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PHYSICAL METALLURGY AND THERMAL PROCESSING OF STEEL

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Course Outline

1.- Physical Metallurgy of Steel
2.- Phase Transformations in Steel
3.- Solidification of Steel
4.- Heat Treatment of Steel
5.- Welding and Surface Treatment of Steel
6.- Supplementary Reading
1.- Physical Metallurgy of Steel

1.1.- Iron
1.2.- Iron-Carbon Alloys
1.3.- Steels
1.1.- Iron

- Thermodynamic Properties
- Phases
- Crystal Structures
1.2.- Iron-Carbon Alloys

• Crystal Structures
• Phases and Microstructures
• Thermodynamic Properties
• Phase Diagram
1.3.- Steels

- Alloying Elements
- Phase Diagrams
- Thermodynamic Properties
- Structural Effects
- Diffusion
- Real Surfaces
Iron, Iron Alloys and Fe-C system

• Iron
  – Medium of first transition series: $\text{Ar}3d^64s^2$
  – Earth Crust contains $\sim 4\%$ Fe
  – $T_f = 1540 \degree C$ ; $T_h \sim 750 \degree C$
  – Useful Phase Transformations (bcc-fcc)
  – Ferromagnetic below 768 C
Iron, Iron Alloys and Fe-C system (contd)

• **Interstitials:**
  – H, B, C, N, O

• **Substitutionals:**
  – Mostly transition series left, right and below of Fe

• **Fe-C system is the basis of steel metallurgy**
Phases and Phase Diagrams

• Equilibrium Phases
  – Ferrite ($\alpha$: $T < 906$, $\delta$: $1401 < T < 1540 \, ^\circ C$)
  – Austenite ($\gamma$: $906 \, ^\circ C < T < 1401 \, ^\circ C$)
  – Liquid ($l$: $T > 1540 \, ^\circ C$)
  – Carbide, Nitride, Oxide Compounds

• Phase Diagrams
  – Graphic display of stable phases as function of temperature.
Crystalline Structures, Microconstituents and Microstructures

• Equilibrium Crystal Structures
  – Ferrite (Body Centered Cubic; BCC)
  – Austenite (Face Centered Cubic; FCC)
  – Carbides, Nitrides, Oxides (Complex)
Crystalline Structures, Microconstituents and Microstructures (contd)

- **Equilibrium Microconstituents**
  - Ferrite
  - Austenite
  - Pearlite (Ferrite-Carbide Micro-Composite)
Crystalline Structures, Microconstituents and Microstructures (contd)

- Equilibrium Microstructures
  - Ferrite (Grains, Allotriomorphs, Widmanstatten Side-Plates)
  - Austenite (Grains - Twinned)
  - Pearlite (Ferrite-Carbide Colonies)
Crystal Defects

• Vacancies
  \[ N_v = C \exp(-U/kT) \]

• Dislocations
  \( \alpha\text{-Fe} \ (a/2)<111> \)
  \( \gamma\text{-Fe} \ (a/2)<110> \)

• Stacking Faults
  \( \alpha\text{-Fe} \ \text{High SFE} \)
  \( \gamma\text{-Fe} \ \text{Low SFE (Twinning)} \)
Crystal Defects (contd)

• Grain Boundaries
  – Low Angle
  – High Angle
• Interstitial and Substitutional Atoms
• Interphase Interfaces
  – Coherent
  – Semi-coherent
  – Incoherent
Crystal Defects (contd)

- Gibbs-Thompson Equation
  \[ \ln \left( \frac{c(r)}{c} \right) = 2 \sigma \frac{V}{r} R T \]

- Surfaces
  - Crystalline arrangement
  - Surface strain
  - Chemical layering
Multilayer Structure of Real Surfaces

Steel
Decarburized steel
Steel-Oxide transition zone
Wustite layer
Magnetite layer
Haematite layer
Effects of Alloying Elements

- Physico-chemical properties
- Mechanical properties
- Magnetic properties
- Corrosion resistant properties
2.- Phase Transformations in Steel

2.1.- Temperature-Time Charts
2.2.- Mathematical Modeling of Thermal Processing of Steel
2.3.- Phase Transformations during Cooling
2.4.- Phase Transformations during Heating
2.5.- Research Techniques
2.1.- Temperature-time Charts

- Casting and Cooling of Liquid Steel
- Heat Treating
- Thermomechanical Processing
2.2.- Mathematical Modeling of Thermal Processing of Steel

- Diffusion
- Heat Transfer
- Fluid and Solid Mechanics
- Electromagnetism
- Microstructural Evolution
2.3.- Phase Transformations during Cooling

- Solidification
- Pearlite Formation
- Ferrite Formation
- Cementite Formation
- Bainite Formation
- Martensite Formation
2.4.- Phase Transformations during Heating

- Recrystallization
- Austenitization
- Tempering
- Melting
2.5.- Research Techniques

- Metallography
- Microscopy
- Crystallography
- Mechanical Testing
- Thermometry
- Mathematical Modeling
Phase Transformations

• Continuum Rate Equations: Convection, Diffusion of Mass, Energy and Electromagnetic Fields, Kinetics
• Phase Transformation Kinetics
• Additional Microconstituents
• Isothermal and Continuous Cooling Transformation Diagrams
Continuum Rate Equations

• Conservation of Mass (Eqn. of Continuity)
• Conservation of Momentum (Eqn. of Motion)
• Conditions of Compatibility
• Conservation of Energy (Energy Eqn.)
Continuum Rate Equations (contd)

- Conservation of Species (Diffusion Eqn. and/or Convection/Diffusion Eqn.)
- Maxwell’s Equations
- Constitutive Equations
- Boundary Conditions
- Arrhenius Rate Equation

\[ r = A \exp(- \frac{E}{kT}) \]
Phase Transformation Kinetics

• Diffusive Nucleation-Growth Transformations

\[ f = \frac{4}{3} \pi S_o^t I G^3 (t - \tau)^3 \, d\tau \]

\[ f = 1 - \exp(- a t^b) \]

• Displacive Transformations (T < Ms)

\[ f = \max \{1 - \exp(- K_0 [Ms - T])\} \]

• Diffusive-Displacive Transformations
Phase Transformation Kinetics (contd)

- **Grain Growth** (\( d = \text{grain diameter} \))
  \[
  \frac{\delta d}{\delta t} = K_1 \exp\left(-\frac{Q}{kT}\right) d^{(1 - \frac{1}{n})}
  \]

- **Precipitate Growth/Dissolution** (diffusion controlled) (\( r = \text{precipitate radius} \))
  \[
  \frac{\delta r}{\delta t} = \{2 D \sigma V c / r R T\}\{1/r_m - 1/r\} 
  \]
Phase Transformation Kinetics (contd)

• Precipitate Growth/Dissolution (interface controlled)

\[ \frac{\delta r}{\delta t} = \left\{ \frac{2 K_2 \sigma V c}{R T} \right\} \left\{ \frac{1}{r_m} - \frac{1}{r} \right\} \]

• Analytical solution (dilute solution)

\[ r^2 - r_o^2 = 2 a C D t \]

where \( C = \frac{(c_i - c_e)}{(c_p - c_e)} \ll 1 \) and

\[ a = 1 + \frac{r_o}{(\pi D t)^{1/2}} \]

Phase Transformation Kinetics (contd)

• Solute balance at a steady state moving solid-liquid interface

\[- D \left( \frac{\delta c}{\delta x} \right) = V \left( c_L^* - c_S^* \right) = V c_o (1/k - 1) \]

i.e.

\[ c(x) = c_o + c_o (1/k - 1) \exp[- V x/D] \]

• Solid-liquid interface stability condition

\[ G < m G_c = m V (c_L^* - c_S^*)/ D \]
Phase Transformation Kinetics (contd)

- Dendritic growth (primary spacing)
  \[ \lambda_1 = K_3 / V^{1/4} G^{1/2} \]
- Dendritic growth (secondary spacing)
  \[ \lambda_2 = K_4 t_s^{1/3} \]
- Eutectic growth (interlamellar spacing)
  \[ \lambda_e = K_5 V^{1/2} \]
Non-Equilibrium Microconstituents

• Martensite
  – Body Centered Tetragonal; BCT
  – C-supersaturated Ferrite
  – Laths, Plates, Needles

• Bainite
  – BCC-BCT
  – Ferrite-Carbide Micro-Composite
  – Laths, Plates
Isothermal Transformation Diagrams

T

f=0.1

f=0.9

path 1

path 2

path 3
Continuous Cooling Transformation Diagrams

T

f=0.1
f=0.9
path 1
path 2
path 3
Properties of Individual Microconstituents in Steel

- **High-purity Ferrite (single crystal)**
  - Theoretical yield shear stress \( \sim 2000 \text{ MPa} \)
  - Actual yield shear stress \( \sim 10 \text{ MPa} \)

- **High-purity Ferrite (polycrystal)**
  - Theoretical yield shear stress \( \sim 6000 \text{ MPa} \)
  - Actual yield shear stress \( \sim 35 - 300 \text{ MPa} \)
  - Grain size dependence  \( \sigma = \sigma_o + K/d^{1/2} \)
Properties of Individual Microconstituents in Steel (contd)

• Pearlite
  – Yield strength  200 - 800 MPa
  – Tensile strength 600 - 1200 MPa

• Bainite
  – Yield strength  800 - 1300 MPa
  – Tensile strength 1300 - 1400 MPa

• Martensite
  – Yield strength  500 - 1800 MPa
Steel as a Composite Material

- Rule of Mixtures
  \[ \sigma = \sigma_a f_a + \sigma_b f_b \]
- Empirical relations (low C steel)
  \[ \sigma = 15.4 \{ 19.1 + 1.8\ (\%\text{Mn}) + 5.4\ (\%\text{Si}) + 0.25\ (\%\text{pearlite}) + 0.5/d^{1/2} \} \]
Steel as a Composite Material (contd)

• Empirical relations (eutectoid steel)

\[ \sigma = -85.9 + 8.3/d^{1/2} \]

where \( d \) = interlamellar spacing (mm)
Strengthening Mechanisms in Steel

- Solid Solution Strengthening
- Dispersion Hardening
- Dislocation Strengthening
- Grain Boundary Strengthening
Thermal Processing Techniques and Thermometry

• Heating and Cooling
  – Induction and Resistance Heaters
  – High Energy Density Beams
  – Molds
  – Quenching Baths

• Thermometry and Dilatometry
  – Temperature Measurement
  – Volume Measurement
Diffractometry/Quantitative Metallography/Image Analysis

• **Diffractometry**
  – X-Rays
  – Electrons
  – Neutrons

• **Microscopy**
  – Optical
  – Electron
  – Field Ion
Diffractometry/ Quantitative Metallography/Image Analysis (contd)

• **Image Analysis**
  – Image acquisition
  – Digital processing
  – Thresholding operations
  – Mathematical morphology operations
  – Measurements
Mechanical Testing

- Hardness test
- Tensile test
- Creep test
- Fracture test
- Fatigue test
Mathematical Modeling and Computer Simulation

- **Hardware**
  - PC
  - Workstations
  - Supercomputers

- **Software**
  - Custom-made
  - Research
  - Commercial
Reading

• Verhoeven et al, JOM, Sept 1998
• Sundman & Agren, MRS Bull, Apr 1999
3.- Thermal Processing of Liquid Steel

3.1.- Liquid-Solid Transformations

3.2.- Microstructure Formation during Solidification

3.3.- Macrostructure Formation during Solidification

3.4.- Mathematical Modeling of Steel Solidification
3.1.- Liquid-Solid Transformations

- Melting and Solidification of Pure Iron
- Solidification of Liquid Steel to Primary Delta-Ferrite
- Solidification of Liquid Steel to Primary Austenite
- Melting of Alloy Additions in Liquid Steel
3.2.- Microstructure Formation during Solidification

- Nucleation of Crystals
- Dendritic Growth
- The Peritectic Transformation during Steel Solidification
- Microsegregation
3.3.- Macrostructure Formation during Solidification

- Formation and Evolution of the Mushy Zone during Solidification of Steel
- Solute Transport and Settling/Floating of Crystals in the Melt
- Macrosegregation
- Contraction during Solidification
- Stresses from Solidification
3.4.-Mathematical Modeling of Steel Solidification

- Heat Transfer
- Solute Transport
- Microstructural Evolution
- Stress Generation
Reading

• Vanaparthy & Srinivasan, Mod. & Sim. in MSE, Vol. 6, 1998
• Schwerdtfeger at al, Met & Matls Trans B, Oct 1998
4.- Heat Treating of Steel

4.1.- Hardenability
4.2.- Austenitizing
4.3.- Annealing
4.4.- Quenching
4.5.- Tempering
4.6.- Mathematical Modeling
4.1.- Hardenability

- Concept of Hardenability
- Physical Foundation of Hardenability
- Measurement of Hardenability
- Influence of Hardenability on Structure and Properties
4.2.- Austenitizing

- Nucleation and Growth of Austenite during Austenitization
- Dissolution of Carbides during Austenitization
- Austenite Grain Growth during Austenitization
4.3.- Annealing

• Phase Transformations during Isothermal Holding
• Nucleation and Growth of Ferrite
• Nucleation and Growth of Pearlite
• Nucleation and Growth of Cementite
4.4.- Quenching

• Phase Transformations during Continuous Cooling
• Nucleation and Growth of Bainite
• The Martensitic Transformation
• Formation of Composite Microstructures containing Multiple Microconstituents
• Dimensional Changes
4.5.- Tempering

• Precipitation and Growth of Carbides during Heating
• Transformation of Retained Austenite during Heating
• Change of Physical Properties during Tempering
• Dimensional Changes
4.6.- Mathematical Modeling of Heat Treatment of Steel

- Heat Transfer
- Solute Transport
- Microstructure Evolution
- Stress Generation
Reading

• Inoue & Arimoto, J. Matls Eng. & Perf., Feb 1997
• Archambault et al, J. Matls Eng. & Perf., Feb 1997
5.- Welding and Surface Treatment of Steel

5.1.- Welding of Steel
5.2.- Case Hardening of Steel
5.3.- Surface Hardening by Rapid Heating and Cooling
5.1.- Welding of Steel

- Welding Process
- Weld Microstructure and Properties
- Mathematical Modeling
5.2.- Case Hardening of Steel

- Case Hardening Processes
- Solute Diffusion from the Surface of Steel
- Decarburization of Steel on Heating
- Nitriding
- Mathematical Modeling
5.3.- Surface Hardening by Rapid Heating and Cooling

• Diffusion of Time-Varying Electromagnetic Fields into Steel
• Surface Heating by Eddy Currents
• Surface Heating by Focused Beams
• Phase Transformations during Rapid Surface Heating
• Mathematical Modeling
Reading

• Mundra et al, Weld. J. WRS, Apr 1997
• Bhadeshia, 1999
• Fuhrmann & Homberg, 1999