Size dependence of incorporation of gas molecules into aerosol nanoparticles

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The influence of size effects on the physicochemical transformations and transfer phenomena in the heterogeneous systems with nanoobjects attracts increasing attention of researchers. These problems are of interest for nanotechnology and atmospheric physics. Size effects can influence the cohesive energy as well as the activation energies of vacancy formation and diffusion of atoms in the nanoscale particles (Vanithakumari and Nanda, 2008). Phase transitions in aerosol systems with nanoscale particles (clusters) also depend on the nanoparticle size (Levdansky *et al*., 2010). Hear we discuss the size dependence of the mass accommodation coefficient in the aerosol system with nanoparticles.

The equation for the mass accommodation coefficient γ can be written as (Hanson, 1997; Crowley *et al*., 2010)

$$\gamma = \frac{\alpha_s k_{abs}}{k_{des} + k_{abs}}, \qquad (1)$$

where α_s is the sticking coefficient, k_{abs} is the rate constant for absorption, k_{des} is the rate constant for desorption.

The sticking coefficient α_s is related to the rate constant for adsorption k_{ads} (Hanson, 1997). The values of k_{ads}, k_{des}, k_{abs} in the general case depend on the nanoparticle size due to the size dependence of adsorption and desorption of molecules (Murzin, 2009) and absorption of adsorbed molecules (Levdansky *et al.*, 2009). The melting temperature and surface tension also depend on the nanoparticle size (Rekhviashvili and Kishtikova, 2006). Taking into account the above-mentioned, we can write the following equation for the mass accommodation coefficient for the nanoparticle γ_p:

$$\gamma_p = \frac{4}{v} \frac{k_{ads,\infty} \exp\left(-\frac{4\alpha_{ads}\lambda\omega}{d}\right) k_{abs,\infty} \exp\left(\frac{4\psi\delta}{d}\right)}{k_{des,\infty} \exp\left[\frac{4(1-\alpha_{ads})\lambda\omega}{d}\right] + k_{abs,\infty} \exp\left(\frac{4\psi\delta}{d}\right)}, \qquad (2)$$

where v is the mean thermal velocity of gas molecules, $k_{ads,\infty}$, $k_{des,\infty}$, $k_{abs,\infty}$ are respectively the rate constants for adsorption, desorption and absorption for bulk matter, α_{ads} is the Polanyi parameter for the adsorption rate constant (Murzin, 2009), d is the particle diameter, δ is the Tolman length (it is assumed that $d >> \delta$), $\lambda = \sigma_\infty V_m/(RT)$, $\psi = Q_{abs,\infty}/(RT)$, $\omega = 1 - 4\delta/d$, σ_∞ is the surface tension for bulk matter, V_m is the molar volume of the substance forming the nanoparticle, R is the gas constant, T is the temperature, $Q_{abs,\infty}$ is the activation energy for the transition of molecules from the adsorption state to the absorption state for bulk matter.

Let us consider the limiting case when $k_{des} >> k_{abs}$. Figure 1 shows the dependence $\gamma^* = \gamma_p/\gamma_\infty$, where γ_∞ is the mass accommodation coefficient for bulk matter, on the dimensionless diameter of the nanoparticle $d^* = d/\delta$ at different values of the parameters ψ and $\varphi = \sigma_\infty V_m/(Q_{abs,\infty}\delta)$. It is seen that γ^* increases with a decrease in d^* and φ and with an increase in ψ.

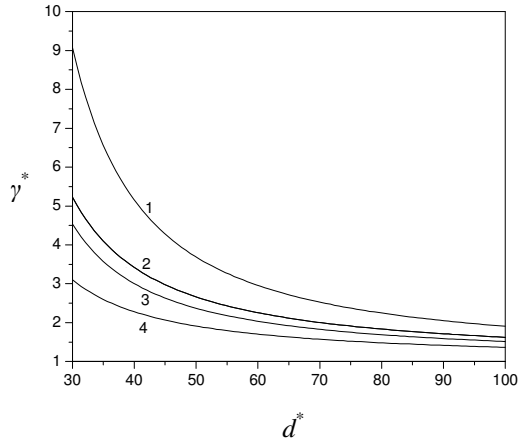

Figure 1. Dependence of γ^* on d^*; 1, 2: $\varphi = 0.2$; 3, 4: $\varphi = 0.5$; 1, 3. $\psi = 20$; 2, 4: $\psi = 15$.

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