Multicomponent nonisothermal nucleation. 3. Numerical results

V.B.Kurasov
Victor.Kurasov@pobox.spbu.ru

We continue the theory presented in preprints 990958 and 990960 in this archive. Now all necessary formulas are known and we shall make some calculations in order to compare our results with the already known theories. All definitions are the same and no special references are given in the text.

1 Numerical results and conclusions

To show the numerical effects of the error approach [8] we shall consider the same situation as it was done in [8]. As far as in has not been declared in [8] what normalizing factor of the equilibrium distribution was used to calculate the stationary rate of nucleation we have to use the isothermal rate of nucleation published in [8] (see Fig.1 there) as some given data.\footnote{The same qualitative picture will be under the arbitrary normalizing factor.} The detailed description of the experimental conditions and data can be found in [8], [12].

The condensation of the ethanol (first component) - hexagonal (second component) is considered. The nucleation rate logarithm over the mean activity \( z = \sqrt{\zeta_1^2 + \zeta_2^2} \) is drawn for the several values of the activity fraction \( q = \zeta_1/(\zeta_1 + \zeta_2) \). In Fig.1. the points correspond to the results of Strey and Visanen [12]. The solid lines show the isothermal rates of nucleation. Two dashed lines presents the nonisothermal nucleation rates for different values of the passive gas (argon) accommodation coefficient \( \alpha_{acc\ g} \). The lower curve...
corresponds to $\alpha_{acc\ g} = 0.01$, the upper corresponds to $\alpha_{acc\ g} = 0.1$ (for all activity fractions).

The values of $q$ are written below the series of experimental points and above the theoretical curves. For small values of $q$ the isothermal and non-isothermal curves practically coincides, but this occurs only due to the big slope of the drawn dependencies. Moreover one can analytically show that the difference in $J$ between isothermal and nonisothermal approaches is growing with the growth of the nucleation rate and, thus, for small $q$ this difference is the greatest.

We omit the comparison with the results of Lazaridiz and Drossinos [7] because their nucleation rates are higher than the classical isothermal results. It lies in contradiction with the principle of stability. It is quite possible that Lazaridis and Drossinos used another input data as the parameters of their theory.

Fig.2 and Fig.3 show the difference between the nucleation rates calculated by Djikaiev et al. [8] and by the formulas presented here. Our results are dotted lines, the results of Djikaiev et al. are dashed lines, the nonisothermal rates logarithms are solid lines. All curves are drawn for $\alpha_{acc\ g} = 0.1$. The greater the nucleation rate is the greater is the manifestation of the thermal effects and the greater is the difference between the nucleation rate calculated by Djikaiev et al. and our results. That’s why we take two situations with the lowest theoretical nucleation rates which corresponds to $q = 0.980$ (Fig.2) and $q = 0.929$ (Fig.3). Certainly, the difference for $\ln J$ isn’t too big, but the correct account of the passive gas cooling changes $J$ in several times in comparison with results of Djikaiev et al. Our results are closer to the experimental data.

To show the qualitative difference we can assume that $\tau_j$, $W_j^+ n_{\infty\ j}$ $\partial F/\partial \nu_j$ have equal values for all components. Then all components can not be separated and we have the nonisothermal nucleation for one component but the passive gas is taken $i_0$ times into account in [8] ($i_0$ is the number of the condensating components). Also we can approximately assume that the main cooling of the embryo occurs due to the passive gas. Then taking into account that the renormalization of the stationary rate is proportional now to the quantity of the passive gas [2] we can see that the error in $J$ attains $i_0$ times (two times in the binary condensation). This error is likely more significant than the difference between the Stauffer approach [13] and the steepens descent method [14].
All necessary limit transitions of the presented theory (to the one component theory, to the nonisothermal theory) are observed and give the correct asymptotes to the already described situations.

To finish our description we can briefly recall the new facts presented here in comparison with other publications. Certainly, the most advanced version of the theory was presented by Djikaiev et al. [8], but even in comparison with this publication the new features are the following ones:

- The theory is now presented for the multicomponent case.
- The shift terms in kinetic equation are obtained. The sense of these terms is clarified, their negligible role is justified. It is shown that their negligible role can be shown only in frames of the initial steps of the Chapman-Enskog procedure. The connection of the vanishing of the shift terms and the possibility to forget about the lattice structure of the distribution domain is shown.
- The common cooling by the passive instead of the separate cooling is considered. This leads to essential numerical difference in the nucleation rate.
- The relaxation in the absence of specific parameter required in [8] is based. It allows to consider by the known Chapman-Enskog approach the situation of the strong thermal effects.
- The wrong parameter of decomposition presented in [8] is now corrected. This clarify the transition to the isothermal multicomponent theory.

The evident weak point of the presented theory is the absence of the surface tension dependence on the temperature. This phenomena will be taken into account in the next publication.
Figure 1.
Figure 2.
Figure 3.
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