Accepted Manuscript

Ab initio study of interstitial cluster interaction with Re, Os, and Ta in W

W. Setyawan, G. Nandipati, R.J. Kurtz

PII: S0022-3115(16)31044-3

DOI: 10.1016/j.jnucmat.2016.11.002

Reference: NUMA 49989

To appear in: *Journal of Nuclear Materials*

Received Date: 14 April 2016

Revised Date: 24 October 2016

Accepted Date: 1 November 2016

Please cite this article as: W. Setyawan, G. Nandipati, R.J. Kurtz, Ab initio study of interstitial cluster interaction with Re, Os, and Ta in W, *Journal of Nuclear Materials* (2016), doi: 10.1016/j.jnucmat.2016.11.002.

Ab Initio Study of Interstitial Cluster Interaction with Re, Os, and Ta in W

W. Setyawan[1,*], G. Nandipati[1], and R. J. Kurtz[1]

[1]*Pacific Northwest National Laboratory, P. O. Box 999, Richland, WA 99352, USA*
[*]*Corresponding author, Tel.: +1(509)3717692; Fax.: +1(509)3753033; E-mail address: wahyu.setyawan@pnnl.gov*

Abstract

The stability of tungsten self-interstitial atom (SIA) clusters is studied using first-principles methods. Clusters from one to seven SIAs are systematically explored from 1264 unique configurations. Finite-size effect of the simulation cell is corrected based on the scaling of formation energy versus inverse volume cell. Furthermore, the accuracy of the calculations is improved by treating the 5p semicore states as valence states. Configurations of the three most stable clusters in each cluster size *n* are presented, which consist of parallel [111] dumbbells. The evolution of these clusters leading to small dislocation loops is discussed. The binding energy of size-*n* clusters is analyzed relative to an $n \rightarrow (n\text{-}1) + 1$ dissociation and is shown to increase with size. Extrapolation for $n > 7$ is presented using a dislocation loop model. In addition, the interaction of these clusters with a substitutional Re, Os, or Ta solute is explored by replacing one of the dumbbells with the solute. Rhenium and Os strongly attract these clusters, but Ta strongly repels. The strongest interaction is found when the solute is located on the periphery of the cluster rather than in the middle. The magnitude of this interaction decreases with cluster size. Empirical fits to describe the trend of the solute binding energy are presented.

Keywords: fusion; tungsten; interstitial cluster; structure; stability; dissociation; solute; binding energy; density functional theory; finite-size scaling; semicore states

1. Introduction

Understanding defect dynamics is fundamental in predicting the evolution of various defect structures in a material. The existence of defects can be beneficial, for instance a dopant in semiconductors, or detrimental, such as solid or gaseous transmutation products in reactor materials. In this research, we focus on the latter case, in particular for tungsten. Current fusion energy system designs utilize tungsten as a plasma-facing material [1-4]. Naturally occurring tungsten is made up of five stable isotopes: ^{180}W (0.1%), ^{182}W (26.3%), ^{183}W (14.3%), ^{184}W (30.7%), and ^{186}W (28.6%). Under fusion neutron irradiation, tungsten undergoes (n, γ) and (n, 2n) transmutation reactions that mainly produce rhenium and osmium isotopes [5, 6]. Neutron absorption in ^{180}W produces traces of Ta through β^+ decay of ^{181}W [5]. Therefore, Re, Os, and to a lesser extent Ta, are the main concerns in regards to the effects of transmutation products on tungsten properties degradation. These solutes will eventually lead to the formation of brittle intermetallic phases that is detrimental to the mechanical properties of tungsten [7, 8].

Transmutation products also influence the nature of atomic displacement damage accumulation during neutron irradiation. Experiments performed in the JOYO reactor found that accumulation