SIMULATION of OSCILLATORY NUCLEATION in VAPORS

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The simulations of heat and mass transfer processes related with kinetics of the phase transitions received new impact from applied research related with novel material production based on a nanoparticles [1]. The homogeneous nucleation is the first stage of nanoparticles creation at vapors mixture.

High rates of a nucleation and nanoparticles growth lead to a depletion effect of vapor density at nucleation zone. In some cases this effect brings to stop of the nucleation process which is extremely sensitive to the supersaturation value. The diffusion mechanism restores the vapor density at nucleation zone in some time if new phase particles have been removed from nucleation zone. Finally, nucleation and particles growth is repeated. Such process is called oscillatory nucleation. It's clear that oscillatory nucleation impacts greatly on the productivity of a devices for nanoparticle production.

The physical and mathematical model of oscillatory nucleation is developed to simulate some parameters of an this process . The mathematical model includes integro-differential equation of the mass transfer processes with source related with growth and motion of a nanoparticles. It have been shown that heat processes have small influence on oscillatory nucleation if pressure carrier gas is much larger the partial vapor pressure. The evolution of the moving source are described by the systems of ODE.

$$\partial_t n(x,t) = \partial_x (D(x)\partial_x n(x,t) - I(R(z(t)), < n(z(t)) >, t) \qquad (1)$$

where n(x,t) is the vapor density, <n(x,t)> is the average vapor density in a spatial domain occupied by nanoparticles, D(x) is a vapor diffusion coefficient, I is general form of moving source, z is the position of the center of mass of a nanoparticles clouds, R(z(t)) is the average radius of nanoparticles. The value of I is directly proportional the number density of nanoparticles.

$$\frac{dz}{dt} = v(R, < n(z(t)) >) \qquad (2)$$

where v is the velocity of nanoparticles. The drag force, gravitational force and thermophoretic force influent on the velocity value.

$$\frac{dR(t)}{dt} = L(R)\left[< n(z(t) > - < n_e(z(t)) >\right] \qquad (3)$$

where $n_e(z(t)$ is the saturated vapor density, L is the known function of Knudsen number.

The theory is illustrated by an example of oscillatory nucleation in diffusion cloud chamber. The spectral variant of Galerkin's method is used for investigation this mathematical model. Results of numerical simulation of oscillatory nucleation are presented. The mass transfer processes are calculated in one-dimensional approximation. In particularly, for oscillatory nucleation at microgravity environment are considered. The comparison of experimental results (Fourier spectra of nanoparticles production rate) and theoretical calculation of the frequencies of periodic nucleation are discussed.

REFERENCES

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