*34th EPS Conference on Plasma Phys. Warsaw, 2 - 6 July 2007 ECA Vol.**31F**, P-2.121 (2007)*

Equations of state for nickel, copper and zinc at high energy densities

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A description of the thermodynamic properties of matter in a wide range of temperatures and densities is of both fundamental and practical interests. The equations of state (EOSs) for metals over the range from normal conditions to extremely high energy densities are required for numerical simulations of hydrodynamic processes in plasmas under pulsed power influences [1].

In this paper, a new semiempirical EOS model, which takes into account the melting, evaporation and ionization effects, is proposed.

The specific free energy of the substance is considered as a sum of three components [2],

$$F(V,T) = F_c(V) + F_a(V,T) + F_e(V,T), \tag{1}$$

describing the cold part of interparticle interaction at $T = 0$ K (F_c) and the thermal contributions by heavy particles (atoms, ions, nuclei) and electrons (F_a and F_e respectively). The first and second components of Eq. (1) have different forms for the solid and liquid phases, but the third is defined identically as in the EOS model [3].

The cold interaction energy for the solid phase is given by the relations [4]. The thermal lattice component of the free energy is defined as follows,

$$F_a(V,T) = RT\left(3\ln\left(1-e^{-\theta_a/T}\right) - D(\theta_a/T)\right), \tag{2}$$

where $R = k_B(Am_u)^{-1}$, k_B is the Boltzmann constant, m_u is the atomic mass unit (amu), A is the atomic mass (in amu), D is the Debye function [5], $\theta_a = \theta_s(V)$ is the characteristic temperature of phonon spectrum [3],

$$\theta_s(V) = \theta_{s0}\sigma^{2/3}\exp\left((\gamma_{s0} - 2/3)\,\frac{{B_s}^2 + {D_s}^2}{B_s}\arctan\frac{B_s\ln\sigma}{{B_s}^2 + D_s\,(\ln\sigma + D_s)}\right), \tag{3}$$

where $\sigma = V_0/V$, V_0 and γ_{s0} are the values of specific volume and Grüneisen coefficient of the solid phase under normal conditions.

The energy of the liquid phase at $T = 0$ K is determined by the relations

$$F_c^{(l)}(V) = F_c^{(s)}(V) + \frac{2{\sigma_l}^2}{1+{\sigma_l}^3}\left(d_0 + \frac{d_n}{n_l}{\sigma_l}^{n_l}\right) \text{ at } \sigma_l \geqslant 1, \quad F_c^{(l)}(V) = \sum_{i=1}^{3}\frac{d_i}{n_i}{\sigma_l}^{n_i} + E_{sub} \text{ at } \sigma_l < 1, \tag{4}$$

where superscripts s and l denote the solid phase and the liquid, $\sigma_l = V_{l0}/V$, V_{l0} is the specific volume of the liquid phase at a chosen point on the melting curve ($P = P_{m0}$, $T = T_{m0}$), the

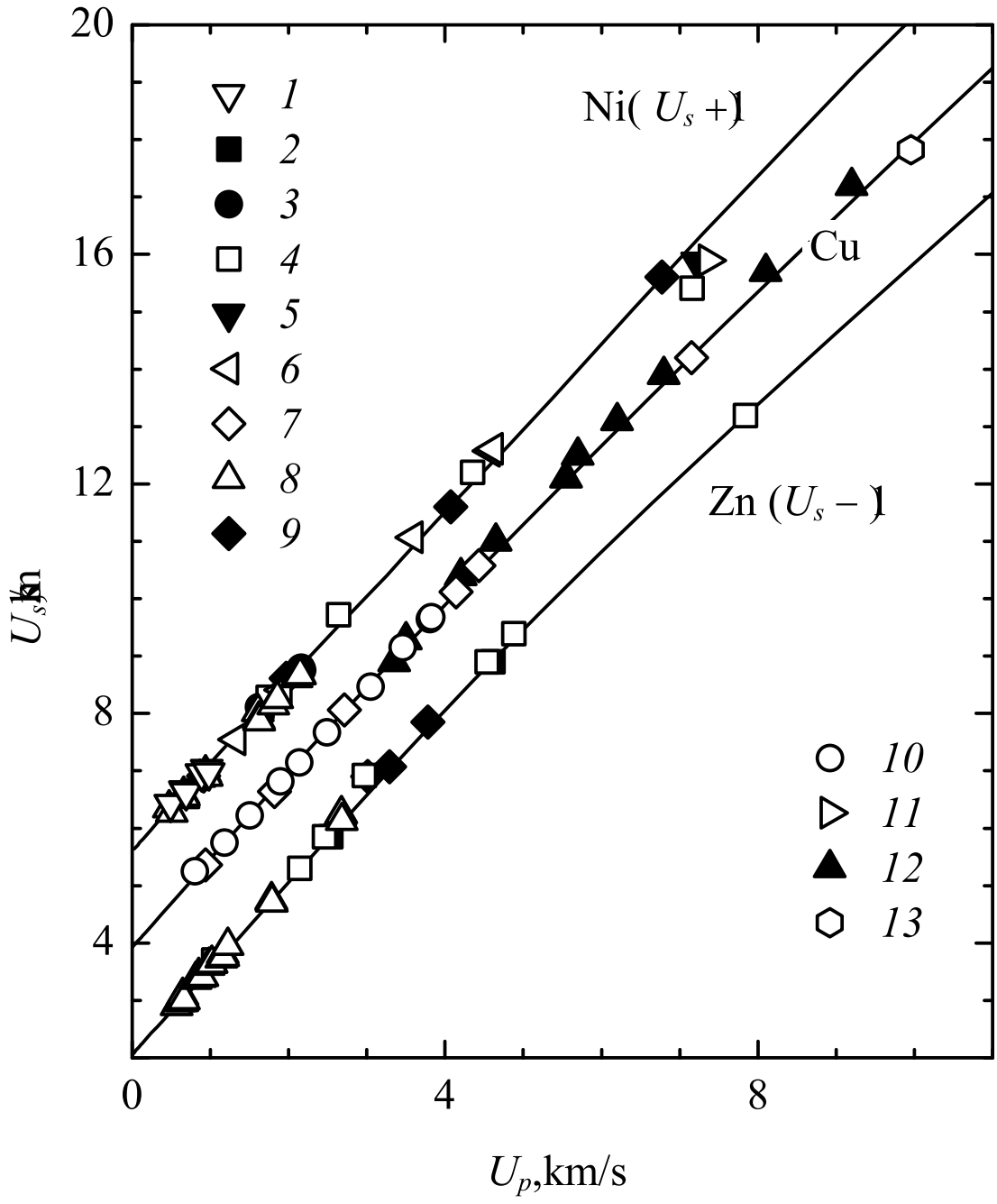

Figure 1: Shock velocity (U_s) versus particle velocity (U_p) on the Hugoniots of nickel, copper and zinc. Experimental data: *1* — [6], *2* — [7], *3* — [8], *4* — [9], *5* — [10], *6* — [11], *7* — [12], *8* — [13], *9* — [14], *10* — [15], *11* — [16], *12* — [17], *13* — [18].

coefficients d_0 and d_n define the volume change under melting at this point, E_{sub} is the sublimation energy. The parameters d_i and n_1 are determined from the requirement of continuity of the function (4) and its three derivatives with respect to volume at $\sigma_l = 1$.

The contribution of thermal movement of heavy particles to the free energy of the liquid

phase is defined in the form of Eq. (2), where $\theta_a = \theta_l(V) + (T_a T {\sigma_l}^{2/3})^{1/2}$, T_a is a constant,

$$\theta_l(V) = \theta_{l0} {\sigma_l}^{2/3} \exp\left((\gamma_{l0} - 2/3) \frac{{B_l}^2 + {D_l}^2}{B_l} \arctan \frac{B_l \ln \sigma_l}{{B_l}^2 + D_l (\ln \sigma_l + D_l)} \right), \qquad (5)$$

the parameter θ_{l0} defines the enthalpy change under melting at $P = P_{m0}$, γ_{l0} is the value of Grüneisen coefficient of the liquid phase at $\sigma_l = 1$.

Wide-range EOSs for nickel, copper and zinc are constructed on the basis of model developed. Calculation results are compared with available experimental data at high temperatures and pressures. The most essential shock-wave experiments [6–18] are described, see Fig. 1. The EOSs obtained can be used efficiently in numerical simulations of different processes at high energy densities.

This work was done under financial support of the Russian Foundation for Basic Research, grant No. 06-02-17464.

References

[1] V. Fortov, I. Iakubov and A. Khrapak, Physics of Strongly Coupled Plasma (New York: Oxford University Press, 2006)

[2] Ya.B. Zel'dovich and Yu.P. Raizer, Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena (New York: Academic Press, 1967)

[3] A.V. Bushman, V.E. Fortov, G.I. Kanel' and A.L. Ni, Intense Dynamic Loading of Condensed Matter (Washington: Taylor & Francis, 1993)

[4] K.V. Khishchenko, Tech. Phys. Lett. **30**, 829 (2004)

[5] L.D. Landau and E.M. Lifshitz, Statistical Physics (Oxford: Pergamon Press, 1980)

[6] J.M. Walsh, M.H. Rice, R.G. McQueen and F.L. Yarger, Phys. Rev. **108**, 196 (1957)

[7] L.V. Al'tshuler, K.K. Krupnikov and M.I. Brazhnik, Sov. Phys.–JETP **7**, 614 (1958)

[8] R.G. McQueen and S.P. Marsh, J. Appl. Phys. **31**, 1253 (1960)

[9] L.V. Al'tshuler, A.A. Bakanova and R.F. Trunin, Sov. Phys.–JETP **15**, 65 (1962)

[10] S.B. Kormer, A.I. Funtikov, V.D. Urlin and A.N. Kolesnikova, Sov. Phys.–JETP **15**, 477 (1962)

[11] W.H. Isbell, F.H. Shipman and A.H. Jones, Mat. Sci. Lab. Report MSL-68-13 (General Motors Corp., 1968)

[12] L.V. Al'tshuler and B.S. Chekin, in: Proc. 1-st All-Union Pulsed Pressures Simposium (Moscow: VNIIFTRI, 1974), v. 1, p. 5

[13] S.P. Marsh (ed.), LASL Shock Hugoniot Data (Berkeley, CA: University of California Press, 1980)

[14] L.V. Al'tshuler, A.A. Bakanova, I.P. Dudoladov, E.A. Dynin, R.F. Trunin and B.S. Chekin, J. Appl. Mech. Techn. Phys. **22**, 145 (1981)

[15] A.C. Mitchell and W.J. Nellis, J. Appl. Phys. **52**, 3363 (1981)

[16] R.F. Trunin, G.V. Simakov, Yu.N. Sutulov, A.B. Medvedev, B.D. Rogozkin and Yu.E. Fedorov, Sov. Phys.–JETP **69**, 580 (1989)

[17] B.L. Glushak, A.P. Zharkov, M.V. Zhernokletov, V.Ya. Ternovoi, A.S. Filimonov and V.E. Fortov, Sov. Phys.–JETP **69**, 739 (1989)

[18] R.F. Trunin, Phys. Usp. **37**, 1123 (1994)