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Modelling self trapping and trap mutation in tungsten using DFT and Molecular Dynamics with an empirical potential based on DFT

J. Boisse[a,b], C. Domain[a,c], A. De-Backer[a,d] C.S. Becquart[a]

[a] Unité Matériaux et Transformations, UMET, UMR 8207, Université de Lille 1, F-59655 Villeneuve d'Ascq, France

[b] Laboratoire d'Energétique et de Mécanique Théorique et Appliquée, LEMTA , UMR 7563, Université de Lorraine, F-54504 Vandoeuvre-lès-Nancy, France

[c] EDF-R&D, Département MMC, Les renardières, F-77818 Moret sur Loing, France

[d] CCFE, Culham Science Centre, Abingdon, Oxon, OX14 3DB, UK

Email address of corresponding author: charlotte.becquart@univ-lille1.fr

Being virtually insoluble in metals, but very mobile, He atoms can be trapped, associate with vacancies, forming platelets and bubbles. He atoms have been shown to contribute to swelling, cause intergranular embrittlement and produce roughening and blistering at metal surfaces. Being repelled by the metal atoms, they form stable clusters, which are also mobile. This tendency to form clusters is so strong that when too many He atoms are aggregated together it can be less costly to relieve the strain created by the interstitial elements by the ejection of one or more matrix atoms leading to the formation of one or more Frenkel Pairs (FP), i.e. vacancies and Self Interstitial Atoms (SIAs). When no vacancy is initially present, the He cluster will be trapped by the vacancy it created, in a self-trapping (ST) event; whereas when one or more vacancies are already associated with the He cluster, the same mechanism is referred to as trap mutation (TM) or loop punching, if more than one SIA is created.

The metal studied in this work is tungsten, candidate for the divertor and currently under heavy investigations experimentally and theoretically. We have investigated the thermodynamics and kinetics of ST and TM using Density Functional Theory (DFT) calculations and Molecular Dynamics with a recently developed potential for W-He adjusted on DFT calculations.

The stability of helium-vacancy clusters (He_nV_m) as well as pure interstitial helium clusters in tungsten results from a competitive process between thermal emission of vacancies, self interstitial atoms and helium atoms, depending on the helium-to-vacancy ratio in mixed clusters or helium number in pure interstitial helium clusters and will be presented in this work. We investigated in particular the ground state configurations as well as the activation barriers of self trapping and trap mutation, i.e. the emission of one SIA along with the creation of one vacancy from a vacancy-helium or pure helium object.