Internship at CEA, year 2019-2020

Multiscale modeling precipitation in nuclear fuels

Scientific Field:

Materials physics

Context:

The nuclear fuels cycle duration is limited by gases produced by fission reactions. The subject is aimed at improving the simulation code of the gas atoms behavior during irradiation. This tool is developed in a multiscale approach [1] and uses parameters based atomistic calculations while others need to be fitted [2,3]. This subject has a "theoretical" axis and an "interpretation" one. The candidate will have the possibility to privilege one axis or the other depending on his preferences and the results. This is also an occasion to get involved in a multi-scale modelling approach and experiment how helpful can be the atomistic techniques to evaluate the input parameters of a simulation tool of large scale phenomena.

1. Skorek, R. (2013). Étude par Dynamique d'Amas de l'influence des défauts d'irradiation sur la migration des gaz de fission dans le dioxyde d'uranium (PhD Thesis). Univ. Aix-Marseille.
2. Andersson D. et al. (2014). Atomistic modeling of intrinsic and radiation-enhanced fission gas (Xe) diffusion in UO2+/-x: Implications for nuclear fuel performance modeling. Journal of Nuclear Materials, 451, 225–242.
3. Le Prioux A. et al. (2016). Empirical potential simulations of interstitial dislocation loops in uranium dioxide. Journal of Nuclear Materials, 479, 576–584.

Goals:

- Interpret annealing experiments of gas implanted samples, using a simulation code
- Improve the fitting method in order to identify the unknown model parameters
- Characterize the impact of each model parameter on the simulation results and prioritize the future work of parameters evaluation

Steps of the work:

- Selection of the most significant experiments for the validation
- Simulation of these experiments
- Critical analysis of the results
- Re-assessment of the model parameters
- Improvement of the fitting procedure using a library of various optimization procedures

Calculation tools, computers (languages, softwares):

Simulation code in FORTRAN90, Mathematica, unix, optimization platform URANIE

Keywords:

Kinetic model, simulation, experiment interpretation, optimization

Duration:

6 months

Location:

CEA Cadarache (13)

Formation required

M1 or M2 in **materials physics**,
Skills and interest for **computer developments** AND interpretation of **experiments**

Possibility to pursue with a PHD thesis

Yes: ☒ No: ☐

Contact

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Application to send 3 months before the beginning of the training course to the person in charge. Consultation of CEA internships on the website: http://portail.cea.fr/emploi