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INFLUENCE OF SIZE EFFECTS ON UPTAKE OF IMPURITY ATOMS BY AEROSOL NANOPARTICLES GROWING IN VAPOR CONDENSATION

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INTRODUCTION

It is known that impurity atoms (molecules) in the main substance can affect its physicochemical properties. Semiconductor doping is paramount in micro- and nanoelectronics. In some cases nanoparticle doping is needed (Erwin *et al.*, 2005). Nanoparticle doping in the general case depends on the size of nanoparticles. Below we consider theoretically size effects in the uptake of impurity (dopant) atoms by the aerosol nanoparticle that grows in the supersaturated vapor.

RESULTS AND DISCUSSION

Let us consider the influence of size effects on the uptake of impurity atoms (molecules) by the growing aerosol nanoparticle in condensation of the supersaturated vapor of the main component. We assume further that the free-molecular regime of gas flow takes place and the concentration of impurity atoms in the nanoparticle is sufficiently small. The uptake coefficient γ for impurity atoms under above-mentioned assumptions according to (Levdansky *et al.*, 2000) is given by:

$$\gamma = \frac{s}{1 + F/I}, \tag{1}$$

where s is the sticking coefficient of impurity atoms on the particle surface, I is the resultant flux density of vapor atoms into the growing aerosol particle, the value of F is related to evaporation of impurity atoms from the particle.

Taking into account the relation between s and the rate constant for adsorption of impurity atoms k_{ads}, as well as the size dependence of k_{ads} (Murzin, 2009) and the surface tension (Rekhviashvili and Kishtikova, 2006), the sticking coefficient for the nanoscale particle s_{p} in the case of $4\delta/d << 1$, where d is the nanoparticle diameter, δ is the Tolman length, can be written as

$$s_{\mathrm{p}} = s_{\infty} \exp\left\{ -\frac{4\alpha\sigma_{\infty}V}{dkT}\left(1 - \frac{4\delta}{d}\right)\right\}. \tag{2}$$

Here σ_{∞} is the surface tension for bulk matter, $s_{\infty} = 4k_{\mathrm{ads},\infty}/v$, $k_{\mathrm{ads},\infty}$ is the value of k_{ads} for bulk matter, v is the mean thermal velocity of impurity atoms in a gas phase, k is the

Boltzmann constant, T is the temperature, V is the volume per atom in the nanoparticle, α is the Polanyi parameter.

The value of F in view of (Levdansky *et al.*, 2000) is given by

$$F = \frac{n_c v}{4} \exp\left\{ -\frac{E_p}{kT} \right\}, \tag{3}$$

where n_c is the total number density of atoms in the nanoparticle that is assumed to be constant, E_p is the activation energy needed to remove the impurity atom from the nanoparticle which decreases with a reduction in the nanoparticle size similarly to the one-component nanoparticle. The last case was examined in (Levdansky *et al.*, 2014).

Let us consider the value of γ for the nanoparticle (γ_p) in the limiting cases when $F/I << 1$ and $F/I >> 1$. In the first case $\gamma_p \approx s_p$ and the uptake coefficient can be described by the equation similar to Eq. (2). The value of γ_p in $F/I >> 1$ can be written as

$$\gamma_p = \frac{4Is_\infty}{n_c v} \exp\left\{ -\frac{4\alpha\sigma_\infty V}{dkT}\left(1-\frac{4\delta}{d}\right)+\frac{E_p}{kT} \right\}. \tag{4}$$

It is worth noting that the value of I will decrease with a reduction in the nanoparticle size due to a decrease in the condensation coefficient of vapor atoms of the main condensing component and the evaporation energy of these atoms. It is seen from Eqs. (2) and (4) that in both above-mentioned cases the uptake coefficient γ_p for impurity atoms and their concentration in the nanoparticle (which is related to the uptake coefficient) will be less for the smaller nanoparticle.

CONCLUSIONS

Thus, it is shown that the size dependence of the sticking coefficient of impurity atoms on the nanoparticle surface and the cohesive energy in the nanoparticle can decrease the uptake coefficient of impurity atoms and their concentration in the nanoparticle growing by vapor condensation.

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