MD Simulations to Evaluate Stable Configurations of Vacancy-type-Defect clusters in Zirconium

*Yilun Hu [1], Kohei Doihara [1], Sho Hayakawa [1], Taira Okita [2], Mitsuhiro Itakura [3]

[1] School of Engineering, the University of Tokyo, [2] Research into Artifacts, Center for Engineering, The University of Tokyo, [3] Center for Computational Science & e-Systems, Japan Atomic Energy Agency

The formation energies of vacancy aggregations containing 19-397 vacancies in zirconium are derived by molecular dynamics simulations to evaluate their stable configuration. In most cases, the formation energy of c-type dislocation loop is lower than that of a vacancy cluster, while the opposite trend is found in the smallest aggregation.

Keywords: fuel cladding, c-component dislocation loop, vacancy cluster, formation energy

1. Introduction

One of the most concerning issues of zirconium alloys, when they are used as the fuel cladding material in light water reactors, is that the amount of the hydrogen absorbed in Zirconium increases significantly after a certain period of irradiation time [1]. The possible reason is considered to be the formation of c-component vacancy dislocation loop, the density of which is also increased after a certain period of time. The present simulation aims at evaluating the formation mechanisms of the loops at the atomic scale.

2. Calculation Method

The MD simulations with lammps code are conducted by using the Mendelev potential [2] or Sheng potential. Initially, a cluster containing 19-397 vacancies is inserted into the cell with X [1,-1,0,0] 30 nm x Y[1,1,-2,0] 30nm x Z[0,0,0,1] 30 nm. A c-type dislocation loop is generated by either of the following relaxation methods; annealing at 600K for 20ps and quench for 20ps, or minimization of the cell. Then, the formation energy is compared between the loop or the cluster at each number of vacancies.

3. Results and Observations

Figure 1 show the morphologies of vacancy aggregations. It is clearly seen that a dislocation loop is formed by collapse of the vacancy aggregation, a process which accompanies the formation of stacking fault. Figure 2 shows the formation energy as a function of the number of vacancies comprised in the aggregation. It is possible to mention that the cluster is more stable for 19-vacancy aggregation, while the loop becomes preferable at the larger size. The results imply that the conversion from a cluster to a loop occurs when the vacancy aggregation becomes a certain size Nv ($19 \leq Nv \leq 37$).

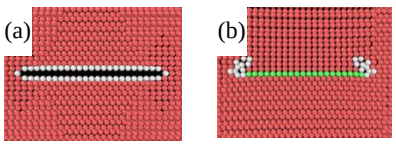

Fig.1 Morphology of (a) vacancy cluster, and (b) c-type dislocation loop

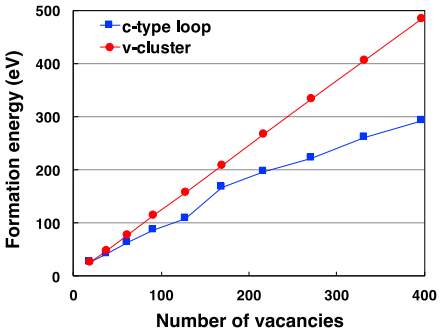

Fig.2 Formation energy as a function of the number of vacancies

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