

# The new calculated data on properties of metals liquid/vapor critical point

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The behavior of metals in a critical point a liquid/vapor is interesting in many tasks of physics of high temperatures. First of all, is important the triad of her basic thermodynamic parameters: the temperature  $T_C$ , density  $\rho_C$ , pressure  $P_C$ . The rather steady meanings of  $T_C$ ,  $\rho_C$ ,  $P_C$  properties are known only for Hg, Cs, Rb, K measured in static conditions. For many other metals the data  $T_C$ ,  $\rho_C$ ,  $P_C$  from dynamic experiments are known, however, with this case had big errors and steady data of  $T_C$ ,  $\rho_C$ ,  $P_C$  came in not. The most part of the known data is received by various calculation methods. However, and in this case disorder of estimations is large, that does not allow reliably to systematize of data and to estimate their probable error.

A basis of our calculations is the specific model of atomic structure of liquid metals. It is supposed in this model, that in a dense liquid at temperature melting  $T_L$  and near to a critical point a liquid metal consists of set steady clusters with number of atoms  $n_{cl} = 1 + Z_1$  in everyone. The quantity  $Z_1$  is number of atoms concerned with central (No. 1) and gather round of it. Such model of structure assumes, that the critical point is the special state of substance, at transition through which connected among themselves  $(1 + Z_1)$ -clusters or break up on free, or are formed from a vapor phase.

The volumetric constant of the van der Waals equation state is determined in this model as  $b_a = 2v_a (1 + Z_1) / Z_1$ , where  $v_a$  - volume of atom. The further transformations show, that the triad of properties  $T_C$ ,  $\rho_C$ ,  $P_C$  is determined only by three parameters: coordination number  $Z_1$ , density  $\rho_L$  at temperature  $T_L$ , and temperature factor of liquid density  $k_L = (d\rho_L/dT)|_{T_L}$ .

The large complex of experimental researches of density  $\rho_L(T)$  of many metals, including area  $\rho_L(T_L)$ , was carried out earlier [1, 2 etc.]. On this basis accounts of a triad of critical properties 37 metals with  $Z_1 = 8$  and  $Z_1 = 12$ : alkaline, alkaline-earth, transitive, rare-earth, platinic, lanthanide (and more others 15 now are carried out, at which experimental data about  $Z_1$  the liquids are insufficiently reliable). It is established, that the new  $T_C$ ,  $\rho_C$ ,  $P_C$  data at Hg, K, Rb, Cs differs from the experimental measured data within the limits of an error. At the majority of other metals the new data is inside a range of estimations of many authors given in [3] and in other reviews.

The accuracy of the received  $T_C$ ,  $\rho_C$ ,  $P_C$  data is determined in the basic errors of measurements data  $\rho_L$  and  $k_L$ . In [1, 2 etc.] the casual errors  $\rho_L$  and  $k_L$  make  $\sim 0,5$  and  $\sim 10\%$  accordingly. It does not mean, that errors in calculated estimations of the  $T_C$ ,  $\rho_C$ ,  $P_C$  is the same but part of systematic errors here excluded those. That determines existence unknown before interrelations of the  $T_C$ ,  $\rho_C$ ,  $P_C$  properties and other properties of metals.

Together with it, new complex calculated data is support a clusters hypothesis of liquid metals structure, including the assumptions [4] about of small atomic clusters near to the  $T_C$ .

[1] A S Basin, *Heat Transfer. Soviet Research* **4** (1972) 32-45

[2] A S Basin, S V Stankus, *Proc. of the 9<sup>th</sup> Europ. Conf. on Thermophys. Prop.* (1984) 176-178

[3] R W Ohse, H Tippelskirch, *High Temperature – High Pressure* **9** (1977) 367-385

[4] F Hensel, *J. Phys.: Condens. Matter* **2** (1990) SA33-SA45