Accepted Manuscript

Dislocation core structures of tungsten with dilute solute hydrogen

Yinan Wang, Qiulin Li, Chengliang Li, Guogang Shu, Ben Xu, Wei Liu

PII: S0022-3115(17)30314-8

DOI: 10.1016/j.jnucmat.2017.09.019

Reference: NUMA 50505

To appear in: *Journal of Nuclear Materials*

Received Date: 28 February 2017

Revised Date: 11 September 2017

Accepted Date: 13 September 2017

Please cite this article as: Y. Wang, Q. Li, C. Li, G. Shu, B. Xu, W. Liu, Dislocation core structures of tungsten with dilute solute hydrogen, *Journal of Nuclear Materials* (2017), doi: 10.1016/j.jnucmat.2017.09.019.

Dislocation Core Structures of Tungsten with Dilute Solute Hydrogen

Yinan Wang[a], Qiulin Li[b], Chengliang Li[c], Guogang Shu[c], Ben Xu[a],*[0], Wei Liu[a,*]

[a] *Key Laboratory of Advanced Materials (MOE), School of Material Science and Engineering, Tsinghua University, Beijing 100084, PR China*

[b] *Graduate School at Shenzhen, Tsinghua University, Shenzhen, China*

[c] *State Key Laboratory of Nuclear Power Safety Monitoring Technology and Equipment, China Nuclear Power Engineering Co., Ltd., Shenzhen 518172, China*

Abstract

In this paper, a combination of quantum mechanical and interatomic potential-based atomistic calculations are used to predict the core structures of screw and edge dislocations in tungsten in the presence of a particular concentration of hydrogen atoms. These configurations of the core structures are the results of two competing energies: the interaction between the partial dislocations and the corresponding generalized stacking fault energy in between the two partial dislocations, which are presented in this work. With this, we can precisely predict the configurations of the hydrogen-doped dislocation core structures.

Keywords: screw dislocation, edge dislocation, QM/MD method, stacking fault energy

1. Introduction

With recent developments in thermonuclear fusion research, tungsten has emerged as one of the most promising plasma-facing materials (PFM). As a PFM, tungsten may be subjected to high magnitudes of heat and particle flux of hydrogen isotopes escaping from the plasma, which would promote the growth of cracks and ultimately result in the deformation and failure of the tungsten. One of the origins of the degradation of mechanical properties is the microscopic changes in the dislocation behavior. In recent MD simulations, the edge dislocations in Ni have been used to demonstrate that hydrogen may influence the distance between partial dislocations[1]. Additionally, the hydride-to-non-hydride transformation could be correlated to the nucleation of micro-cracks at the tips of dislocation pile-ups[2]. According to the results of another MD simulation performed on Fe, a high concentration of hydrogen imparts a unique core structure to screw dislocations, while in edge dislocations, the core energy and Peierls potential decrease as a function of the hydrogen concentration[3]. In the DFT work of D. Terentyev et al.[4], the authors demonstrated that H atoms are strongly bound to the screw dislocation core in body-centered cubic (bcc) W and exhibit fast one-dimensional migration along the dislocation line. Additionally, they observed the formation of a jog on the dislocation line introduced by the transformation of a cluster of eight H atoms into an immobile configuration. Another MD work by Petr Grigorev et al[5] suggested a strong and localized attraction of H to the core of edge dislocations, although the results fully depend on the potentials. To summarize the limitation of the above research, the empirical potentials for MD calculations[6] were not developed specifically to include the interactions between hydrogen and dislocation cores in tungsten, and thus, the possible deviated structure could be predicted. Moreover, it is still a challenge for DFT simulation due to the long range stress field of edge dislocations. Therefore, a reliable algorithm that suitably includes the interactions between dislocations and hydrogen atoms is needed for the prediction of core structures . With this, it is highly recommend to evaluate the dislocation core structures in the presence of H atoms as empirical potentials are developed in the future. Additionally, since the mobility of dislocations is strongly dependent on their core structure, such work substantially increases our ability to understand the possible mechanism of hydrogen embrittlement in tungsten.

2. Method

2.1. QM/MD method

In this paper, a systematic study using a quantum mechanics/molecular mechanics (QM/MD)[7] method determines the stable core structures of screw and edge dislocations with a certain concentration of hydrogen atoms. Then, the generalized stacking fault energy (γ_{SFE}) is discussed to characterize the influence of hydrogen on γ_{SFE}, which is vital for understanding the non-split phenomenon

Email addresses: xuben@mail.tsinghua.edu.cn (Ben Xu[a],*), liuw@tsinghua.edu.cn (Wei Liu[a,*])