MD and Adaptive Kinetic Monte Carlo Study of Hydrogen and Helium Diffusion/Trapping/Clustering in First–Wall Tungsten

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Abstract
The core question for plasma-wall interaction in fusion devices is focused on two main concerns – Erosion (lifetime of PFC; damage, impurity) and Hydrogen (Tritium) issues (such as deposition, retention, migration). Radiation damage of first wall material and transmutation effects are also of interest and concern, along with structural questions due to embrittlement of material. Integrated modeling including dynamic evolution of first wall materials, such as, Be-W (ITER, JET); C-steel (W7-X), W-based alloy (DEMO), full W PFC (EAST) is desired for future designs. Although most fusion devices are designed to be carbon free the National Spherical Torus Experiment Upgrade (NSTX-U) has carbon walls with lithium coatings and high-z materials in select region of the spherical tokamak. Due to the presence of carbon based first-wall material the formation of hydrocarbon flakes (H:C), their transformation into flakes with different H:C ratio, and, their deposition in remote regions of machine is still a crucial problem for fusion devices [1].

The current study presented here is focused on Molecular Dynamics (MD) and Kinetic Monte Carlo (KMC) study of hydrogen and helium diffusion, trapping and clustering in tungsten using classical and quantum mechanical (DFT) methods. This study advances earlier large-scale classical molecular dynamics (MD) simulations that have been used to evaluate He bubble nucleation and its impact on tungsten surfaces. MD results indicate highly mobile He atoms self traps and form He clusters with varying size distribution and mobility, which are temperature dependent. The influence of implantation flux on cluster size distribution as a function of depth and impact of radiation/thermal damage is still to be resolved.

We use classical MD with W-H-He embedded atom method potential of Bonny and Terentyev [2] to study the formation of helium cluster and interaction of hydrogen with helium in a tungsten matrix under different helium fluence and substrate temperatures. Helium/Hydrogen cluster size distribution, depth distribution, and mobility of the cluster are calculated in bulk and W-surface. Adaptive Kinetic Monte Carlo (aKMC) method is used to perform saddle point searches and use harmonic transition state theory to model state-to-state dynamics of atomic cluster. Many limitations of KMC are relaxed in aKMC with the exception that reaction mechanism available to the system is not *a priori* but instead found during the simulation. The method is described as adaptive because the list of possible events in KMC is not fixed. Once saddle point is located the reaction rate for the corresponding event is computed using harmonic-TST. KMC method is used to simulate millions of events with modest computational work, however, this approach is limited by the number of states; reaction mechanism connecting predefined states and the reaction rates which can be determined from potential energy surface using transition state theory (TST).

He-H interaction in tungsten matrix is also investigated and the effect of this interaction on trapping of tritium (or hydrogen) will be presented. This could influence recycling, retention and radioactive dust in fusion devices. The effect of He gas cluster on H/D/T retention is studied.

Reference:

[1] A. R. Sharma, R. Schneider, and U. Toussaint, "Hydrocarbon radicals interaction with amorphous carbon surfaces," *Journal of Nuclear Materials*, vol. 363, pp. 1283–1288, 2007.
[2] G Bonny, P Grigorev, and D Terentyev, "On the binding of nanometric hydrogen–helium clusters in tungsten," *Journal of Physics: Condensed Matter,* Vol. 26, Number 48, pp. 485001, 2014.