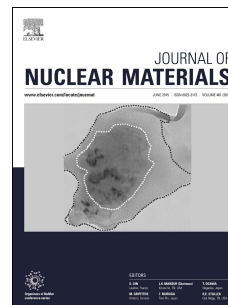


# Accepted Manuscript

The trapping and dissociation process of hydrogen in tungsten vacancy: A molecular dynamics study

Baoqin Fu, Mingjie Qiu, Jiechao Cui, Min Li, Qing Hou



PII: S0022-3115(18)30200-9

DOI: [10.1016/j.jnucmat.2018.05.065](https://doi.org/10.1016/j.jnucmat.2018.05.065)

Reference: NUMA 50995

To appear in: *Journal of Nuclear Materials*

Received Date: 8 February 2018

Revised Date: 28 May 2018

Accepted Date: 28 May 2018

Please cite this article as: B. Fu, M. Qiu, J. Cui, M. Li, Q. Hou, The trapping and dissociation process of hydrogen in tungsten vacancy: A molecular dynamics study, *Journal of Nuclear Materials* (2018), doi: 10.1016/j.jnucmat.2018.05.065.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

# 1 The trapping and dissociation process of hydrogen in 2 tungsten vacancy: a molecular dynamics study

3 Baoqin Fu, Mingjie Qiu, Jiechao Cui, Min Li, Qing Hou\*

4 *Key Laboratory for Radiation Physics and Technology, Institute of Nuclear Science and Technology, Sichuan*  
5 *University, Chengdu 610065, PR China*

## 7 Abstract

8 Tungsten (W) is a primary candidate for plasma facing materials (PFM) for future fusion  
9 devices. The interaction between hydrogen (H) and vacancy (V) is the key for understanding many  
10 material behaviors under irradiation. Therefore, it is necessary to study carefully the kinetic  
11 process between H and W vacancy. In this work, the dynamical parameters, including effective  
12 capture radii (ECRs) and dissociation coefficients, for various trapping and dissociation processes  
13 ( $VH_x + H \rightleftharpoons VH_{x+1}$ ), have been investigated using an ingenious method based on molecular dynamics  
14 (MD) simulations. It was found that the parameters are dependent not only on the reaction types  
15 but also on the temperatures. The ECRs decrease gradually as the increase of the trapped H atoms  
16 in the W vacancy, and decrease roughly with increasing temperature for  $T < 1200\text{K}$ . The  
17 dissociation energies decrease gradually as the increase of the trapped H atoms in the W vacancy.  
18 The evolution of concentration of the trapped H atoms in W vacancy was investigated by coupling  
19 the trapping process and dissociation process and using the dynamical parameters calculated by  
20 the MD simulations. The H retention in W obviously depends on the state of trapping sites and the  
21 temperatures. These results should be potentially applicable for the long-term simulation methods  
22 such as kinetic Monte Carlo (KMC) and rate theory (RT) models.

23  
24 **Key words:** Tungsten; Molecular dynamics; Hydrogen retention; Vacancy;

\*Corresponding author.

[qhou@scu.edu.cn](mailto:qhou@scu.edu.cn) (Q. Hou), [bqfu@scu.edu.cn](mailto:bqfu@scu.edu.cn) (B.Q. Fu).

Download English Version:

<https://daneshyari.com/en/article/7963069>

Download Persian Version:

<https://daneshyari.com/article/7963069>

[Daneshyari.com](https://daneshyari.com)