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On finding the diffusion coefficient of an impurity on the results of evaporation refining

A.I. Kravchenko

National Science Center "Kharkov Institute of Physics and Technology",
Academic st, 1, Kharkiv, 61108 Ukraine

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The fundamental possibility of calculating the diffusion coefficient D of an impurity in a substance based on the results of evaporation refining at a given temperature is shown - using the formula $D = vX/Pe$, where Pe is the Peclet number, v is the linear evaporation rate, X is the size factor of the refined material.

Keywords: diffusion coefficient, distillation, sublimation, Peclet number

Про знаходження коефіцієнта дифузії домішки за результатами випарного рафінування. *Кравченко О.І.*

Показано принципову можливість обчислення коефіцієнта дифузії домішки D в речовині за результатами випарного рафінування при заданій температурі - за допомогою формули $D = vX/Pe$, де Pe - число Пекле, v - лінійна швидкість випаровування, X - розмірний фактор матеріалу, що рафінується.

1. Introduction

Knowledge of the coefficient D of the diffusion of an impurity in a substance at a given temperature is required to solve various problems. Despite the fact that both methods for the experimental determination of D and methods for calculating D have been developed, finding the values of D remains a difficult task: database on the value of D is small, and the calculated and experimental data on D are not in good agreement [1-3] . In this regard, it is of interest to consider new possibilities for experimentally finding D, for which various processes can be considered, the occurrence of which depends on D.

Recently, attention has been paid to the development of the theory of distillation and sublimation refining using the Peclet number - which includes D. In relation to simple distillation and sublimation, a method for calculating the refining of a two-component substance has been developed, which takes into account two factors: the equilibrium separation coefficient β_0 (the ratio of impurity concentrations in vapor and in the evaporized substance) and Peclet number

$$Pe = vX/D,$$

where v is the linear velocity of the evaporation surface, D is the impurity diffusion coefficient, X is the dimensional factor of the evaporated material (for example, the initial thickness of the liquid layer in the crucible) [4-8]. The process of evaporation of matter is described by a system of complex equations, but solutions can be found by numerical methods.

Some results of calculations for the refining of substances with different values of β_0 are presented in Fig. 1 [9, 10] in the form of graphs of the dependence of the relative purity of the condensate C/C_0 on the yield g of the process with a flat phase interface (C is the average impurity concentration in the condensate, C_0 is the initial impurity concentration. At the beginning refining process, at $g \approx 0$, $C/C_0 \approx \beta_0$). In

particular, using these graphs, an analysis of experimental data on the refining of Pb from Sb by distillation was performed, which made it possible to estimate the value of *Pe* in the process under consideration [11].

The purpose of this work was to consider the possibility of finding the value of the impurity diffusion coefficient *D* on the results of evaporation refining.

2. Experimental

The following possibility of finding *D* from the result of evaporation refining of a substance with a given *X* in the *Pe* at temperature *T* with a known rate *v* of process is being considered. An experimentally constructed graph of the dependence of C/C_0 on g allows one to determine the value $ß_0 \approx C/C_0$ at $g \approx 0$. For the value of $ß_0$ found in this way and for different values of *Pe*, using method [5] graphs of the dependence of C/C_0 on *g* should be constructed, with which the experimental data can be compared graph of C/C_0 on *g*. As a result, the experimental value of *Pe* can be established (similar to what was done when analyzing experimental data on the distillation of the Pb-Sb substance [11]) and the value of *D* can be calculated using the formula

$$D = vX/Pe.$$

3. Results and discussion

The fundamental possibility of measuring the diffusion coefficient of an impurity in a substance on the results of evaporation refinig at a given temperature is shown, based on measuring the Peclet number in a real process of evaporative or crystallization refining.

For a given temperature and *X*, two experiments are enough to find *D*: measurement of C/C_0 at $g \approx 0$ (to find the value of $ß_0$) and measurement of C/C_0 at some large value of *g* (for example, at $g = 0.8$) are required. With the established values of $ß_0$ and C/C_0, the corresponding value of *Pe* can be calculated (using the specified method for calculating refining [5]) and $D = vX/Pe$ is found if *v* in the process under consideration is established. In a container of simple shape the linear rate *v* of evaporation of a substance can be determined by the change in the liquid level during the process. In this case $v = w/ρ$, where ρ is the density of the substance, and *w* is the rate of evaporation of the substance per unit surface. As a result, the value of *D* will be found at temperature *T* and impurity concentration ~ C_0.

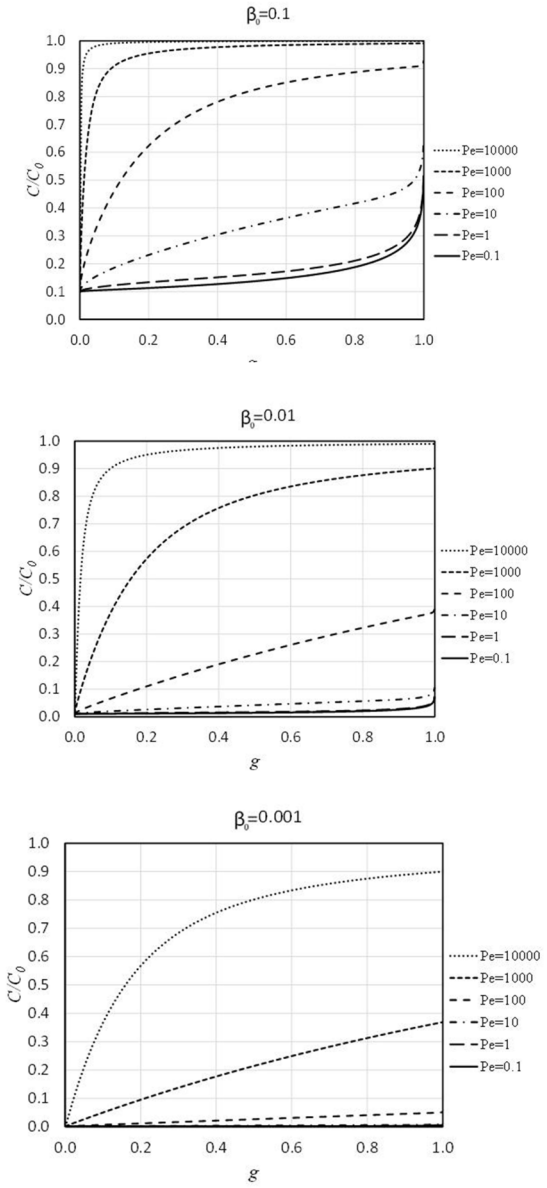

Fig. 1. Dependence of C/C_0 on *g* at different $ß_0$ and *Pe* in a vacuum evaporation refining with a flat and constant evaporation surface.

It should be noted that finding *D* for impurities in substances by the method under consideration cannot be based on literature data on refining parameters (*g*, *T*, *v*, *X*) due to the incompleteness or inaccuracy of these data, and special experiments and detailed development of the method are required. Obviously, more reliable results can be obtained by using sublimation rather than distillation, since distillation is characterized by convection, which is not taken into account in the refining calculation method [5]. Finding *D* on distillation results requires the use of special techniques that suppress convection.

4. Conclusions

The fundamental possibility of calculating the diffusion coefficient D of an impurity in a substance at a given temperature on the results of evaporation refining is shown - using the formula $D = vX/Pe$ and the measurement Pe in an actual refining process.

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