Regularities of the distribution of H and O atoms in bacteria LEPTOTHRIX.

D.M. Mirzayeva[1,2], S.P. Kaplina[1,2], M.V. Gustova[2], I.Z. Kamanina[1,2]

[1]Dubna State University, Dubna, Moscow distr., Russian

[2]Joint Institute for Nuclear Research, Dubna, Moscow distr., Russian

dunyamirzayeva@gmail.com

At present, due to the increase in the anthropogenic load on the environment, the search for new natural sorbents for wastewater treatment both in the natural environment and under production conditions becomes relevant. Methods for cleaning the environment using microorganisms are of great interest in solving scientific and technological problems. Iron-forming bacteria of the genus Leptothrix are of great interest, since in the course of their growth they produce extracellular formations containing iron oxides and oxyhydroxides, which can be used for environmental purposes. Positron annihilation is characterized by high sensitivity to vacancy-type defects, which makes it a method commonly used in materials science and materials technology research. In the crystal lattice, the positrons have captured all the vacancy-type defects that could exist under the conditions accompanying the metabolism of the bacteria under study. Positrons penetrating in a solid may be trapped in defects that show sites in the crystal lattice where the atomic density is less than the average density in the volume, i.e. vacancies, vacancy clusters (consisting of voids) and dislocations. The annihilation aspects of a positron trapped in free space or empty nanocavities are different from those of a positron trapped in nanocavities containing hydrogen. To calculate the positron lifetime, we used the MIKA package with local density approximation (LDA) method, which works without relaxation in a conventional scheme and uses TCDFT. With the help of model calculations, we can make a study of supposed effects in the ongoing processes in Fe, Fe_2O_3 and Fe3O4 in the conditions of synthesizing balance, as observed in the environment where the bacterium lives. Figure 1 shows Fe, Fe_2O_3 and Fe_3O_4 vacancy defects with implantation as expected to be available in the current situation.

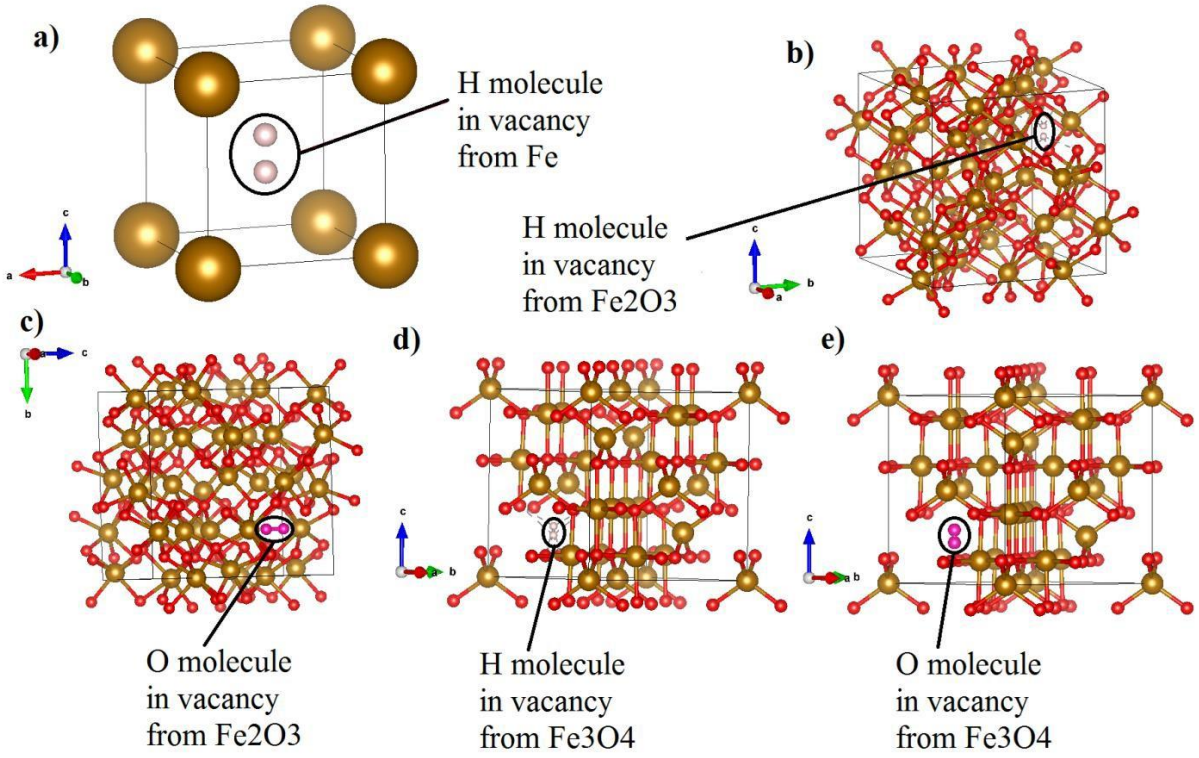

Figure 1. Schematic position of defects and impurities atoms in lattices of Fe, Fe_2O_3 and Fe_3O_4

In an aqueous environment, there is expected to be an accumulation of hydrogen and oxygen molecules in the free clusters. Through a virtual experiment that simulates real statistics, for the three materials we study, we investigate the change of the positron lifetime in a single-vacancy cluster in which the number of hydrogen atoms grows.