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

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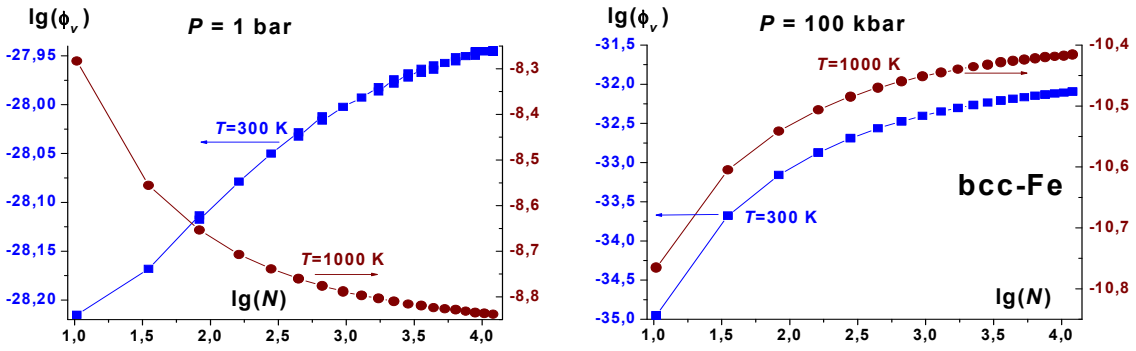
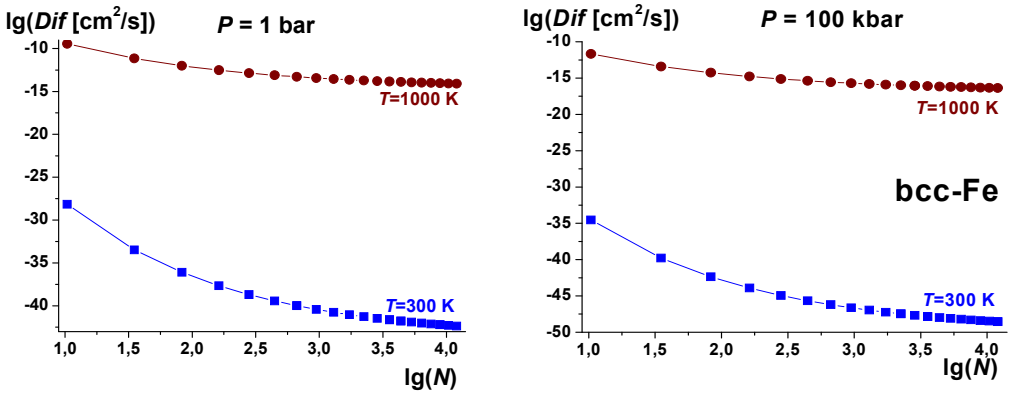
The previously proposed RP-model [1, 2] was generalized to the case of the vacancies and the delocalized (i.e. diffusing) atoms presence, which are uniformly distributed throughout the volume of the simple matter nanocrystal with *N*-atoms. On the basis of the generalized RP-model, the vacancy formation probability (ϕ_v) and the atom delocalization probability (x_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 ($Dif \sim x_d$) 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

[1] M.N. Magomedov: *Study of interatomic interaction, vacancy formation and self-diffusion in crystals.* Moscow: Fizmatlit (2010). [in Russian]

[2] M.N. Magomedov: *On dependences of the thermoelastic properties on size and shape of an iron nanocrystal.* Nanotechnologies in Russia, **10**, *# 1-2*, 89-99 (2015).