The study of diffusion mechanisms of self-interstitial atom (SIA) and vacancy in bcc iron has been carried out using molecular statics and molecular dynamics simulations. Temperature dependences of defects diffusion $D_d(T)$ and corresponding self diffusion $D'(T)$ coefficients and tracer correlation factor $f_{tr}$ have been calculated in temperature ranges (1000 - 1800) K and (250 - 1800) K for vacancy and SIA, respectively.

The obtained temperature dependences of vacancy diffusion coefficients are described well by Arrhenius equation:

$$D_d(T) = 8.49 \times 10^{-3} \exp(-0.733 eV/k_BT) \text{ cm}^2/\text{s},$$

$$D'(T) = 5.35 \times 10^{-3} \exp(-0.720 eV/k_BT) \text{ cm}^2/\text{s},$$

$k_B$ is Boltzmann constant. Additional migration mechanisms are activated at high temperatures, at which the vacancy migrates to the 3rd and the 5th nearest neighbors (nn) positions, besides the ordinary mechanism of migration to the 1st nn position. The approximation of the temperature dependences of jump frequencies, corresponding to these migration mechanisms, by Arrhenius equation gives the values of the activation energies: 0.730 eV, 1.401 eV and 1.664 eV for the jumps to the 1st, 5th and 3rd nn positions, respectively. These values agree with the corresponding static barriers: 0.735 eV, 1.406 eV and 1.743 eV. The calculated value of $f_{tr}$ agrees with its theoretical value 0.727 within the limits of inaccuracy at $T \leq 1600$ K. At higher temperatures, some weak systematic decrease of $f_{tr}$ is observed which is concerned with the activation of two mentioned above less energetically favorable migration mechanisms.

The temperature dependences of SIA diffusion coefficients sufficiently differ from Arrhenius type in the considered temperature range. The effective migration energies are $\sim (0.22 - 0.23)$ eV at $T < 300$ K. These values are close to the calculated values of static barriers of $<110>$ dumbbell migration and $<110>$ to $<111>$ dumbbell reorientation processes (0.246 eV and 0.250 eV, respectively) and in agreement with the experimental value $\sim (0.25 - 0.30)$ eV. The effective migration energy decreases with the temperature reaching the value 0.09 eV at $T \sim 1000$ K. The SIA has a complex 1D and 3D migration mechanism. The value of $f_{tr}$ is constant within the limits of inaccuracy through the considered temperature range and equals to 0.27, which is the evidence of the complex diffusion mechanism not changing with the temperature.