Modeling of Niobium and Titanium Carbides precipitates in Cluster Dynamic

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Abstract

The paper is focused on applying Cluster Dynamic to model the precipitation kinetics of niobium and titanium carbides. The simulation was carried on for niobium carbides in austenite and ferrite and titanium carbide in austenite. The results were compared with available experimental data and were analyzed for dependency on initial cluster distribution. The analysis showed that initial distribution does not affect the simulation after a certain point in time. It has also been shown that the case when only monomers present in very dilute alloys has significantly different behavior compare to other cases.

Keywords: Cluster Dynamics, precipitates, titanium carbide, niobium carbide

1. Introduction

The addition of titanium and niobium into steels is widely used in metallurgy due to its beneficial effects on the steel. In solid solution, titanium/niobium combines with carbon and forms carbide precipitates, which are known to limit the formation of chromium carbides and, thereby, prevent intergranular corrosion [1, 2]. Also carbides precipitates increase strength of the alloy at high and low temperatures [2, 3], if present in a steel as a fine dispersion. However, for nuclear grade steels (steels used in nuclear power plans) the titanium and niobium carbides play even more significant role. These precipitates act as point defect recombination centers and as competitive to grain boundaries sinks for helium, thus reduce void swelling and helium embrittlement [3, 4, 5, 6, 7, 8, 9, 10]. Besides, TiC/NbC precipitates stabilize the dislocation network, and as the result enhance creep resistance of the steel [4, 5]. Titanium carbides are especially known for the above effects, which is reflected in the developing of 15-15Ti steel in 1970s [11] for nuclear reactor application. The steel is well known for its high resisting to irradiation swelling and creep and have been chosen as a structural material for several Generation IV nuclear reactors. Therefore, the simulation of titanium/niobium carbides is to be especially important.

To simulate the precipitation behavior of the carbides Cluster Dynamics (CD) was used. CD is an effective method to predict microstructural evolution of a material due to its low computational cost while allowing long term simulation. The drawback of CD is that the distribution of the cluster in space is not considered. The efficiency of the method and its drawback come from the assumption that clusters exist in a mean-field environment.

The paper is organized as follows. In Section 2 a brief description of the CD method is given. In Section 3 we present our simulation results for niobium carbides in austenite and ferrite and titanium carbide in austenite. In Section 4 we also present a comparison of obtained results with available experimental data. In Section 4 a summary of our study is given.
2. Methodology

In the Cluster Dynamics (CD), the evolution of precipitates is governed by Master equations described below. The system of ordinary differential equations (ODEs) Eq. (1-2) assumes that only monomers are mobile. In general, small clusters are mobile too. However, for dilute alloys, such assumption is reasonable [12].

\[
\frac{dC_n}{dt} = \beta_{n-1} C_1 C_{n-1} - (\alpha_n - \beta_n C_1) C_n + \alpha_{n+1} C_{n+1}, \quad n \neq 1, \tag{1}
\]

\[
\frac{dC_1}{dt} = -2\beta_1 C_1 C_1 + \alpha_2 C_2 + \sum_{i=2}^{N_{\text{max}}} [\alpha_i - \beta_i C_1] C_i, \tag{2}
\]

where \( n \) is size of a cluster, \( N_{\text{max}} \) is maximal size of clusters, \( C_n \) is concentration of clusters with size \( n \), \( C_1 \) is concentration of monomers, \( \alpha_n \) is rate of monomer emission from cluster of size \( n \), \( \beta_n \) is rate of monomer absorption by cluster of size \( n \), which are calculated by following equations:

\[
\beta_n = 4\pi r_n D/V_{\text{at}}^m, \tag{3}
\]

\[
\alpha_n = \beta_{n-1} C_{eq} \exp \left[ A \left( \sigma n^{2/3} - \sigma (n-1)^{2/3} \right) \frac{kT}{n} \right], \tag{4}
\]

where \( V_{\text{at}}^m \) is atomic volume of matrix, \( r_n \) is radius of cluster with size \( n \), \( D \) is thermal diffusion coefficient of solute atom in the system, \( A \) is geometrical factor, \( \sigma \) is interfacial energy between precipitate and matrix, \( C_{eq} \) is equilibrium concentration of solute atom in system, \( T \) is temperature in Kelvins, \( k \) is Boltzmann constant. Radius of a cluster with size \( n \) is equal to

\[
r_n = \left( \frac{3nV_{\text{at}}^p}{4\pi} \right)^{1/3}. \tag{5}
\]

Although, CD is an efficient method, it consumes more and more computational power and time with increase of \( N_{\text{max}} \) (\( N_{\text{max}} \gtrsim 100 \)). A traditional method to overcome this obstacle is to transform Master equations into partial differential equation of the Fokker-Planck type:

\[
\frac{\partial C_n}{\partial t} = -\frac{\partial}{\partial n} \left[ (\beta_n C_1 - \alpha_n) C_n \right] + \frac{1}{2} \frac{\partial^2}{\partial n^2} \left[ (\beta_n C_1 + \alpha_n) C_n \right], \tag{6}
\]

The discretization of the Fokker-Planck equation with central difference method change Eq. (6) into the following form:

\[
\frac{dC_{n,j}}{dt} = \frac{C_{n,j-1}}{n_{j+1} - n_{j-1}} \times \left[ (\beta_{n,j-1} C_1 - \alpha_{n,j-1}) + \frac{\beta_{n,j-1} C_1 + \alpha_{n,j-1}}{n_{j} - n_{j-1}} - \frac{C_{n,j}}{n_{j+1} - n_{j-1}} (\beta_{n,j} C_1 + \alpha_{n,j}) \times \left[ \frac{1}{n_{j+1} - n_{j}} + \frac{1}{n_{j} - n_{j-1}} \right] + \frac{C_{n,j+1}}{n_{j+1} - n_{j-1}} \times \left[ -(\beta_{n,j+1} C_1 - \alpha_{n,j+1}) + \frac{\beta_{n,j+1} C_1 + \alpha_{n,j+1}}{n_{j+1} - n_{j}} \right] \right], \tag{7}
\]

where \( n_j \) is defined as follows:

\[
\begin{cases}
  n_j = j, \forall j \leq N_{tr}, \\
  n_j = N_{tr} + \frac{1 - \lambda}{1 - \lambda} (N_{tr} - j), \forall j > N_{tr},
\end{cases} \tag{8}
\]

The above system has a property that with \( n_j = j \), it reduced to initial Master equations. The evolution of monomer concentration is evaluated by the next equation:

\[
\frac{dC_1}{dt} = -2\beta_1 C_1 C_1 + \alpha_2 C_2 + \sum_{j=2}^{N_{tr}} [\alpha_j - \beta_j C_1] C_j + \sum_{j>N_{tr}} [\alpha_j - \beta_j C_1] C_j \frac{n_{j+1} - n_{j-1}}{2}. \tag{9}
\]

This numerical scheme does not strictly conserve the matter, as the Master equations do. Therefore, one must check that losses are small and acceptable. To solve the system of ordinary differential equations (ODEs) the ODEINT solver [13] was used in the study.
Another point that needs a discussion is the diffusion coefficient of the solute atoms in a matrix. In the study, we assume that the diffusion coefficient of titanium/niobium carbide is determined by the diffusion coefficient of the most resistive element. Hence, in the simulation, we have taken diffusion coefficients of Ti and Nb. It was mentioned in [14] and [15], that TiC/NbC precipitation kinetic is strongly affected by dislocation enhancement of the diffusion coefficient because the diffusion of Ti and Nb atom along dislocation is much faster than that in the lattice (such effect named in the literature as pipe diffusion). Effect of dislocations is included in the model (in Eq.3) as modified effective diffusivity [15]:

\[ D_{\text{eff}} = D_{\text{pipe}} \pi R_{\text{core}}^2 \rho + D(1 - \pi R_{\text{core}}^2 \rho), \tag{10} \]

where \( D_{\text{pipe}} \) is the pipe diffusion coefficient, equals to \( D_{\text{dist}} \), \( \alpha_{\text{dist}} \) is dislocation enhance coefficient and defined according to [16], \( R_{\text{core}} \) is the radius of the dislocation core, and \( \rho \) is the dislocation density.

The results of the simulation are time-evolution of mean radius, \( \bar{r} \), volume fraction, \( f_v \), and number density of precipitates, \( N_{\text{tot}} \), which are calculated by the following equations.

- Mean radius

\[ \bar{r} = \left( \frac{3n V_f}{4\pi} \right)^{1/3}, \tag{11} \]

where \( V_f \) is atomic volume of precipitate, and \( n \) is mean size of precipitation clusters find by Eq.12

\[ n = \frac{\sum_{j=0}^{N_{\text{max}}} n_j C_j \Delta n_j}{\sum_{j=0}^{N_{\text{max}}} C_n \Delta n_j}, \tag{12} \]

where \( \Delta n_j = n_j - n_{j-1}, j_{\text{cut}} \) was take such as \( r_{j_{\text{cut}}} = 1 \text{nm} \) for TEM data, because declared resolution limit [17] [18], and \( r_{j_{\text{cut}}} = 0.5 \text{nm} \) for SANS data.

- Volume fraction

\[ f_v = \frac{V_f}{V_{\text{mat}}} \sum_{j=0}^{N_{\text{max}}} n_j C_j \Delta n_j \times 100\%. \tag{13} \]

- Number density

\[ N_{\text{tot}}(t) = \frac{1}{V_{\text{mat}}} \sum_{j=0}^{N_{\text{max}}} C_n(t) \Delta n_j, \tag{14} \]

where \( V_{\text{mat}} \) is atomic volume of matrix.

In the study we have used initial cluster distribution described by the following equations

\[
\begin{align*}
C_1 &= xC_0, \\
C_n &= \frac{(100-x)C_0}{n \sum_{n=1}^{M} \Delta n} & 2 \leq n \leq M \\
C_n &= 0, & n > M
\end{align*}
\tag{15}
\]

where \( C_0 \) is a concentration of the alloying element in steel, \( x \) is a part of the alloying element which exist as monomers, \( M \) is the maximal size of a cluster that assumed to exist in the steel at the moment of \( t = 0 \). In the next section we study the dependence of CD results on initial state of the system.

### 3. Results and Discussion

In this section, we present the results of our CD simulation for NbC and TiC in ferrite and austenite and compare it with available in literature experimental data. The parameters used in the simulations are given in Tables 1 and 2. In Table 1 material parameters for TiC, NbC and iron matrix are presented. Meanwhile, Table 2 gives references to the experimental data and condition in which this data was obtained.

#### 3.1. Niobium Carbide

An interesting point in any simulations is the sensitivity of the model to the initial state of the system. Figures 1–3 show the dependence on initial cluster distribution for time-evolution of precipitates mean radius and number density. The initial cluster distribution for our simulation is described by Eq.15. For better clarity in the figures, we use radius \( r_M \), which corresponds to \( M \) (maximal size of a cluster initially existing in the system), rather than \( M \) itself. We have also used cluster distribution with “shape” differ from Eq.15 such as Poisson-like and step-function. However, the simulation results for those distributions are the same as for Eq.15. Therefore, we can conclude that there is no dependence on the distribution “shape”. Taking into account mentioned above, we present only results with initial distribution described by Eq.15

Figure 1 shows time-evolution of precipitates mean radius and number density for 4 cases, in which concentrations of monomers and other clusters (see Eq.15) was varied, while \( r_M \) was kept the same. On a contrary, Figures 2 and 3 present
Table 1: Material parameters for Titanium and Niobium carbides and Iron matrix

| Parameter | Symbol | Units | Value | Reference |
|-----------|--------|-------|-------|-----------|
| TiC       |        |       |       |           |
| Lattice parameter | $a$ | nm   | 0.433 | [19] |
| Diffusion coefficient | $D^{Ti}$ | $m^2/s$ | $0.15 \cdot 10^{-4} \exp\left[-251000/RT\right]$ | [20] |
| Interfacial energy solubility limit | $\sigma$ | $J/m^2$ | 0.2 | [21] |
| $\gamma_{Fe}$ |        |       |       |           |
| Diffusion coefficient | $D^{Ti}$ | $m^2/s$ | $0.15 \cdot 10^{-4} \exp\left[-251000/RT\right]$ | [20] |
| Interfacial energy solubility limit | $\sigma$ | $J/m^2$ | 2.97 – 6780/T | [22] |
| NbC       |        |       |       |           |
| Lattice parameter | $a$ | nm   | 0.445 | [23] |
| Diffusion coefficient | $D^{Nb}$ | $m^2/s$ | $0.75 \cdot 10^{-4} \exp\left[-264000/RT\right]$ | [24] |
| Interfacial energy solubility limit | $\sigma$ | $J/m^2$ | 2.06 – 6770/T | [25] |
| $\alpha_{Fe}$ |        |       |       |           |
| Diffusion coefficient | $D^{Nb}$ | $m^2/s$ | $1.27 \cdot 10^{-5} \exp\left[-224000/RT\right]$ | [26] |
| Interfacial energy solubility limit | $\sigma$ | $J/m^2$ | 0.5 | [26] |
| $\sigma$ |        |       |       | [22] |
| $\log\left[M C\right]$ |       |       | 2.97 | |
| $\log\left[M C\right]$ |       |       | 1.05 | |
| $\log\left[M C\right]$ |       |       | 0.54 | |
| Matrix    |        |       |       |           |
| Lattice parameter | $a_{\gamma_{Fe}}$ | nm | 0.358 | |
| Lattice parameter | $a_{\alpha_{Fe}}$ | nm | 0.287 | |
| Dislocation enhance coefficient | $\alpha_{disl}(\gamma_{Fe})$ | | 0.643 | |
| Dislocation enhance coefficient | $\alpha_{disl}(\alpha_{Fe})$ | | 0.0133 | |

Table 2: Concentrations and temperatures of datasets

| Reference | Ti/Nb concentration | C concentration | Temperatures | Matrix |
|-----------|---------------------|-----------------|--------------|--------|
| TiC       |                     |                 |              |        |
| [18]      | wt%Ti=0.31          | wt%C=0.1        | T=750 °C     | $\gamma_{Fe}$ |
| [27]      | wt%Ti=0.1           | wt%C=0.05       | T=925 °C     | $\gamma_{Fe}$ |
| [21]      | wt%Ti=0.4           | wt%C=0.07       | T=900 °C     | $\gamma_{Fe}$ |
| NbC       |                     |                 |              |        |
| [17]      | wt%Nb=0.031/0.095   | wt%C=0.1/0.1    | T=900/950 °C | $\gamma_{Fe}$ |
| [28, 26]  | wt%Nb=0.040/0.079   | wt%C=0.058/0.1  | T=600/700/800 °C | $\alpha_{Fe}$ |

As one can see from Figures 1 through 3, initial cluster distribution play role only on small time (with exception of 0.031wt%Nb-steel with monomers and very small clusters). After a time equal to 1000 s, there is no effect of the initial cluster distribution and all simulation results are indistinguishable from each other. The interesting case is 0.031wt%Nb-steel with monomers and very small clusters presented (see Fig.3). We should mention, that such behavior also was observed for other cases (TiC in $\gamma_{Fe}$, NbC in $\alpha_{Fe}$). The possible explanation might be that in such dilute alloy there are not many precipitation centers, as it could be with higher solute concentration, and those few centers have the opportunity to grow faster than in case of higher solute concentration. But the amount of such clusters remains small (see upper Fig.3). However, if we introduce higher clusters into initial distribution, the precipitate kinetic follows its standard pattern.

The comparison of our simulation results with the experimental data for niobium carbide precipitations in austenite [17] are presented in Fig.4. According to [17] for the steel with 0.095wt% of niobium only 73% of Nb existed as monomers, meanwhile, there were only monomers in steel with 0.031wt% of niobium. However, the simulation result with the assumption that only monomers exist in 0.031wt%Nb-steel contradicts to experimental data [17]. Therefore, we assume that in 0.031wt%Nb-steel 90% of niobium exists as monomers and remained 10% is distributed between clusters with $r_M < 1$nm, hence, invisible to TEM.

It should be mentioned, to simulate NbC precipitation in austenite for case described in [17], there was no need in correction for dislocation enhancement of diffusion (Eq.10). The authors did not find dislocation density for the steel used in [17].
However, in the paper [17] the authors mentioned that the steel was well annealed. The dislocation density of such steel is usually in the range of $10^{11} - 10^{12}\text{ m}^{-2}$. The diffusion enhancement effect for such small dislocation density is negligible, that could be observed in the simulations.

For niobium carbide precipitations in ferrite, the simulation results and experimental data are depicted in Fig. 5. As one can see, our model with the set of parameters given in Table 1 matches relatively well the data given in [26, 28] except for volume fraction: our model tends to predict faster clustering of precipitations than observed in the experiments. From Fig. 5 one also could notice that the simulation results have better agreement with...
the experimental data for low temperatures than for high temperatures. The possible explanation of such discrepancy is that at high temperature there is enough energy to activate diffusion of small clusters along with monomers, however, model used in this study assumes that only monomers are mobile.

3.2. Titanium Carbide

The simulation results for TiC precipitates in austenite and experimental data available in the literature are presented in Fig. 6. For cases of experimental data at high temperature (900°C [21] and 925°C [27]), the simulation results follow the same pattern as experimental data, but disagree in time. Therefore, we could suggest that the observed discrepancy might be an effect of the incorrect value of such parameters as diffusion, dislocation density, etc. It should be mentioned, that for these cases no exact dislocation densities were given in [21] and [27], hence for simulation we used dislocation density the same as for case at low temperature from [18]. For low-temperature case (750°C [18]), the pattern of simulation results and the experimental data differ significantly. Such difference cannot be explained by incorrect parameters and might suggest another mechanism that controls the growth of TiC precipitations.

In [18] was mentioned that the pinning of mobile dislocation affects TiC precipitation kinetics in temperature range 650–900°C. However, the
Figure 6: Comparison of simulation results with experimental data for TiC precipitations in austenitic stainless steel. The dots represent experimental data taken from [18, 21, 29].

CD is applied only for the diffusion-controlled growth of precipitations clusters. To overcome this obstacle, the model for the time-evolution of mobile dislocation density should be introduced alongside with the dependency of diffusion on mobile dislocation density. Unfortunately, the authors did not find those properties, therefore, did not simulate the described effect. Note, the data itself is very scarce for TiC precipitations. We think that there is a necessity for more experimental and theoretical work on TiC precipitates.

4. Conclusion

In the present paper, Cluster Dynamic has been applied to model the precipitation kinetics of niobium and titanium carbides. The kinetic of NbC precipitates have been simulated for ferrite and austenite iron matrix. The obtained results are in agreement with experimental data. The simulation results have been analyzed for dependency on initial cluster distribution, where we considered various types of distributions and monomers concentration. The analysis has shown that initial distribution play role only on a small time range. After a certain point in time, all simulations follow the same pattern. The analysis also has shown the “special” behavior of precipitates if only monomers present in very dilute alloys: the fast growth of mean particle diameter, while number density remains small. We have suggested that in dilute alloy fewer precipitation centers are created and they have less competition, that allows those centers to grow faster.

For TiC at high temperature, the simulations and data have the same pattern but disagree in time. Such disagreement might be a consequence of incorrect values of parameters used for modeling. Similar situation was with CD modeling of Cu precipitation in ferrite iron [30]. The copper diffusivity obtained by the authors [30] allows CD simulation has a better agreement with the data. However, we have decided not to adjust parameter’s values but used those found in the literature, as this issue may need more detailed study, that lies out of the scope of this paper. Meanwhile, for TiC at low temperature, the simulation results and the experiment differ significantly, that might be explained by another controlling mechanism than diffusion. Such mechanism could be mobile dislocation and its pining, which was suggested in [18]. The authors, however, have not found a way to incorporate this effect into modeling, therefore, was unable to verify this suggestion. The verification of this suggestion is postponed to further study. The authors believe, that more experimental and theoretical work is needed to correctly model titanium carbide precipitates kinetics.

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