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Cluster dynamics modeling of the effect of high dose irradiation and helium on the microstructure of austenitic stainless steels

Daniel Brimbal [a, *], Lionel Fournier [a], Alain Barbu [b]

[a] AREVA NP, Tour AREVA, 1 Place Jean Millier, 92084 Paris La Défense, France
[b] Alain Barbu Consultant, 6 Avenue Pasteur Martin Luther King, 78230 Le Pecq, France

HIGHLIGHTS

- Irradiation of steels with helium is studied through a new cluster dynamics model.
- There is only a small effect of helium on cavity distributions in PWR conditions.
- An increase in helium production causes an increase in cavity density over 500 °C.
- The role of helium is to stabilize cavities via reduced emission of vacancies.

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ABSTRACT

A mean field cluster dynamics model has been developed in order to study the effect of high dose irradiation and helium on the microstructural evolution of metals. In this model, self-interstitial clusters, stacking-fault tetrahedra and helium-vacancy clusters are taken into account, in a configuration well adapted to austenitic stainless steels. For small helium-vacancy cluster sizes, the densities of each small cluster are calculated. However, for large sizes, only the mean number of helium atoms per cluster size is calculated. This aspect allows us to calculate the evolution of the microstructural features up to high irradiation doses in a few minutes. It is shown that the presence of stacking-fault tetrahedra notably reduces cavity sizes below 400 °C, but they have little influence on the microstructure above this temperature. The binding energies of vacancies to cavities are calculated using a new method essentially based on *ab initio* data. It is shown that helium has little effect on the cavity microstructure at 300 °C. However, at higher temperatures, even small helium production rates such as those typical of sodium-fast-reactors induce a notable increase in cavity density compared to an irradiation without helium.
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1. Introduction

Neutron irradiation of metals produces quantities of point defects far in excess of equilibrium concentrations. At intermediate temperatures, these point defects are mobile and may react with each other and with other elements of the microstructure such as surfaces, grain boundaries, dislocations, and other defect sinks. In the temperature regime which extends from the onset of thermally-induced vacancy emission from vacancy clusters up to temperatures at which large interstitial clusters become thermally unstable, i.e. from about 300 °C to about 700 °C, self-interstitial atoms (SIAs) may agglomerate to form Frank loops while vacancies may form dislocation loops, cavities or stacking-fault tetrahedra (SFT) in austenitic stainless steels. Frank loops with a significant size may annihilate by reaction with each other or with the pre-existing dislocation network which eventually reaches a steady state density.

The accurate prediction of the evolution of all these elements of the microstructure to high dose is of crucial importance for the understanding of the mechanisms controlling irradiation assisted stress corrosion cracking (IASCC), swelling, and irradiation creep in austenitic stainless steels in the context of pressurized water reactors (PWRs) aging and life extension. It is also of particular interest for fast breeder reactor applications.

Today, only mean field models, based on the rate theory, are able to simulate the evolution of materials under irradiation up to high doses. Their main purpose is to describe the evolution of clusters under irradiation. They are all based on the discrete master

* Corresponding author.
E-mail address: Daniel.brimbal@areva.com (D. Brimbal).

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equation [1]:

$$\frac{dC_j}{dt} = \sum_k w(k,j)C_k - \sum_k w(j,k)C_j + G_j - L_j \quad (1)$$

where C_j is the density of clusters of type j (j = SIA clusters, voids, stacking fault tetrahedra, etc.), $w(k,j)$ the rate per unit density of transition of clusters k to clusters of type j. G_j is the production rate of clusters of type j. L_j is the loss of clusters of type j at sinks (dislocations, grain boundaries, etc.).

One approach, intensively used in the past century, is based on the classical nucleation and growth theory developed to describe the phase separation in gases and extended to solid solutions. In this method, the cluster distribution is separated into two parts, (i) the sub-critical nucleus that tends to decrease in size and, (ii) the super-critical nucleus that tends to increase in size. A stationary nucleation rate is calculated by setting all fluxes of clusters in the space of configurations equal to a constant value (the stationary nucleation flux), and assuming the detailed balance approximation for rate coefficients. The growth rate of super-critical clusters is obtained considering the simple classical rate equation [1]. The evolution of the clusters distribution may be obtained using several approaches. The simplest one consists in considering only two quantities: the total number density of super-critical clusters and their mean radius [2]. Several size classes have also been considered in order to obtain a distribution of cluster sizes [3].

The other approach, called cluster dynamics, consists in directly solving the whole set of ordinary differential equations (ODEs). In this approach, nucleation, growth and possibly coarsening don't have to be treated separately. There is no distinction between sub- and super-critical nuclei and there is no need to use the stationary nucleation rate approximation. However, the number of equations becomes rapidly extremely large as soon as the targeted dose increases and large cluster sizes must be taken into account. To overcome this difficulty, the discrete equations are maintained up to cluster sizes large enough so that nucleation and growth are correctly dealt with. For larger sizes, either the master discrete Equation (1) is transformed into a continuous Fokker–Planck type equation, solved numerically with a discretization mesh which increases with cluster size [4,5], or a valuable grouping method is used [6].

To model void swelling of austenitic steels, the generation of helium under irradiation cannot be ignored as it has an important impact on cavity stability [7–11]. Indeed, the densities of cavities of a given size, not only depend on their number of vacancies, but also on the number of helium atoms they contain. Several models have been proposed to address this issue. They are either based on the classical nucleation and growth theory [3,12] or more recently by considering directly the whole set of master equations [5,13]. In the former approach, the difficulty is that there are several nucleation paths in the two dimensional configuration space. The most accomplished model based on the classical nucleation and growth approach was given by Parker and Russell [3]. In the latter approach, the number of equations increases considerably and, up to now, it seems that there are some difficulties to reach high doses using either the Fokker Planck or grouping approximation, especially when substitutional He atoms are mobile. In between these two approaches, a lot of models based on approximations more or less controlled and more or less *ad hoc* were developed. Among them, there are those that consider that the critical nucleus is at equilibrium and contains three helium atoms and some vacancies, the density of which is obtained by solving typically four discrete equations. The evolution of the helium-vacancy clusters containing more than three helium atoms are treated considering only the continuous Fokker–Planck equation [14,15], the first and the second moments of the distribution [16,17] or a kind of grouping method [18,19]. Some other new approaches have been recently proposed. The first one [20] is based on the stochastic simulation algorithm. This method can easily handle clusters with multiple species and also enables the addition of new clusters or new species without the need to rewrite the whole set of equations. However, it cannot yet be used to calculate the evolution of the microstructure under irradiation to 100 dpa for conditions typical of a PWR environment. The second one [21] is based on the classical cluster dynamics ODE approach: the originality of the method is to reduce the number of ODEs by delimiting a reduced formation path for helium-vacancy clusters around the mean He/V ratio that has been determined for small cluster sizes in a preliminary calculation. The later method has been applied to the case of pre-implantation of helium ions at room temperature followed by thermal annealing at high temperature. It remains to be proven that this method can be applied to the case of a continuous irradiation typical of nuclear reactor structural materials.

In this paper a new approach is proposed in order to overcome the difficulty of calculating densities of large cavities in a two dimensional configuration space with a computation time remaining small. Instead of considering that these cavities are characterized by two parameters, they are characterized only by the mean number of helium atoms they contain. The dimension of the configuration space passes from N^2 to 2N. This is justified only if the distribution of helium atoms in cavities is leptokurtic. This kind of approach has already been used [22] but considering the mean number of helium atoms in cavities for all sizes. Unfortunately, using this approximation, it appears that nucleation is not accounted for properly, particularly at high temperatures. In the new model, densities of small cavities depend on both variables (number of vacancies and number of helium atoms), and the mean number of helium atoms in cavities is only used for large cavities. In the next section, this new 2D/1D model is described. In the third section, the model is thoroughly discussed and some examples of calculations with the same set of input parameters as Fournier et al. [23] are presented.

2. Model description

2.1. Basic principles

The objects considered in this model are helium-vacancy clusters in the form of cavities, pure vacancy clusters in the form of SFT, SIA clusters in the form of dislocation loops, the dislocation network and grain boundaries.

Helium is produced in the interstitial position and described by a cluster containing a single helium atom and no vacancy. Substitutional helium atoms are described by a cluster containing a single helium atom and a single vacancy. Helium-vacancy clusters can only emit mono-vacancies containing no helium and mono-interstitial helium atoms.

A schematic description of the model for only helium-vacancy and SIA clusters is shown in Fig. 1. Small helium-vacancy clusters are noted (n_v, p), with p the number of helium atoms and n_v the number of vacancies. For $n_v < N_v^{2D}$ and $p < N_p^{2D}$, their density, noted $C(n_v, p)$, is calculated following a so-called two dimensions (2D) approach.

For large helium-vacancy clusters with $n_v > N_v^{2D}$, their density, $C(n_v)$, as well as $y(n_v)$, the mean number of helium atoms in clusters of size n_v, are calculated, following a so-called one dimension (1D) approach as already described in Ref. [23]. For $n_v > N_v$, the

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