The dependencies of self-diffusion coefficient on the size and shape of the nanocrystal at different $P$-$T$-conditions

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The previously proposed RP-model \([1, 2]\) was generalized to the case of the vacancies and the delocalized (i.e. diffusing) atoms presence, which are uniformly distributed throughout the volume of the simple matter nanocrystal with $N$-atoms. On the basis of the generalized RP-model, the vacancy formation probability ($\phi_v$) and the atom delocalization probability ($\chi_d$) dependencies on the size and shape of BCC-iron nanocrystal at different $P$-$T$-conditions were studied.

It is shown that when an isothermal pressure increases, the function $\phi_v(P)$ decreases more significantly for nanocrystal than for bulk crystal, and at a certain pressure, the probability of vacancy formation in nanocrystal becomes smaller than in bulk crystal. At the isobaric-isothermal nanocrystal growth under atmospheric pressure and temperature 300 K, the nanocrystal contains fewer vacancies per atom than the bulk crystal. However, at 1 bar and 1000 K, the size reduction of crystal leads to higher probability of vacancy formation (Fig. 1, left). At nanocrystal formation under $P = 100$ kbar the nanocrystal contains fewer vacancies per atom than the bulk crystal both at 300 K and at 1000 K (Fig. 1, right).
At nanocrystal size reduction the probability of the atom delocalization ($x_d$) and the self-diffusion coefficient ($D_{if} \sim x_d$) are increasing at any pressure and temperature (Fig. 2).

At the nanocrystal shape deviation from the most optimal shape (for RP-model – from the cubic shape), the size dependences of the activation parameters for the nanocrystal are increasing.

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**References**
