# Atomistic study to evaluate interactions between helium bubbles and an edge dislocation in iron

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Abstract

We investigated bubbles coalescence through pipe-diffusion along an edge dislocation in iron from atomistic scale. We have observed two typical bubble structures during the coalescence along the $1/2a_0[1\ 1\ 1]$ dislocation even within the MD timescale, the corresponding relative system energy calculated was ranging from -14.6 eV to -4.1 eV.

**Keywords:** Molecular dynamics, blanket, bubbles migration, activation energy

## 1. Introduction

One important mechanism of the hardening of Ferritic/martensitic stainless steels used in nuclear energy facilities is believed to be caused by the nanosized helium bubbles as an obstacle for dislocation movement. When the bubble distance is not short, it is thought that the migration and coalescence are difficult to happen in bulk iron using atomic simulations usually within microsecond or shorter timescale because of the large migration barrier of nanosized bubbles in bulk iron. Therefore, to clarify the hardening mechanism caused by the interactions between helium bubbles and dislocation, the pipe diffusion of helium bubbles along the dislocation was discussed varying the temperature and bubble pressure, and the change in the bubble shape with system energy during bubble coalescence was evaluated.

## 2. Calculation Method

All the simulations in the study were carried out using MD program LAMMPS [1]. In these computations, the Fe-Fe interactions were described using the Embedded Atom Method potential of Ackland [2]. The pair-wise interactions of Fe-He and He-He were described according to the pair potential of Juslin [3] and that of Beck [4], respectively. An edge dislocation with the Burgers vector of $1/2a_0[1\ 1\ 1]$ and the line direction of [1 1 -2] was introduced in the center of the simulation cell, with two identical 4 $a_0$ diameter bubbles along the dislocation at temperature ranging from 100 K to 600 K. Also, when the helium bubbles with an initial distance of about 1.2 nm begin pipe-diffusion along the dislocation and physical contact, their structure was plotted using OVITO software [5] and the corresponding relative system energies were estimated.

## 3. Results

During the pipe diffusion of helium bubbles, there are two typical bubble structures observed. At the beginning of the bubbles physical contact along the z axis, the dumbbell-like structure was formed with a larger amount of helium atoms located at upper and lower side of the coalesced bubble (Figure 1 (a)). With the pipe diffusion of helium atoms in the bubble, more amount of He atoms located at the two sides diffuse into the middle part of the bubble, causing the cylinder-like structure was formed (Figure 1 (b)).

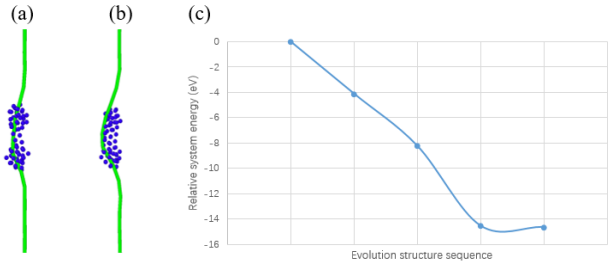


Figure 1 Typical bubble structures along the dislocation (a)-(b) that involve a change in (c) relative system energy ΔE. (a) dumbbell shape with ΔE=-4.1 eV ; (b) cylinder shape ΔE=-8.1 eV.

Figure 1 (c) shows the system energy of possible bubble structures caused by the pipe diffusion of bubble as a result of that the helium atoms inside the two bubbles diffuse to the middle along the dislocation. The cylinder bubble seems to cause a larger decrease in system energy than dumbbell bubble.

**References**

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