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Thermodynamic properties and phase transitions of metals at high temperatures

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Abstract – Thermodynamic approach to modeling of equation of state for metals with taking into account the polymorphic phase transformations, melting and evaporation effects is proposed. Multiphase equations of state for some materials are constructed on the basis of developed model. Calculation results for aluminum, iron, tin and lead are compared with experimental data at high temperatures and pressures. The most essential thermophysical experiments are described. The obtained equations of state can be used efficiently in simulations of processes at high energy densities.

A description of the thermodynamic properties of materials in a wide range of parameters is of both fundamental and practical interests. Equations of state for metals over the range from normal conditions to extremely high pressures and temperatures are required for numerical simulations of hydrodynamic processes in condensed media under pulsed power influences [1].

In this paper, a new thermodynamic approach to modeling of equation of state for metals with taking into account the polymorphic transformations, melting and evaporation effects is proposed. Multiphase equations of state for aluminum, iron, tin, lead and some other metals are obtained on the basis of the model. Results of calculations for these materials are given in comparison with experimental data over a wide range of temperatures, pressures and densities. For example, calculated phase diagrams for aluminum and tin are shown in figures 1 and 2.

The proposed multiphase equations of state provide for a reliable description of properties of metals in a wide range of thermodynamic parameters. That gives an opportunity to effectively use the equations of state in numerical simulations of unsteady-state hydrodynamic processes at high energy densities.

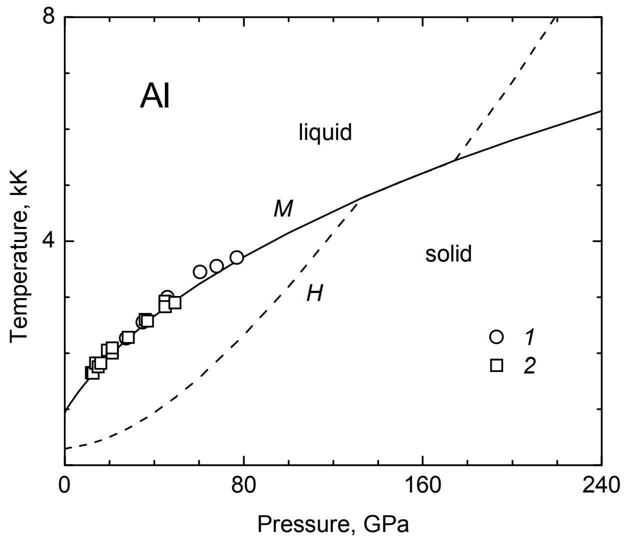

Figure 1: Phase diagram of aluminum at high temperatures and pressures. Solid line *M* is the melting curve calculated in this work. Dashed line *H* is the calculated Hugoniot curve. Markers *1* and *2* denote experimental data on melting in diamond anvil cells: *1* — [2], *2* — [3].

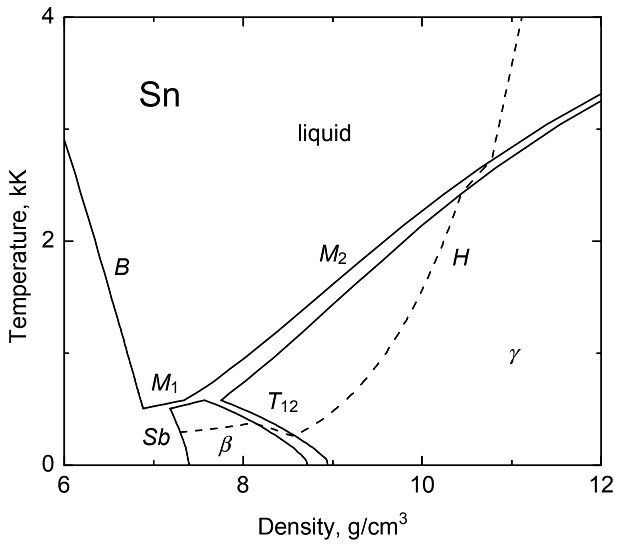

Figure 2: Calculated phase diagram of tin. Solid lines are the boundaries of phase transitions: M_1 and M_2 — melting of the white tin β and the body-centered tetragonal γ phases, respectively; T_{12} — the β–γ polymorphic transformation; *Sb* — sublimation, *B* — evaporation. Dashed line *H* is the Hugoniot.

[1] A. V. Bushman, V. E. Fortov, G. I. Kanel and A. L. Ni. Intense Dynamic Loading of Condensed Matter. Taylor & Francis, Washington, 1993.
[2] R. Boehler and M. Ross. Earth Planet. Sci. Lett. 153 (1997) 223.
[3] A. Hänström and P. Lazor. J. Alloys Comp. 305 (2000) 209.