. UCRL-50108, 1977.
[17] K. Miyanishi et al., Laser-shock compression of magnesium oxide in the warm-dense-matter regime, *Phys. Rev. E*. vol. **92**, 023103, 2015, doi: 10.1103/PhysRevE.92.023103
[18] C. Renero, and F. E. Prieto, Shock induced temperature in MgO, Ag, and Ta, *Shock Waves*, vol. **2**, 201, 1992, doi: 10.1007/BF01414642
[19] A.M. Dziewonski and D.L. Anderson, Preliminary reference Earth model, *Phys. Earth Planet. Inter.*, vol. **25**, 297, 1981, doi: 10.1016/0031-9201(81)90046-7
[20] S.K. Srivastava, S.K. Sharmaa, K. Vinod, and V.S. Malik, *J. Phys. Chem. Solids*., vol. **69**, 1029, 2008, doi: 10.1016/j.jpcs.2007.10.005
[21] K.K. Maevskii, Modeling of shock-wave loading of magnesium silicates on the example of forsterite, *Technical Physics*, vol. **67**, 1580, 2022, doi: 10.21883/TP.2022.12.55193.77-22
[22] K.K. Maevskii, Magnesium silicates at high dynamic loading, *Vestnik Tomskogo Gosudarstvennogo Universiteta, Matematika i Mekhanika. – Tomsk State University Journal of Mathematics and Mechanics*, vol. **72**, 111, 2022, doi: 10.17223/19988621/79/10
[23] M. Kumazawa, H. Sawamoto, E. Ohtani, and K.Mazaki, Postspinel phase of forestenite end evolution of the Earth's mantle, *Nature*, vol. **247**, 356, 1974, doi: 10.1038/247356A0
[24] T. Sekine et al., Shock compression response of forsterite above 250 GPa, *Sci. Adv.*, vol. **2**, e1600157, 2016, doi: 10.1126/sciadv.1600157
[25] D.K. Spaulding et al., Erratum: Evidence for a phase transition in silicate melt at extreme pressure and temperature conditions, *Phys. Rev. Lett*., vol. **108**, 065701, 2012, doi: 10.1103/PhysRevLett.119.139903