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Modeling of helium bubble nucleation and growth in austenitic stainless steels using an Object Kinetic Monte Carlo method

A. De Backer [a,b,*], G. Adjanor [c], C. Domain [c], M.L. Lescoat [c], S. Jublot-Leclerc [d], F. Fortuna [d], A. Gentils [d], C.J. Ortiz [e], A. Souidi [f], C.S. Becquart [a]

[a] UMET, UMR 8207, Université Lille 1, Villeneuve d'Ascq, France
[b] CCFE, Culham Centre for Fusion Energy, Abingdon, Oxon, United Kingdom
[c] EDF R&D, MMC Centre des Renardières, Moret-sur-Loing, France
[d] CSNSM, Univ Paris-Sud, CNRS/IN2P3, Orsay, France
[e] CIEMAT, Laboratorio Nacional de Fusión por Confinamiento Magnético, Madrid, Spain
[f] Université Dr. Tahar Moulay de Saida, Saida, Algeria

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ABSTRACT

Implantation of 10 keV helium in 316L steel thin foils was performed in JANNuS-Orsay facility and modeled using a multiscale approach. Density Functional Theory (DFT) atomistic calculations [1] were used to obtain the properties of He and He-vacancy clusters, and the Binary Collision Approximation based code MARLOWE was applied to determine the damage and He-ion depth profiles as in [2,3]. The processes involved in the homogeneous He bubble nucleation and growth were defined and implemented in the Object Kinetic Monte Carlo code LAKIMOCA [4]. In particular as the He to dpa ratio was high, self-trapping of He clusters and the trap mutation of He-vacancy clusters had to be taken into account. With this multiscale approach, the formation of bubbles was modeled up to nanometer-scale size, where bubbles can be observed by Transmission Electron Microscopy. Their densities and sizes were studied as functions of fluence (up to 5×10^{19} He/m^2) at two temperatures (473 and 723 K) and for different sample thicknesses (25–250 nm). It appears that the damage is not only due to the collision cascades but is also strongly controlled by the He accumulation in pressurized bubbles. Comparison with experimental data is discussed and sensible agreement is achieved.

1. Introduction

In the internal components of the present generation nuclear reactors, helium can be produced due to transmutation reactions. In service conditions, helium production is small. However, real conditions vary widely from in service condition to the different experimental reactors and numerical modeling is necessary to predict the long term evolution of steel microstructure. These models need to be validated using dedicated ion irradiation experiments, leading to non activated samples. The CoIrrHeSim project [5] aims to study three conditions using the dual ion beam in-situ TEM facility JANNuS-Orsay: He beam only, He-damage dual beam and damage only beam. This work reports experimental and modeling results of the He-only implantation of 316L steel thin foils. In these extreme conditions, helium accumulates on microstructure defects and precipitates into bubbles. After a short presentation of some experimental results, the multiscale model is described. Finally, simulation results obtained at 473 K and 723 K are presented and analyzed.

2. Experimental results

In-situ 10 keV He ion implantations were performed on 316L austenitic stainless steel thin foils in the JANNuS-Orsay facility at two elevated temperatures, namely 473 and 723 K, to a fluence of 5×10^{19} m^{-2}. At 473 K, very small bubbles at the limit of detection (<0.8 nm) are observed as revealed by the opposite white/black contrast in under and over focus conditions shown on Fig. 1a (some of the visible bubbles have been circled in red). It is very likely that a high concentration of smaller bubbles have formed in the sample. These small bubbles are either not visible due to detection limits or not distinguishable from an amorphous oxide layer that has formed on top of the specimen and which gives a similar black/white contrast. For these reasons, it was not possible to determine their concentration.

* Corresponding author at: CCFE, Culham Centre for Fusion Energy, Abingdon, Oxon, United Kingdom.
E-mail address: andree.debacker@ccfe.ac.uk (A. De Backer).

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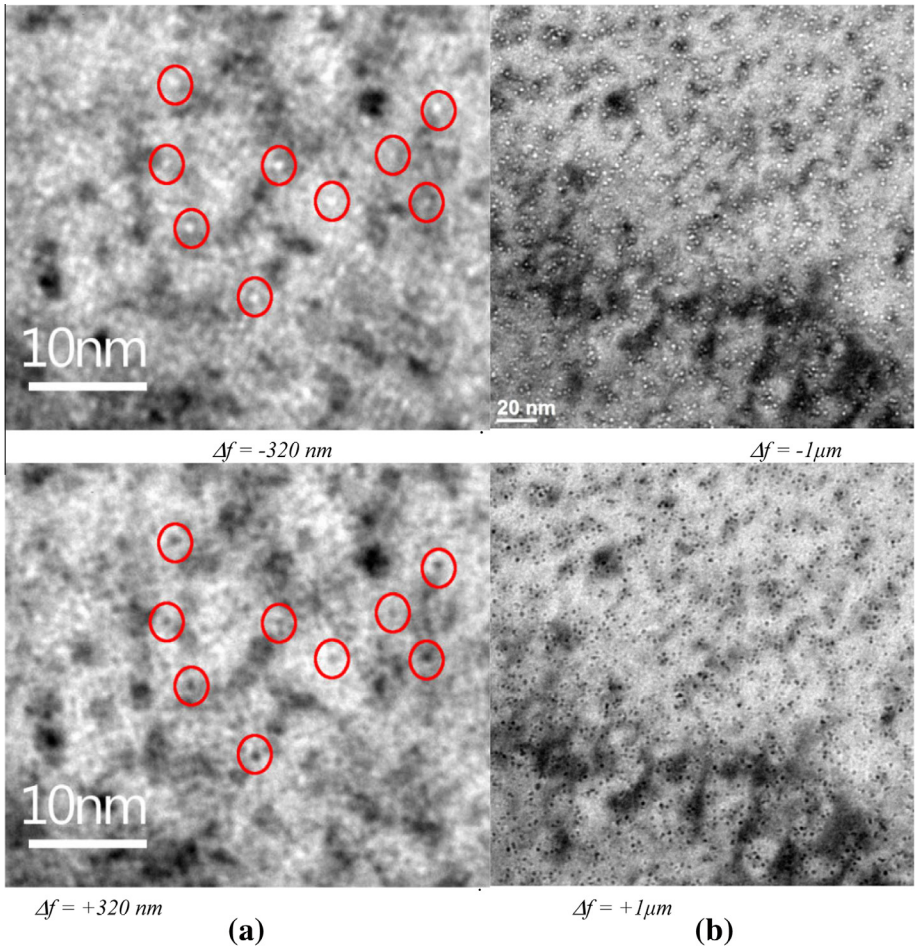

Fig. 1. TEM bright-field images of He bubbles in 10 keV He ion implanted 316L at 473 K; (b) at 723 K. Δf is the value of the defocus used. Bubbles appear white at a negative Δf, and black at a positive Δf.

At 723 K, a large concentration of bubbles is clearly visible (Fig. 1b) and their size ranges from 1.0 to 2.7 nm. Their concentration was estimated to a value between 4.8 and 5.8 $\times$ 10^{23} bubbles/m^3 in a 60 nm thick region. The same range of concentration was obtained in a thicker region (90 nm). At lower thicknesses of the thin foil, lower concentrations were obtained showing a "free surface effect" which was obvious in regions thinner than 40 nm where no bubble was observed. No extended defects such as dislocation loops were observed. From our experimental investigations as well as previous experimental works on the subject [6], we concluded that the higher the implantation temperature, the lower the nucleation but the larger the bubbles.

3. He implantation and He-point defects interaction modeling

For this work, the multiscale approach that we adopted mainly consists in (1) the evaluation of the damage using the MARLOWE code based on the Binary Collision Approximation (BCA), (2) the description of the processes (diffusion, recombination and clustering of defects and helium atoms) implemented in the OKMC model and (3) the development of a parameterization based on Density Functional Theory (DFT) calculations from [1] for the thermally-activated processes taken into account in the OKMC.

3.1. Evaluation of the damage: the displacement cascades

MARLOWE is based on the BCA and makes possible the elimination of unstable created Frenkel (FP) pairs using a critical distance called recombination radius. This method mimics remarkably well the different processes that occur during the thermal spike and replacement sequences and has been applied in BCC iron and W [2]. For this project, 10 keV He cascades in a FeNiCr FCC lattice were calculated. The amount of FP as a function of their separation distance is shown Fig. 2a. It decreases rapidly from 15 to 1 for a recombination radius of 5 lattice units. To determine the recombination radius, the same method used in Fe and W was applied by comparing the damage predicted by MARLOWE to Primary Knock-On Atom (PKA) cascades calculated using Molecular Dynamics (MD) [7]. The MD cascades were obtained with a FeNiCr potential derived in [8] and hardened in the framework of the PERFORM-60 project [9]. A recombination radius equal to $4a_0$ lattice unit was chosen which gives on average 1.2 Frenkel pairs (FP) per 10 keV He.

30,000 MARLOWE cascades were then calculated at 473 and 723 K and post processed using this recombination radius. The comparison with SRIM [10] (using a displacement energy of 40 eV and the "monolayer" option) is illustrated Fig. 2b. Both MARLOWE and SRIM predict similar implantation (~50 nm) and damage (~20 nm) peaks. MARLOWE takes into account the crystal structure and predicts some channeling which causes a deeper penetration of the He atoms. The main difference is the amount of FP per He atom: SRIM predicts 38 FP per He atom while MARLOWE predicts 1.2 FP on average. MARLOWE also gives details on the cascade: 1/3 of them contain only one He atom, 1/3 contains one He and one FP and the last third contains one He and 2–4 FP.