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APPLICATION OF METHOD OF GIBBS CHEMICAL POTENTIALS IN FERROUS METALLURGY

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The analysis of the use of method of Gibbs chemical potentials in modern ferrous metallurgy is executed. It is shown that this method and all its practical applications is based on strict foundation of chemical thermodynamics.

Keywords: chemical potential, thermodynamics, Gibbs method, Gibbs energy, reverse task.

Introduction. In works of professor A. Ponomarenko [1] beginning to practical application of method of Gibbs chemical potentials in the calculations of steel-smelting processes was fixed. Dignity of this method was abandonment from the use of compounds (oxides, sulfides etc.) as components of liquid slag in physical and chemical calculations. It was instead suggested to use the elements of the D.I. Mendeleyev Periodic system. Afterwards, this approach got experimental confirmation, when by it was not succeeded to educe some stoichiometrical connections by the methods of X-ray structural analysis in a liquid slag [2].

For the practical use of Gibbs method equation of the state of the multicomponent system «metal-slag-gas» of general view

$$\mathbf{F}(\mathbf{m},\bar{\mathbf{m}}_{[]},\bar{\mathbf{m}}_{0},\bar{\mathbf{m}}_{\{\}},p,T)=0\ , \qquad (1)$$

where $\mathbf{m}$, $\bar{\mathbf{m}}_{[]}$, $\bar{\mathbf{m}}_{0}$, $\bar{\mathbf{m}}_{\{\}}$ – vectors of the masses of elements respectively in the system, metal, slag and gas; p, T – pressure and absolute temperature in the system, it is necessary to formulate in terms of chemical potentials as a system $2k + 2$ equations:

$$\begin{cases} \Delta\mu_{[i)}=0\ ,\ i=1..k; \\ \Delta\mu_{[i\}}=0\ ,\ i=1..k; \\ \sum\limits_{i=1}^{k}\tilde{o}_{(i)}\nu_i=0; \\ \Delta H=\Delta Q, \end{cases} \qquad (2)$$

where $\Delta\mu_{[i)}$, $\Delta\mu_{[i\}}$ – differences of chemical potentials of elements on a interphase border respectively «metal-slag» and «metal-gas»; $x_{(i)}$ – mole fractions of elements in a slag; ν_i - valences of elements in a slag; ΔH – a change of enthalpy of the system «metal-slag-gas»; ΔQ – a quantity of eaten up an or lost by the system heat with a corresponding sign; k – a quantity of chemical elements.

An important step in development of practical appendixes of method of Gibbs chemical potentials was simplification of the system of equations (2) to three nonlinear equations the quantity of which already did not depend on the number of chemical

elements [3]. Equation of enthalpy thermal balance was later added to these three equations [4].

Simultaneously with this simplification and possibility analytically to express differential coefficients mastering, having a key value in the decision of reverse task of thermodynamics analysis of steel-smelting processes appeared due to its.

The differential coefficients of mastering (DCM) appear by the elements of square matrix and in general case are calculated by accounts the method of non-obvious differentiation of equation of the state (1):

$$U_{ij} = \frac{\partial m_{[i]}}{\partial m_j} = -\left[\frac{\partial F_i}{\partial m_{[j]}}\right]^{-1} \cdot \left[\frac{\partial F_i}{\partial m_j}\right], \qquad (3)$$

Thus, became possible to decide the reverse task of thermodynamics analysis of steel-smelting processes in full volume. Presently the decision of reverse task is successfully used in the control steel-smelting production the personal computer system «Master» [5] and educational-research programmatic complex «Excalibur» [6].

In the system of equations (2) chemical potentials of components in some phase are expressed through to activity of chemical elements:

$$\mu_i = \mu_i^0 + R \cdot T \cdot \ln a_i \ , \qquad (4)$$

where μ_i^0 – standard chemical potential of clean component; R – universal gas permanent; a_i – activity of chemical elements in multicomponent solution.

To the present time the most adequate model of liquid metallic phase is a model, got from the configuration statistical sum of the microstates of phase taking into account interparticle energies of co-operation [7]. Advantage of this model is possibility of the use of large array of experimental data on the pair parameters of Wagner co-operation of and coefficients of activity in infinitely dilute solutions. In addition, within the framework of this model interconsistencal formulas for the integral and partial sizes of Gibbs energy, enthalpy, entropy and heat capacity of mixing are got.

For a multicomponent liquid slag phase an analogical thermodynamics model, additionally taking into account valences of elements which in general case can be variable quantities depending on the temperature of the system [8], is offered.

Conclusions. The method of Gibbs chemical potentials, based on strict foundation of chemical thermodynamics, finds all increasing application in ferrous metallurgy. By means of this science intensive and perspective method there are developed and inculcated new technologies of melting and out-of-furnace steel treatment. In particular, successful realization of reverse task of thermodynamics analysis of steel-smelting processes, id est task of optimization of the masses of materials and quantity of power mediums, necessary for the assured receipt of the set composition and temperature of the prepared steel or half-finished material became possible. Presently a method of Gibbs is not only the reliable instrument of metallurgist-researcher, but by means of application in programmatic complexes becomes the instrument of practical metallurgist-worker.

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