

Modelling of Precipitation Kinetics in Ultra High Strength Stainless Steels



Netherlands Institute
for Metals Research

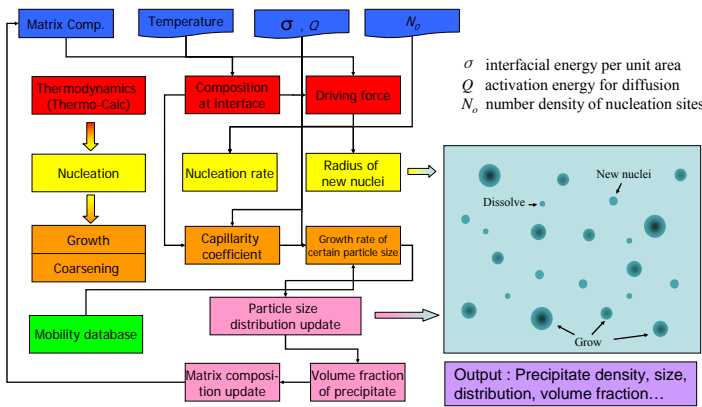


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Fundamentals of Advanced Materials

General strategy

Precipitation strengthened materials derive their mechanical properties from microstructural features such as their particle volume fraction, average radius, average separation and their morphology. The evolution of precipitates is controlled by both thermodynamic and kinetic principles. The modelling of precipitation kinetics typically establishes an artificial boundary separating nucleation, growth and coarsening stages. The model presented here accounts for the concomitant effects of these regimes, in an effort to produce a computing scheme to maximise the properties of precipitation hardened ultra high strength stainless steels through the control of their thermal treatment.



Methodology of the precipitate evolution modelling

Model development

Thermodynamics: Thermo-Calc calculation based on CALPHAD

Nucleation: Classical nucleation theory

$$I = \frac{dN}{dt} = N_0 \frac{kT}{h} \exp\left[-\frac{(\lambda_1 G^* + Q^*)}{kT}\right] \quad r_c = -\frac{2\sigma}{\Delta G}$$

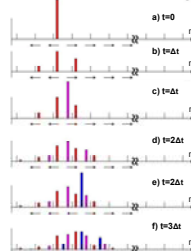
Growth: Growth rate accounting for capillarity effects

$$v(r, t) = \frac{\partial r}{\partial t} = -\frac{2D\sqrt{Dt}(2c^{\gamma}\Gamma - \bar{c}r + c^{\gamma}r)}{r(2c^{\gamma}\Gamma + c^{\gamma}r - c^{\gamma}r)[-2\sqrt{Dt} + \sqrt{\pi}e^{-r^2/4Dt} \operatorname{erfc}(r/2\sqrt{Dt})]}$$

$$\Gamma = \left(\frac{\sigma\gamma}{kT}\right) \left(\frac{1-c^{\gamma}}{c^{\gamma}-c^{\gamma}}\right) \quad D = D_0 \exp(-\lambda_2 Q/RT)$$

Coarsening: KWN numerical model

$$\frac{\partial N}{\partial t} = -\frac{\partial Nv}{\partial r} + I$$



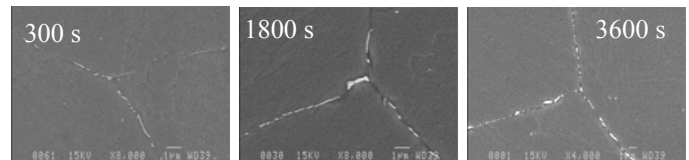
- G^* free energy required to overcome the barrier for nucleation
- λ_1 scaling factor used for G^*
- λ_2 reflects lower energy for diffusion at the grain boundary
- \bar{c} average solute concentration in the matrix
- c^{γ} concentration of the matrix (γ) in equilibrium with precipitate (χ)
- c^{χ} concentration of the precipitate (χ) in equilibrium with matrix (γ)

Application of the model

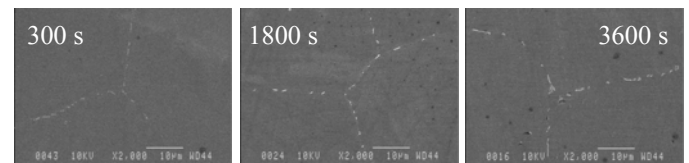
The model is applied to simulate the evolution of Chi (χ) ($\text{Fe}_{36}\text{Cr}_{12}\text{Mo}_{10}$) precipitation in Nanoflex[®] maraging steel.

Specimens were heated to 1100 °C, for 5 and 30 minutes, then cooled down at 50 °C/s to 900 °C and held for different times (120, 300, 900, 1800 and 3600 s) to study the precipitation kinetics, and further cooled down to room temperature at 50 °C/s. The measured average grain size was 40 μm and 120 μm for 5 and 30 minutes solution heat treatment, respectively. SEM images of specimens aged for 300, 1800 and 3600 s are shown below.

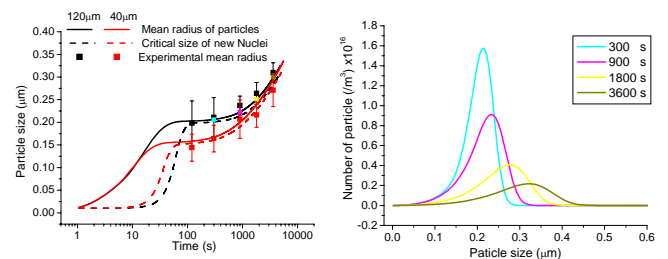
5 minutes solution heat treatment and then tempering



30 minutes solution heat treatment and then tempering

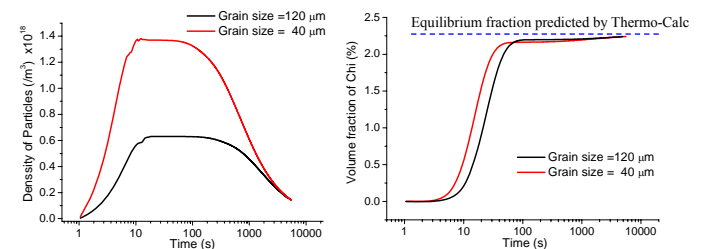


The alloy composition was taken as Fe-12Cr-4Mo-9Ni wt% in the calculation. The number density of nucleation sites was assumed to be 10^{18} and $0.33 \times 10^{18}/\text{m}^3$, following the average grain size of 40 μm and 120 μm . The interfacial energy was assumed to be 0.1 J/m².



Evolution of average particle size, new nuclei size and comparison with experimental data

Particle size distribution of 300, 900, 1800, 3600s of the sample tempering for 30 minutes



Evolution of density of Chi particles

Evolution of volume fraction of Chi phase

For further contact and collaborations please contact us at p.rivera@lr.tudelft.nl



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