

**THERMODYNAMIC MODELLING OF EVAPORATION PROCESSES
OF LUNAR AND METEORITIC SUBSTANCE.**

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Knowledge of how melt composition evolves during evaporation is very important to reconstruct the possible thermal evolution of lunar and meteoritic materials, composition of which can be described within a frame of CaO–MgO–Al₂O₃–FeO–TiO₂–SiO₂ oxide system.

The evaporation process of complex oxide compounds is a combination of evaporation reactions of oxides and reactions forming gaseous complex oxides. Both solid and liquid pure oxides, with a few exceptions, evaporate without changing the composition of the condensed phase. Similarly, evaporation of solid oxide compounds also does not affect the composition of the condensed phase [1]. However, evaporation of molten oxide compounds (or their solid solutions) changes the composition of the condensed phase and the process can be described by the Hertz-Knudsen equation:

$$\Delta q_i = \alpha_i p_i M_i / \sqrt{2\pi RT}, \quad (1)$$

which allow to calculate the amount of evaporated *i*th component of the melt (Δq_i) with a molecular weight M_i at a temperature T if its equilibrium partial pressure (p_i) is known. The partial evaporation coefficient (α_i), characterizing the change in the structure of a molecule during its transition to the gas phase, in this case is equal to 1 [2].

The values of p_i can be determined from the activity of a component (a_i) in the melt according to Lewis equation [3]: $p_i = a_i p_i^\circ$, where p_i and p_i° are the partial pressures of the *i*th component of the gas phase over the melt and over the individual substance (pure component), respectively. Since values of p_i° are well known [4], and values of a_i can be determined both experimentally [5] and theoretically [6] with sufficient accuracy, this method of calculations of p_i seems to be the optimal.

In this case, the simplest approach is to use models which are based on the theory of ideal associated solutions [7]. In these models the standard Gibbs energies of formation of condensed phases (ΔG_i°) of a multicomponent system, which can be formed from an arbitrary number of components, are used as a model parameters. When the system reaches an equilibrium state, the mixing energy (ΔG^m) is at a minimum, that is equivalent to solving the system of mass balance equations of components for all reactions occurring in the system at a given composition. According to this approach, the equilibrium conditions are calculated based on the following equation [8, 9]:

$$\Delta G^m = \sum_i \left(\Delta G_i^\circ + RT \ln a_i \right). \quad (2)$$

Calculations of a_i in CaO–MgO–Al₂O₃–FeO–TiO₂–SiO₂ melts requires having a reliable thermodynamic database which was carefully selected and then tested making sure that the selected values of ΔG_i° of the condensed phases of the most important binary and ternary subsystems of the melt are correct. The thermodynamic database is mainly based on the experimental data obtained by high-temperature Knudsen mass spectrometry effusion method in the temperature range 1600–2500 K [10].

By comparing the model calculations and experimental data on evaporation of lunar basalt and meteoritic materials of different nature [11–14] it is shown the high accuracy of the developed thermodynamic approach, which allows to calculate not only the thermodynamic properties of a multicomponent oxide melt, but also the changes in the melt composition during evaporation. The observed evaporation regularities of the considered multicomponent oxide melt are in agreement with variations in activities of oxides in the residual melt, thus confirming the correctness of the choice of the ΔG_i° values used in the model.

Thermodynamic approach to describe evaporation of chondritic materials was first used by Grossman et al. [15]. The details of the model and results will be discussed during presentation.

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