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Interaction of hydrogen with dislocations in tungsten: An atomistic study

Petr Grigorev[a,b,*], Dmitry Terentyev[a], Giovanni Bonny[a], Evgeny E. Zhurkin[c], Guido Van Oost[b], Jean-Marie Noterdaeme[b]

[a]*SCK•CEN, Nuclear Materials Science Institute, Boeretang 200, Mol, 2400, Belgium*
[b]*Ghent University, Department of Applied Physics EA17 FUSION-DC, St.Pietersnieuwstraat, 41 B4 B-9000, Gent, Belgium*
[c]*Department of Experimental Nuclear Physics K-89, Institute of Physics, nanotechnology and telecommunications, St.Petersburg State Polytechnical University, 29 Polytekhnicheskaya str., 195251, St.Petersburg, Russia*
*Corresponding author email: petr.grigorev@sckcen.be

Abstract

The interaction of interstitial hydrogen with a dislocation and point defects in tungsten is studied by means of atomistic simulations. Two different types of interatomic potentials were tested by comparing their results with available ab initio data. The recently developed embedded atom method potential showed a better agreement with ab initio results than the bond order potential. Static calculations involving screw and edge dislocations showed that hydrogen is attracted to the dislocation core in both cases. It is also found that hydrogen atoms prefer to arrange themselves as elongated clusters on dislocation lines. Molecular dynamics simulations of hydrogen migration along the edge dislocation core confirmed the results of the static calculations and demonstrated a strong attraction to the dislocation core and one-dimensional migration along it.

1. Introduction

Tungsten (W) is one of the currently considered in-vessel plasma-facing materials for ITER [1]. During ITERs exploitation, cyclic thermal stresses coupled with radiation damage and trapping of plasma components (retention) impose a serious uncertainty regarding the lifespan of the components made of W. Hydrogen (H) retention is a specific problem, since it has a dual impact defining the degradation of W-based components. On the one hand, the maximum retention is limited by the safety limits, and on the other hand, the storage of hydrogen provokes further embrittlement to be added to the detrimental effect of neutron irradiation and thermal fatigue.

Despite significant efforts done in past investigations to explore the main mechanisms of H retention in W [2-6], a complete physical model capable of describing a broad set of experimental data does not yet exist. In our recent works [7, 8], we have drawn attention to the role played by dislocations in the trapping, transport and nucleation of hydrogen bubbles. Based on the *ab initio* calculations we have proposed the so-called 'jog-punching' process as the mechanism to explain the transformation of a meta-stable hydrogen cluster into a stable hydrogen-vacancy cluster – nucleus for a future hydrogen bubble [7].

The idea of the jog-punching mechanism and the obtained *ab initio* data was then implemented in a new theoretical model for the H retention based on H trapping at dislocations and transport to the surface via the dislocation network [8]. Such a model was used to explain the experimentally observed saturation of H retention with dose in different W grades under high flux plasma implantation conditions. One of the principal conditions of this model was the assumption about transport of hydrogen atoms along a dislocation network. Although the *ab*