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Integrated modeling of second phase precipitation in cold-worked 316 stainless steels under irradiation

Mahmood Mamivand [a], Ying Yang [b], Jeremy Busby [b], Dane Morgan [a, *]

[a] Department of Materials Science and Engineering, University of Wisconsin-Madison, USA
[b] Materials Science & Technology Division, Oak Ridge National Laboratory, USA

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ABSTRACT

The current work combines the Cluster Dynamics (CD) technique and CALPHAD-based precipitation modeling to address the second phase precipitation in cold-worked (CW) 316 stainless steels (SS) under irradiation at 300–400 °C. CD provides the radiation enhanced diffusion and dislocation evolution as inputs for the precipitation model. The CALPHAD-based precipitation model treats the nucleation, growth and coarsening of precipitation processes based on classical nucleation theory and evolution equations, and simulates the composition, size and size distribution of precipitate phases. We benchmark the model against available experimental data at fast reactor conditions (9.4×10^{-7} dpa/s and 390 °C) and then use the model to predict the phase instability of CW 316 SS under light water reactor (LWR) extended life conditions (7×10^{-8} dpa/s and 275 °C). The model accurately predicts the γ′ (Ni_3Si) precipitation evolution under fast reactor conditions and that the formation of this phase is dominated by radiation enhanced segregation. The model also predicts a carbide volume fraction that agrees well with available experimental data from a PWR reactor but is much higher than the volume fraction observed in fast reactors. We propose that radiation enhanced dissolution and/or carbon depletion at sinks that occurs at high flux could be the main sources of this inconsistency. The integrated model predicts ~1.2% volume fraction for carbide and ~3.0% volume fraction for γ′ for typical CW 316 SS (with 0.054 wt% carbon) under LWR extended life conditions. This work provides valuable insights into the magnitudes and mechanisms of precipitation in irradiated CW 316 SS for nuclear applications.

1. Introduction

Austenitic stainless steels (SS) are major structural materials in a reactor core because of their high strength, corrosion resistance, and formability. In a reactor core, structural materials experience a relatively harsh environment (>250 °C and neutron irradiation), which leads to materials degradation. One form of austenitic SS degradation is precipitation of second phases in the matrix. Precipitation in austenitic SS under irradiation could lead to steel hardening and embrittlement and finally limiting their operation lifetime [1–3].

Precipitation in austenitic SS under irradiation has been subject of several experimental studies especially for temperatures higher than 400 °C [4–8]. It was thought for some years that no significant precipitation may happen in austenitic SS at temperatures lower than 400 °C [5]. However, later experimental observations showed that phases like carbides ($M_{23}C_6$ and M_6C), γ′ (Ni_3Si), and G-phase ($M_6Ni_{16}Si_7$) could form in austenitic SS under irradiation at temperature lower than 400 °C and specifically in the temperature range experienced by todays Light Water Reactor (LWR) core-internal components (275–340 °C) [9–13].

Most of the available experimental data come from irradiated specimens at fast reactors and the precipitation in austenitic SS under LWR conditions is less well studied. The possibility of life limiting effects of precipitates becomes a particular concern under LWR extended life conditions, as there is limited experimental data to address the materials behavior under such low-flux, high-fluence conditions. In the absence of experimental data, modeling techniques can help us to gain insight into materials behavior under LWR extended life conditions.

There are two recent works with an emphasis on thermodynamic and kinetic modeling of austenitic SS precipitates under nuclear power plants conditions. Yang and Busby [14] used the CALPHAD (Calculation of Phase Diagram) approach and developed

* Corresponding author.
E-mail address: ddmorgan@wisc.edu (D. Morgan).

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a thermodynamic database, OCTANT (ORNL Computational Thermodynamics for Applied Nuclear Technology), for austenitic stainless steels with a focus on reliable thermodynamic modeling of precipitate phases in AISI 316. Then they coupled the thermodynamic database with precipitation kinetics simulation (using MatCalc package [15]) to study the thermal aging of 316 SS. They found that by increasing dislocation density, the precipitation kinetics of phases such as $M_{23}C_6$ and Ni_3Si can be greatly enhanced. Shim et al. [16] used the same methodology (CALPHAD database and MatCalc) to study the thermal aging of 316 SS at 400 °C. They also studied the aging behavior of alloys with the addition of radiation induced segregation (RIS) composition to gain insight into radiation induced precipitates (RIP), and demonstrated that RIS can play a critical role in 316 SS precipitates. In both works authors commented on the lack of correct radiation enhanced diffusion (RED) and proper dislocation evolution in their modeling as the key missing information which held them back from more accurate modeling of 316 SS under irradiation. A valid estimation of RED is critical in obtaining correct time scales of precipitation as the diffusion controls many aspects of precipitate growth. Dislocations evolution is also essential to a precipitation model for multiple reasons. First, to develop an accurate RED model a realistic dislocation density is necessary, as it provides a sink density in the defect evolution equations. Furthermore, dislocations will influence the RIS through their impact on overall sink density and their ability to generate RIS near the dislocation core. Finally, dislocations can serve as fast diffusion channels and nucleation sites for precipitates. We seek to integrate RED and dislocation models into precipitate evolution models to gain insight into the mechanisms, time scales, and extent of precipitations in CW 316 SS.

To address the aspects lacking in previous works we developed an integrated model which combines the Cluster Dynamics (CD), precipitation modeling (MatCalc), thermodynamic database (OCTANT), and mobility database (mc_fe_v2.006). We use multiple programs as no one set of codes provides all the necessary modeling tools. The CD code was written by ourselves and tracks the evolution of defects under irradiation and gives us the evolution of single vacancy (and consequently RED) and total dislocation concentrations. The CD predicted RED and dislocation density go into MatCalc as input data. In MatCalc the evolution of the thermodynamic system is based on the framework of the Kampmann–Wagner model [17] which breaks the total time history into small isothermal segments. The nucleation kinetics is based on classical nucleation theory extended for multicomponent systems [18] and the growth is evaluated based on the evolution equations for the radius and composition of the precipitate derived by Svoboda et al. [18] which is based on a mean-field approach utilizing the thermodynamic extremal principle [19,20]. More detail reading about MatCalc can be found in Ref. [21].

For radiation induced phases (RIPs), which occur primarily around dislocation loops, we use a simple model that assumes that RIPs form inside a cylindrical region around the dislocations loops, where this region is assumed to have the appropriate RIS composition. Using the RIS composition to study the RIP is similar to the approach used by Shim et al. [16]. However, in this work, we use a more quantitative cylindrical model to address the RIP (details are given in Section 3.2.4).

2. Methods

2.1. Cluster dynamics: governing equations

Cluster Dynamics (CD) is a computational technique for predicting microstructural evolution and it is frequently applied to precipitation problems or defect cluster evolution in materials under irradiation. In CD, the system is described as a gas of non-interacting clusters. The clusters are defined by a single parameter, their size (or equivalently, the number of atoms they contain).

In CD modeling of defect clusters the principle of the model is to describe a population of defects by their size distribution. The evolution of these populations is obtained through 'chemical kinetics' in a homogeneous medium, where the probability of a cluster of size n to become a cluster of size $n+1$ or $n-1$ depends on its rate of absorption or emission of a vacancy or an interstitial. These kinetics depend on the available population of mobile defects.

The main parts of the CD model developed here are:

- Rate of defect production from irradiation cascade,
- Recombination rate of point defects,
- Absorption and emission rates of point defects by the defect clusters (loops and voids),
- Annihilation kinetics on fixed sinks like grain boundaries,
- Annihilation kinetics on dislocations,
- Frank loops un-faulting,
- Network dislocation evolution.

The model contains a series of coupled ordinary differential equations that capture the evolution of point defects and larger clusters. The solution of these equations is obtained by direct integration of equations using the CVODE solver [22]. Our approach to building this model will be to use existing models and then alter them as needed to yield agreement with known data on loop evolution.

The modeling approach is taken from Refs. [23–29]. The generation of defects from the cascade is taken from Ref. [30] which considers the formation of clusters of size higher than 4 unlikely. The defect generation terms are

$$\begin{aligned} G_{i(v)}(1) &= \eta G_{dpa}\left(1 - f_{i(v)2} - f_{i(v)3} - f_{i(v)4}\right), \\ G_{i(v)}(2) &= \frac{\eta G_{dpa} f_{i(v)2}}{2}, \\ G_{i(v)}(3) &= \frac{\eta G_{dpa} f_{i(v)3}}{3}, \\ G_{i(v)}(4) &= \frac{\eta G_{dpa} f_{i(v)4}}{4}, \\ G_{i(v)}(n>4) &= 0. \end{aligned} \tag{1}$$

G_{dpa} in these equations is the damage rate in the reactor, η is cascade efficiency and $f_{i(v)n}$ is the fraction of clusters on size n and type $i(v)$ surviving the reorganization events following the cascade.

Assuming that only monomer defects are mobile the governing equations for defect evolution would be as follows [23–27].

$$\begin{aligned} \frac{dC_{i(v)}(1)}{dt} =& G_{i(v)}(1) - R_{iv}C_i(1)C_v(1) - \rho D_{i(v)}Z_{i(v)}\left[C_{i(v)}(1) - C^e_{i(v)}\right] \\ & - 6D_{i(v)}\frac{\sqrt{S_m^{i(v)}}}{d_g}\left[C_{i(v)}(1) - C^e_{i(v)}\right] \\ & - \left[\sum_{n=2}\beta_{i(v),i(v)}(n)C_{i(v)}(n) + \sum_{n=2}\beta_{v(i),i(v)}(n)C_{v(i)}(n) \right. \\ & \left. + 4\beta_{i(v),i(v)}(1)C_{i(v)}(1)\right]C_{i(v)}(1) + \sum_{n=3}\alpha_{i(v),i(v)}(n)C_{i(v)}(n) \\ & + 4\alpha_{i(v),i(v)}(2)C_{i(v)}(2) + \beta_{i(v),v(i)}(2)C_{i(v)}(2)C_{v(i)}(1) \end{aligned} \tag{2}$$