



Irradiation-induced precipitation modelling of ferritic steels

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ABSTRACT

In high strength low alloy (HSLA) steels typically used in reactor pressure vessels (RPV), irradiation-induced microstructure changes affect the performance of the components. One such change is precipitation hardening due to the formation of solute clusters and/or precipitates which form as a result of irradiation-enhanced solute diffusion and thermodynamic stability changes. The other is irradiation-enhanced tempering which is a result of carbide coarsening due to irradiation-enhanced carbon diffusion. Both effects have been studied using a recently developed Monte Carlo based precipitation kinetics simulation technique and modelling results are compared with experimental measurements. Good agreements have been achieved.

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1. Introduction

Several studies exist of the precipitate distribution in pressure vessel steels used for nuclear reactor applications [1–4]. In addition, Buswell [5] completed a comprehensive metallographic study of such materials in 1983. The steels are typically C–Mn steels or MnMoNi steels, but some with a certain amount of unintended copper. The Ni/Cu ratio has been recognised as a critical parameter in controlling the response of the microstructure to neutron irradiation. The experimental observations confirm that there are three major types of precipitate seen in both unirradiated and irradiated materials. These are Fe_3C , Mo_2C , and a strained Cu-rich phase with a basic BCC crystal structure. Mn and Ni also play a role in determining the stability of the Cu-rich phase, where fewer Cu atoms are associated with such cluster phases and the levels of Mn and Ni are raised [2].

In recent years progress in building models of precipitation as a function of time and temperature has been highly successful. The thermodynamic data for determining the relative stabilities of different phases in commercial alloys has become available in digital format through such packages as Thermocalc, Dictra, and MTDATA [6]. The mechanisms for nucleation and growth have become better understood and considerable progress has been made with identifying the mechanisms of heterogeneous nucleation and growth, particularly on grain boundaries. This has allowed the development of iterative computer-based analysis of the kinetics of nucleation and growth of precipitates in a wide range of metallic materials. One such model proposed by Yin and Faulkner [7,8] allows the prediction of precipitate size, volume fraction, and inter-precipitate spacing as a function of both time and tempera-

ture. The separate precipitation sequences at grain boundaries and within the grains also can be considered in the model. This is a very powerful tool because the evolving precipitate size distribution information can be fed directly to continuum damage mechanics models of high temperature mechanical strength and the result is that the precipitation models can be used to predict creep rate at any specified time and temperature. Thus, creep life can be forecast. This provides a very effective tool in assisting alloy design with respect to providing materials with improved creep strength [9,10]. As mentioned earlier, the underlying thermodynamics of the precipitate evolution are provided by powerful software which analyses the stability of all potential phases at the temperature concerned and in the alloy of interest. Small changes in chemical composition can alter the thermodynamic stabilities by considerable amounts, and these factors are accurately taken into account in the thermodynamic assessment. There is also the prospect of feeding the evolving precipitate distribution into hardening models and combining fracture initiator distribution to give fracture toughness distributions.

Previously, phase transformations under irradiation had only been treated in a semi-quantitative fashion [11]. Until this current work was undertaken, no attempts had been made to accurately alter the thermodynamics of phases present as a function of neutron irradiation effects. In principle this should be straightforward, so long as the additional energy input to the system coming from the neutron irradiation is known. The effects of introducing this energy to thermodynamic modelling of ferritic steels have been reported [12]. The main findings were the reversion of approximately 25% of the ferrite to austenite under high dose, fast reaction neutron energy spectrum irradiation conditions ($E > 1$ MeV). These results were confirmed experimentally. However, the characteristics of the remaining ferrite do not differ very much from those without the extra energy input, i.e. without irradiation.

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It is also well known that irradiation generates a high density of vacancies in the material and this results in faster diffusion of solute atoms within the material. This paper shows that the effect of irradiation-enhanced diffusion can be introduced to the precipitation kinetics model and that the model output reflects well the real situation for second phase particles in irradiated steels. Examples of the application of the new method to RPV steels will be given and the effects of the predicted differences in precipitate distribution as a function of Ni/Cu ratio and absolute Ni concentration will be highlighted.

2. Model details

2.1. Precipitation model

The precipitation model without considering irradiation effects has been described in full detail elsewhere [7,8]. However, a brief description is given here below.

The simulation is carried out in a representative body of the material termed the simulation cell, which includes both matrix and grain boundaries. The model considers the formation, growth and coarsening of inter- and intra-granular precipitates separately. Quench induced solute segregation to the grain boundaries is then calculated according to the non-equilibrium segregation model developed by Faulkner to give the solute concentration in grain boundaries of the simulation cell [13]. This contribution depends on the cooling rate employed in any initial heat treatments used to either solution treat or normalise the alloy. The pre-service heat treatment and service (or test) durations at different temperatures are divided into small time intervals Δt . In each step, possible nucleation, growth and dissolution options are considered. Nucleation of precipitates is considered using classical theory and nuclei are generated both on grain boundaries and inside the grains according to the corresponding activation energies for nucleation. The number of nuclei generated in each time step is calculated according to the classical nucleation theory of Russell [14], and the grain boundary precipitates are assumed to be cap-shaped with a contact angle with the precipitate and the grain boundary of 57° , while intra-granular particles are assumed spherical. The activation energy for nucleation, ΔG^* , and the nucleation rate, I , are as follows [14]:

$$\Delta G^* = \frac{16\pi\sigma_{\alpha\theta}^3}{3\Delta G_v^2} K_j \quad (1)$$

$$I = Z\beta^* \left(\frac{N}{x_\theta}\right) \exp\left(-\frac{\Delta G^*}{kT}\right) \exp\left(-\frac{\tau}{t}\right) \quad (2)$$

where $\sigma_{\alpha\theta}$ is the nucleus-matrix interfacial energy, K_j is a shape factor related to the contact angle, equal to unity for a sphere, and ΔG_v is the driving force for the transformation. Z is the Zeldovitch factor, concerned with the rates of change of phase free energy with temperature, β^* is the rate at which solute atoms are added to the nucleus, N is the number of atomic nucleation sites per unit volume, x_θ is the mole fraction of solute atoms in the nucleus, k is Boltzmann's constant, T is the absolute temperature, t is time and τ is the incubation time for nucleation. Usually τ is very small (1–2 s) and so for realistic ageing times the exponential term tends to unity.

The model constructs an array of potential nuclei using a Monte Carlo random sampling algorithm so that a distribution of spatially defined particles are formed and monitored throughout the lifetime of the material at the temperature concerned. Nuclei of critical size are generated and located randomly both inter- and intra-granularly according to the respective activation energies for nucleation. At each time step, the number of nuclei generated, ΔN , is limited by $\Delta N = I\Delta t$, where I is the nucleation rate deter-

mined using Eq. (2). Because the decreasing solute concentration decreases the activation energy for nucleation, ΔG^* , and reduces the supply term, β^* , the nucleation rate approaches zero as the solute saturation level approaches equilibrium.

The generated nuclei are then allowed to either grow or dissolve. The growth or dissolution rate of a particle is determined by the diffusion constants for the slowest moving solute species (called rate controlling elements) and the concentration gradient existing between the matrix solute level and the interface concentration in equilibrium with the precipitate particle and the matrix at the temperature concerned. The volume increase, ΔV , of an intra-granular spherical particle in time interval $t \sim t + \Delta t$ is [7–9,15]

$$\Delta V = D_V S g \frac{\rho_\alpha}{C_\theta \rho_\theta - C_r \rho_\alpha} \Delta t \quad (3a)$$

where $S = 4\pi r^2$ is the surface area of the spherical particle with a radius of r , g the solute concentration gradient at the interface, D_V the volume diffusion coefficient, ρ_θ the density of the precipitate phase, ρ_α the density of the matrix, C_r the solute concentration at the interface and C_θ the solute concentration in the precipitate phase. For grain boundary precipitates, solute atoms can migrate by both grain boundary diffusion and volume diffusion. Therefore, the increase in the volume of a grain boundary particle in time interval $t \sim t + \Delta t$ can be calculated using [15]

$$\Delta V_{GB} = (D_V S_M g_M + D_{GB} S_{GB} g_{GB}) \frac{\rho_\alpha}{C_\theta \rho_\theta - C_r \rho_\alpha} \Delta t \quad (3b)$$

where S_M and S_{GB} are the surface areas of the parts of grain boundary particle within the matrix and inside the grain boundary, respectively and therefore $S_M + S_{GB}$ is the total surface area of the inter-granular particle, D_{GB} is the grain boundary diffusion coefficient, g_M and g_{GB} are solute concentration gradients at the surface of the grain boundary particle from the matrix and along the grain boundary, respectively and are calculated using average inter-particle spacing data, average solute concentration and interfacial solute concentration individually for each particle.

The concentration gradient, g , is determined by [7–9]

$$g = \frac{C_t - C_r}{d} \quad (4)$$

where d is the mean inter-particle spacing and C_t is the mean matrix solute composition at the particular time being considered and is calculated using

$$C_t = C_g - \frac{V_f \rho_\theta N_r}{\rho_\alpha} \quad (5)$$

where V_f is the volume fraction of precipitate, N_r is the number of rate controlling atoms per precipitate molecule (e.g. for Mo_2C , the rate controlling element is Mo and $N_r = 2$), and C_g is the initial matrix grain solute concentration.

The concentration, C_r , is determined by the heats and entropies of formation, the radius of the precipitate, and the Gibbs-Thomson curvature effect, which depends on the radius of curvature of the precipitate [16]

$$C_r = C_\infty \exp\left(\frac{2\sigma_{\alpha\theta} V_\theta}{RT\bar{r}}\right) \quad (6)$$

where $\sigma_{\alpha\theta}$ is the particle-matrix interfacial energy, V_θ is the molar volume of the precipitate phase. C_∞ is the equilibrium solute interface concentration determined from thermodynamic data contained within the MTDATA software [6]. MTDATA is also adapted in this work to take account of irradiation-induced phase instability. The method used is described in [12].

The nucleation/growth (or dissolution) process at each time step is repeated for all time intervals until the required time duration is reached and results containing average particle size, particle

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