The modelling of helium segregation at grain boundaries in Fe-Cr alloys for fusion applications

Description for the general public

The rapid population growth on Earth cause the ever-increasing demand for electricity. In order to provide it, various physical and chemical phenomena are used, such as redox reactions in galvanic cells, photovoltaic effect in solar panels or electromagnetic induction phenomena in generators. Increasing of the efficiency of current power plants and creating numerous new energy sources is undoubtedly an important domain of many researchers. Nevertheless, if we seriously want to stave off the problem of shortage of energy for many generations ahead, then we must use the energy derived from the Einstein's equation $E = mc^2$, where m is an invariant mass, and c^2 is the speed of light squared. Since the middle of last century, mankind has successfully used heavy nuclear fission in power plants, where about 0.09% of the original mass is converted into energy. The next step, for the 21st century, is the use of light elements in the thermonuclear reaction, which from the beginning of our existence provides us with solar energy. Nucleosynthesis, converting even about 1% of mass into energy, has been the subject of research for several decades, but it still did not result in a functioning fusion reactor. Both physicists and material engineers have a lot of work ahead of them.

The thermonuclear reactor will be made of a number of materials that will be exposed to such factors as elevated temperature, helium and hydrogen corrosion, or irradiation of high-energy neutrons. The great care should be paid to helium segregation at the grain boundaries, because this process leads to the formation of nanometric helium bubbles, which results in brittleness and in a significant limiting the lifetime of such material. A presence of hardly detectable helium and the fact those phenomena occur at atomic scale causes it is extremely difficult to provide valuable empirical study.

In the ITER project (International Thermonuclear Experimental Reactor), a large number of reactor components from various steels are planned to be made. Designing materials for such applications is possible only in the way of deep understanding of basic knowledge about the processes occurring in the crystal structure. For this reason, the main objective of the project is to determine the impact of the presence of radiation defects and chemical composition on the process of segregation of helium atoms at the grain boundaries in Fe-Cr alloys. The conducted theoretical research will pay special attention to the alloys with a chromium content of up to 10% atomic, which will be a good model of the so-called EUROFER steel. In addition, three special goals were formulated in the project: 1) development of program code for Atomistic Kinetic Monte Carlo (AKMC) method; 2) description of how point defects interact with the grain boundaries; 3) investigation of the local environment influence on grain boundary properties.

To reach this goals, calculations based on quantum chemistry, and more precisely on the density functional theory, will be carried out. The results of these calculations will be used to determine the properties characterizing various defects of the crystal structure as well as to refine the developed AKMC code. A Monte Carlo simulations enable to study the kinetic processes taking place in the material and also provide the possibility to test the alloys in a wide range of chemical compositions.

The research planned in this project goes beyond the results obtained by other researchers, and therefore there is a great opportunity to publish the results in journals from Journal Citation Reports list such as: Journal of Nuclear Materials, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, Physical Review B, Physica Status Solidi, or Acta Materialia.