Equations of State of Matter at Extreme Conditions

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Physical processes arising under conditions of extreme energy densities, such as hypervelocity impacts, action of powerful energy fluxes on condensed matter and others, are of interest for fundamental investigations and for numerous practical applications. The typical features of these phenomena are complicated character of 3D gas dynamic flow and big gradients of flow parameters. The numerical modeling of processes at extreme conditions supports experimental investigations in this area [1,2]. On the other hand, it is the only tool for investigating phenomena which can not been carried out at laboratory conditions [3]. The dramatic progress in the computer industry in past 20 years resulted to the development of high-performance computers and efficient numerical schemes as well. The equation of state (EOS) governing the system of gas dynamic equations defines significantly accuracy and reliability of results of numerical modeling.

The current state of the problem of a theoretical description of thermodynamic properties of matter at high pressures, high temperatures is given in a set of publications [1-3]. In spite of a significant progress achieved on construction of EOS in solid, liquid and plasma state with the use of the most sophisticated "first-principle" theoretical approaches (classic and quantum methods of self-consisted field, diagram technique, computer's Monte-Carlo and molecular dynamics methods) the disadvantage of these theories is their regional character [2]. The range of an applicability of each theory is local and, rigorously speaking, no one of them allows to provide for a correct theoretical calculation of thermodynamic properties of matter on the whole phase plane from the cold crystal to liquid and hot plasmas. The principal problem here is the necessity to take into account correctly the strong collective interparticle interaction in disordered media, which meets especial difficulties in the region occupied by dense disordered non-ideal plasmas [2].

In this case experimental data at high pressures, high temperatures are of peculiar significance, because they serve as reference points for theories and semi-empirical models. Data obtained with the use of dynamic methods (see [4] and references therein) are of the importance from the practical point of view. Shock-wave methods allow to study a broad range of the phase diagram from compressed hot condensed phase to dense strongly coupled plasma and quasigas states. Available experimental data on the shock compression of solid and porous metals as well as isentropic expansion embrace to nine orders with respect to pressure and four to density. The extension of studied range of the phase diagram to greater relative volumes, in comparison with the principal Hugoniot, is achieving in the investigation of the shock compressibility of porous samples [4]. Nevertheless, difficulties of a work with ultradispersive targets and singularities of the heat transfer in multi-phase non-equilibrium media restrict the possibility of an advance on the density scale. The method of isentropic expansion of shocked matter allows, depending on the magnitude of the shock pressure, and, respectively, the entropy provided, to pass in one experiment states from a hot metallic liquid and strongly coupled plasma to two-phase region liquid-gas and Boltzman's weakly ionized plasma and an ideal gas [2]. The complex of available

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experimental and theoretical information is shown on Figure 1 on 3D relative volume-temperature-pressure surface calculated by semi-empirical multi-phase EOS [5].

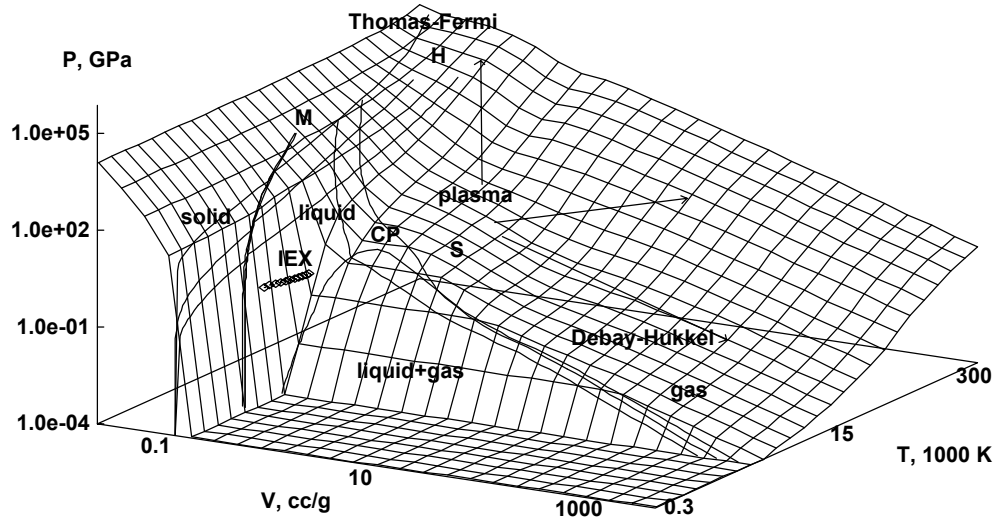

Fig. 1. 3D volume-temperature-pressure surface for copper in the investigated region of the phase diagram. M - melting region, H - principal and porous Hugoniots, IEX - isobaric expansion data, S - release isentropes, CP - the critical point. Shown are phase states of metal; arrows indicate the direction of the nonideality decreasing.

This EOS [5] fully assigns the free energy thermodynamic potential for metals over entire phase diagram region of practical interest. It accounts for solid, liquid, plasma states as well as two-phase regions of melting and evaporation. Some coefficients in EOS, included in the analytical expressions, are constants characteristic for each metal (atomic weight and charge, density at normal conditions and other) and are found from tabular data, while the rest serve as fitting parameters and their values are found from the optimum description for the available experimental and theoretical data and providing for correct asymptotes to calculations on the base of Debay-Hukkel and Thomas-Fermi theories. It should be emphasized that, even though the number of coefficients in the EOS model [5] is large, most of them are rigidly defined constants whose values are assigned explicitly or implicitly from the fulfillment of various thermodynamic conditions at specific points on the phase diagram. A few coefficients (about ten) serve to characterize the densities and temperatures on transition from one typical phase-plane region to another and are found empirically. To construct EOS, used was following information at high pressures, high temperatures: measurements of isothermal compressibility in diamond anvil cells, data on sound velocity and density in liquid metals at atmospheric pressure, IEX measurements, registration of shock compressibility for solid and porous samples in incident and reflected shock waves, impedance measurements of a shock compressibility under condition of an underground nuclear explosion, data on isentropic expansion of shocked metals, calculations by Debay-Hukkel and Thomas-Fermi models, evaluations of the critical point.

Available now are wide-range multi-phase EOS for 30 simple and transition metals of the most usage like Li, Be, Al, Cu, ε-Fe, Mo, W, Au, and others. Their direct usage in computer codes leads to complicated and not economy calculations, so they are usually involved in numerical modeling in tabular form. The EOS code for calculation of tables can produce the complete set of thermodynamic derivatives (such as pressure, sound velocity, heat capacity) using any one of input pairs: volume-temperature, volume-internal energy or volume-pressure. The input grid can be linear, logarithmic or arbitrary; each point in 2D output tables is marked by

symbol which indicates the physical state, i.e. is it solid, liquid, gas, plasma or mesh (solid-liquid, liquid-gas).

These tabular EOS have been successfully implemented in gas dynamic codes. We present here results of numerical modeling obtained with the use of modified method of "individual particles" which has been developed for solving the system of gas dynamic equations in 3D setup. The continuous media in this approach is represented as an ensemble of finite-size particles, which carry all flow parameters. The special algorithm for splitting and merging of particles belonging to the same eulerian cell has been developed. It made it possible to solve common for PIC-type methods problems with the memory loading and unphysical oscillations. The computation procedure in the modified "individual particles" method performs calculations with the only one particle per cell, while splitting particles are smoothly redistributed in the rarefaction regions. Physical models library includes advanced equations of state for 150 structural materials (metals, alloys, polymers, composites, rocks and minerals), and constitutive relations.

The developed gas dynamic code has been tested in the regime of massive parallel computations. Figure 2 illustrates results of solution of the Riemann problem depending on amount of processors. The amount of cells in this test calculations was of the order of 10^7 which corresponds to the dimension of 3D area of 200x200x300. The performance of the code has approximately linear dependence on the amount of processors. The maximum amount of processors was to 768.

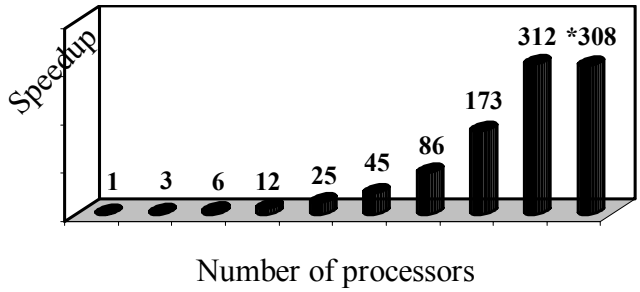

Fig. 2. The speedup of modified "individual particles" method in tests.

We present results of numerical modeling of hypervelocity impact process in 3D setup. The calculations were carried out for different initial velocities and shapes of impactor. Also the materials of impactor and target were varied. The comparison of the results of simulations with experimental X-ray photographs has been done.

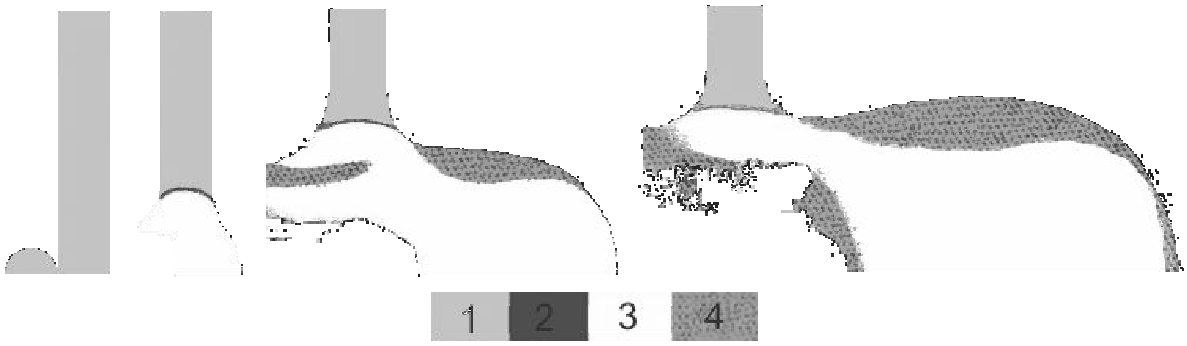

Fig. 3. Vertical cross-sections of density during hypervelocity impacts process. Regions marked 1,2,3,4 corresponds to solid, liquid, melted and evaporated material.

Shown on Figure 3 are cross-sections of density profiles in different time moments corresponding to the impact of lead ball on lead plate with velocity of 6.6 km/s. Along with physical properties like pressure, energy and others it is possible also to visualize physical states and to match the propagation of melting and evaporating effects. So the usage of advanced physical models of matter in numerical modeling improves the quality of calculations.

References

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