2 years post-doctoral position

Object Kinetic Monte Carlo and Finite Element developments for the creation of a Macroscopic Rate Equation model of fusion reactor walls

This 2 years post-doctoral position is offered in the framework of the collaborative project WHeSCI (piim.univ-amu.fr/amidex/whesci), financed by the A*MIDEX foundation (amidex.univ-amu.fr) and proposed in the context of the International Thermonuclear Experimental Reactor (ITER), the international project that aims to demonstrate the technological and scientific feasibility of fusion energy with the Tokamak design (www.iter.org). The WHeSCI project seeks to describe the interactions of the fusion fuel (deuterium (D) and tritium (T)) and ashes (helium (He) and neutron) with the walls of the exhaust of the reactor (the divertor made of Tungsten, W). The induced material properties modifications are indeed critical for the reactor operation and safety and the successful operation of ITER requires a detailed understanding of the plasma-wall interactions.

In this context, the post-doctoral fellow will be involved in the further development of the MHIMS and HIIPC Macroscopic Rate Equation (MRE) models [1-4], which are describing so far the D/T fuel trapping in bulk metals, in absence or in presence of bubbles in the micrometre range. In particular, he/she will study and implement synergistic effects between D/T/He implantations and neutron-induced defects in tungsten materials. Object Kinetic Monte Carlo (OKMC) simulations will be used to obtain a dynamical insight onto temporal and thermal evolution of D/T/He and defects in W. Ultimately, OKMC simulations will provide information on bubble nucleation. The input parameters for the OKMC code LAKIMOCA [5] will come from the literature but also from several WHeSCI project partners: atomic-scale events energies and attempt frequencies will come from DFT calculations, spatial distribution of defects and D/T/He species will come from experiments. Once bubble nucleation is understood, its growth will be investigated with Finite Element Methods (FEM) [6]. Based on this numerical approach, D/T/He trapping and bubble growth will be included in the MRE simulations. This work will be done in close collaboration with a PhD student at CNRS/LSPM who is currently developing the Abaqus Finite Element Method (FEM) code as well as a staff of the CEA group working on the MHIMS program.

The candidate should have a PhD in computational physics, a solid background in solid state physics and show skills in the field of metallic materials. At least one experience of OKMC or FEM simulations is required. As the candidate will have to interact with the various actors in the project, good oral and written communication skills are necessary and the ability to work in a collaborative research environment is essential. Knowledge of French would be appreciated but is not mandatory.

The 1st year of the contract will be located in Lille (France) and will focus on OKMC simulations with Charlotte Becquart (CNRS/UMET - University Lille). The 2nd year will be located in Paris and will focus on FEM and MRE implementations with Yann Charles and Jonathan Mougenot (CNRS/LSPM - University Paris 13). Christian Grisolia (CEA/IRFM) will coordinate the simulation work. The postdoctoral contract is financed by the WHeSCI project (coordinated by Régis Bisson, Aix-Marseille University/PIIM). Application is open until May 31 and the earliest starting date is July 1 2018. Questions should be sent directly to the following contact persons:

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[1] E.A. Hodille *et al* Nucl. Fusion **57** 076019 (2017)
[2] E.A. Hodille *et al* Phys. Scr. **T167** 014011 (2016)
[3] C. Sang *et al* Nucl. Fusion **52** 043003 (2012)
[4] C. Quiros *et al* Nucl. Mat. Ener. **12** 1178-1183 (2017)
[5] C.S. Becquart *et al.* J. Nucl. Mater. **403** 75-88 (2010)
[6] Y. Charles *et al* IJHE **42** 20336-350 (2017)