Pearlite in multicomponent steels: phenomenological steady-state modeling

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Outline

• Austenite-to-pearlite transformation
  – Assumptions for modeling

• Steady-state growth rate: driving-force–dissipation balance
  – Finite interfacial mobility
  – Constrained carbon equilibrium and “optimal pearlite”
  – Solute drag

• Grain boundary nucleation rate
  – Effect of grain boundary segregation

• Summary
The austenite-to-pearlite transformation and assumptions for modeling

- Cooperative eutectoid transformation
- Continuous lamellar composite in spherical colonies
  - Divorced (degenerate) or rod microstructure not considered
- Constant (steady-state) growth rate and lamellar spacing
  - Divergent pearlite (due to soft impingement) not considered

Fe–2.46C–3.50Mn (at.%) 5h at 625°C (α+θ two-phase region)
C.R. Hutchinson, R.E. Hackenberg, and G.J. Shiflet: Acta Mater., 2004, vol. 52, pp. 3565–85.
Steady-state growth rate: a driving-force–dissipation balance approach

\[
G_m^\gamma - [(1 - f^\theta)G_m^\alpha + f^\theta G_m^\theta] = \frac{2\sigma V_m}{S} + \frac{v}{M^I} + (1 - f^\theta) \sum_{j=1}^{m} \Delta G_{m,j}^{SD} + \frac{v S (f^\theta)}{2} \sum_{i=1}^{n} \left( \frac{u^0_i - u^\theta_i}{M^I_i + \frac{2(k M^{B/\|\delta\|})_i}{S}} \right)
\]

- Driving force \(\Delta G_m\)
- \(\gamma \rightarrow \alpha + \theta\)
- TCFE database

- Driving force depends on \(\alpha\) and \(\theta\) compositions (to be revisited)

This equation defines \(v\) as a function of \(S\)
Comparison to previous modeling approaches

- Previous models all have advantages and simplifications for different model ingredients. In comparison, we have ...
- Simplified capillarity consideration
  - Not considering equilibrium of surface tension at \(\gamma/\alpha/\theta\) trijunction
- Simplified volume diffusion field
  - Not looking for local equilibrium at \(\gamma/\alpha\) or \(\gamma/\theta\) interface
- Added finite interfacial mobility and solute drag
Significance of finite interfacial mobility

• Critical spacing: \( S_c = 2\sigma V_m / \Delta G_m \), where \( \nu = 0 \)

• Can obtain unique \( \nu \) and \( S \) by \( d\nu / dS = 0 \)

• For infinite interfacial mobility, \( S / S_c \rightarrow \cdots \)
  – 2 for volume-diffusion control
  – 1.5 for boundary-diffusion control
  – 1.5~2 for mixed control

• Finite interfacial mobility allows \( S / S_c > 2 \)
  – Previously \( \sigma^{\alpha/\theta} > 1 \text{J/m}^2 \) (too high) for \( S \) to agree with experimental value
  – With finite \( M' \), \( \sigma^{\alpha/\theta} \) can be 0.5J/m\(^2\) (reasonable)
Temperature dependence of interfacial mobility

- Non-Arrhenius temperature dependence of interfacial mobility
  - First discovered in 1976*
  - Parameterized empirically in this work
  - Can possibly be modeled based on ledge mechanism of growth as observed** (future work)

*F. Togashi and T. Nishizawa: J. Japan Inst. Met., 1976, vol. 40, pp. 691–700

**For example, D.S. Zhou and G.J. Shiflet: Metall. Trans. A, 1991, vol. 22A, pp. 1349–65
Constrained Carbon Equilibrium (CCE)

• In alloyed steel, driving force (and then growth rate) depends on the $\theta:\alpha$ partition coefficient(s) $K_i^{\theta/\alpha}$ of substitutional alloying elements
  
  $K_i^{\theta/\alpha}$ from orthoequilibrium (OE):
  orthopearlite, usually at high $T$

  $K_i^{\theta/\alpha} = 1$ (paraequilibrium, PE):
  parapearlite, usually at low temperature

• In general they are two special cases of CCE under an arbitrary $K_i^{\theta/\alpha}$

Fe–0.69C–1.80Mn (wt.%) $T=900K$
“Optimal pearlite”

- Can maximize $\nu$ wrt $S$ and $K_i^{\theta/\alpha}$: “optimal pearlite”
- Can realize a smooth transition from orthopearlite to parapearlite from high-T to low-T

Fe–0.69C–1.80Mn (wt.%) $T=900K$
Dissipation mechanisms

- Interface- and diffusion-mixed control (even for Fe-C)
- Element generating most dissipation by diffusion: M for orthopearlite, C for parapearlite, M→C for optimal pearlite

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Solute drag

• Using Cahn’s model (1962) for simplicity
• Can describe the “bays” on growth curves for Cr- and Mo-containing alloys

Fe–0.6C–1.78Cr (wt.%) Optimal pearlite
GB nucleation rate is modeled and fitted to overall kinetics
  - Time-independent GB nucleation rate is enough to describe overall kinetics
  - Direct measurement of GB nucleation rate is scarce but shows time dependence (not understood physically!)

*J.W. Cahn: Acta Metall., 1956, vol. 4, pp. 449

Fe-0.93C (wt.%)
Grain boundary segregation and nucleation rate

- GB nucleation rate should depend on GB concentration
- GB concentration modeled by equilibrium McLean isotherm

\[ u_i^{GB} = u_i^0 \exp \left( \frac{E_i^{GB}}{RT} \right) \]

- Can describe the dramatically retarded transformation below the nose for Cr-steels
Summary

- Steady-state modeling of pearlite growth and nucleation
  - Suitable for multicomponent steel using CALPHAD databases
- Finite interfacial mobility and solute drag are introduced for growth
- “Optimal pearlite”: Partitioning of substitutional elements in pearlite can be optimized, which realizes an ortho-para transition
- GB nucleation rate (with effect of GB segregation) and overall kinetics are modeled

J.-Y. Yan, J. Ågren, J. Jeppsson, Metall Mater Trans A (2020), accepted

Notes after presentation: Paper published in Vol. 51A pp. 1978-2001
Thermo-Calc implementation

- Pearlite Property Model in Thermo-Calc since Version 2019a

Example
PM_Fe_03

Growth rate

TTT diagram

Including Fe, C, Mn, Cr, Mo, W, Si, Al, Ni, Co