Mécanique Physique des Matériaux

Changements de phase

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Lecture objectives

What this lecture is not

- Detailed presentation about one well defined topic

Patchwork

- Overview of several aspects
- Some energetic concepts
- Different scales
- Semi-empirical approaches
- Numerical approaches
- Experiments
- Applications to additive manufacturing

Only scratch the surface !

Lecture outline

Lecture outline

Forming and fabrication processes

- Selected examples
- Requirements
- Material properties

Selected examples

Variety of processes

- Casting
- Machining
- Forging
- Rolling
- Friction Stir Welding
- Welding
- Additive manufacturing

Selected examples

Casting

Selected examples

Forge

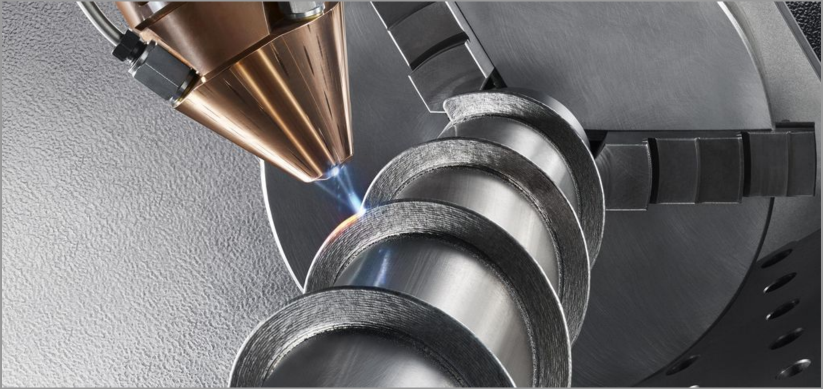
Selected examples
Rolling process

Selected examples

Welding

Selected examples

Additive manufacturing



Forming and fabrication processes

- Selected examples
- Requirements
- Material properties

Requirements

- Geometrical tolerances
- Defects
- Porosity
- Roughness
- ...
- Phase transformations (this lecture)
- Residual stresses (next lecture)

Forming and fabrication processes

- Selected examples
- Requirements
- Material properties

Material properties

Microstructures

- Material properties are not only a matter of chemical composition
- Microstructure plays a critial role
  - Grain size distribution
  - Grain shape (sphericity) distribution
  - Crystal arrangement distribution (fcc,bcc etc. phases)
  - Crystal orientation distribution
  - Crystal disorientation distribution
  - Diffusion of alloying elements
  - Segregation at grain boundary joints
  - ...

Material properties

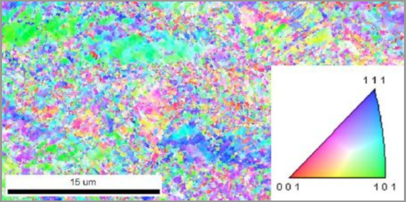
Microstructure vs overall properties

- Anisotropy
- Yield stress
- Hardening behavior
- Hardness
- Ductility
- Toughness
- ...

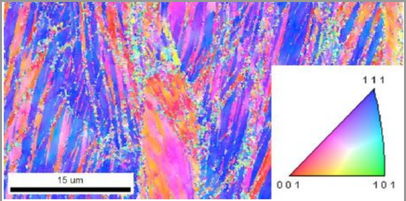
Material properties

Odnobokova et al. 2014

Forging : 316L

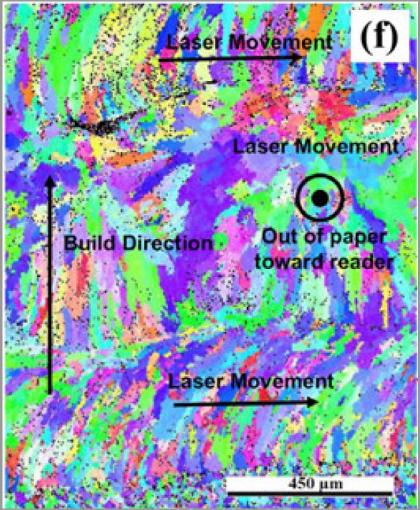


Rolling : 316L



Yadollahi et al. 2015

Additive manufacturing : 316L



Lecture outline

1. Forming and fabrication processes
2. Grain growth during solidification
3. Grain growth during annealing
4. Solid-state phase transitions

Grain growth during solidification

- Basic thermodynamics
- Surface energy
- Growth rate
- Grain morphology

Basic thermodynamics

First law

- E_T : total energy
- C : kinetic energy
- U : internal energy

$$U = E_T - C$$

- Postulate : first thermodynamic law

Production of total energy = 0

- Power brought to the system
  - W_{ext} : Power of external forces
  - Q : Heat (all the rest)
- Hence :

$$\dot{E}_T = \dot{C} + \dot{U} = Q + W_{\text{ext}}$$

Basic thermodynamics

First law

- Principle of virtual power

$$W_{\text{int}} + W_{\text{ext}} = W_{\text{acc}}$$

- After simple calculation

$$\dot{C} = W_{\text{acc}}$$

- Internal energy balance

$$\dot{U} = Q - W_{\text{int}}$$

- $-W_{\text{int}}$ can be seen as a production of internal energy.

Basic thermodynamics

Second law

- S : entropy
  - number of microscopic arrangements
  - same macroscopic state
- Entropy balance
  - Q/T : entropy brought to the system
  - P_S : entropy production

$$\dot{S} = \frac{Q}{T} + P_S$$

- Postulate : second thermodynamic law

Entropy production : $P_S \geq 0$

Basic thermodynamics

Balance

- Internal energy balance

$$\dot{U} = Q - W_{\text{int}}$$

- Entropy balance

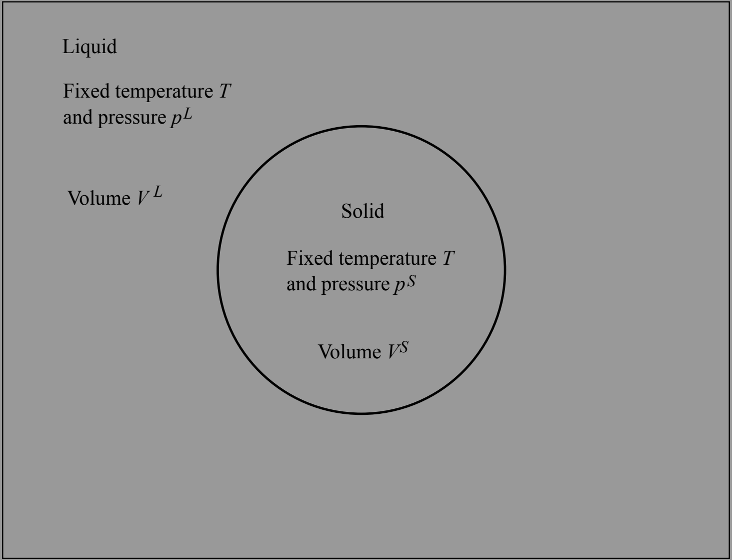
$$T\dot{S} = Q + \underbrace{TP_S}_{D}$$

- Balance equation

$$\boxed{-W_{\text{int}} - (\dot{U} - T\dot{S}) = D \geq 0}$$

Basic thermodynamics

Phase transition liquid/solid



Basic thermodynamics

Internal power

- State variables : p, V, T

$$W_{\text{int}} = -\int_V \underline{\underline{\sigma}} : \underline{\underline{\dot{\varepsilon}}} \mathrm{d}V = -\underline{\underline{\sigma}} : \underline{\underline{\dot{\varepsilon}}}$$

- Hydrostatic loading : $-\underline{\underline{\sigma}} = p\underline{\underline{1}}$
- Volume variation : $\underline{\underline{1}} : \underline{\underline{\dot{\varepsilon}}} = \text{tr}(\underline{\underline{\dot{\varepsilon}}}) = \frac{\dot{V}}{V}$
- Hence :

$$W_{\text{int}} = p\dot{V}$$

Basic thermodynamics

Phase transition liquid/solid

- Internal energy : $U = U^S + U^L$
- Entropy : $S = S^S + S^L$
- Dissipation : $D = D^S + D^L$
- Volume : $V = V^S + V^L$
- Balance equation in solid and liquid

$$\begin{cases} \dot{U}^S - T\dot{S}^S + p^S\dot{V}^S = -D^S \leq 0 \\ \dot{U}^L - T\dot{S}^L + p^L\dot{V}^L = -D^L \leq 0 \end{cases}$$

- Balance equation in the mixture

$$\boxed{\dot{U} - T\dot{S} + p^S\dot{V}^S + p^L\dot{V}^L = -D \leq 0}$$

Basic thermodynamics

Phase transition liquid/solid

- Free energy : $E = U - TS$
- Enthalpy : $H = U + pV$
- Gibbs free energy : $G = H - TS$
  - $G = G^S + G^L$
  - where $G^S = U^S + p^S V^S - TS^S$ and $G^L = U^L + p^S V^L - TS^L$
- Balance equation in the mixture

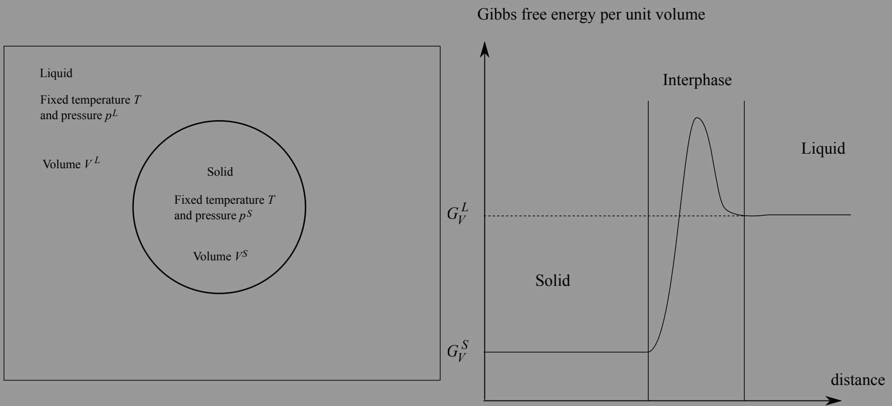
$$\boxed{\dot{G} = -D \leq 0}$$

- G is decreasing during the phase transition
- At the equilibrium G is minimum

$$\boxed{\dot{G} = 0}$$

Basic thermodynamics

Phase transition liquid/solid



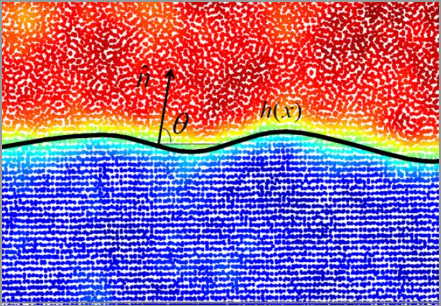
- Driving force : $\Delta G_V = G_V^L - G_V^S$

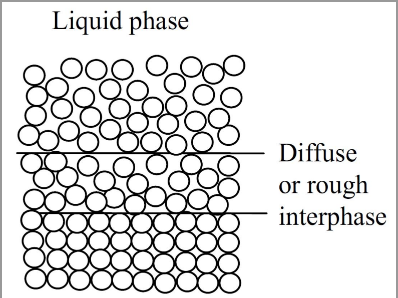
Grain growth during solidification

- Basic thermodynamics
- Surface energy
- Growth rate
- Grain morphology

Surface energy

Asadi et al. 2015

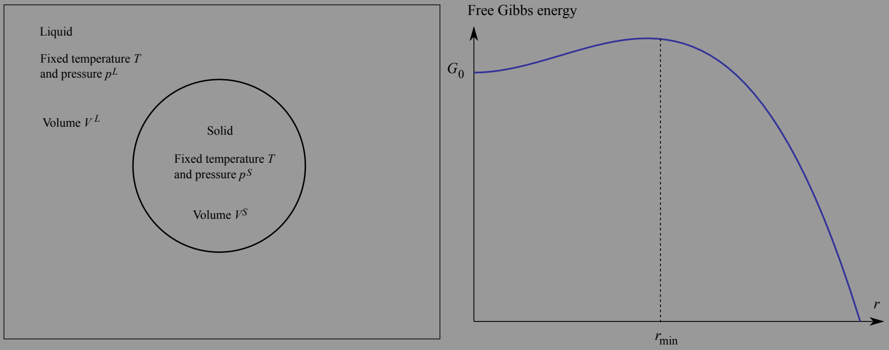




- Inter-phase structure
- Energy per unit area γ

Surface energy

Nucleation size

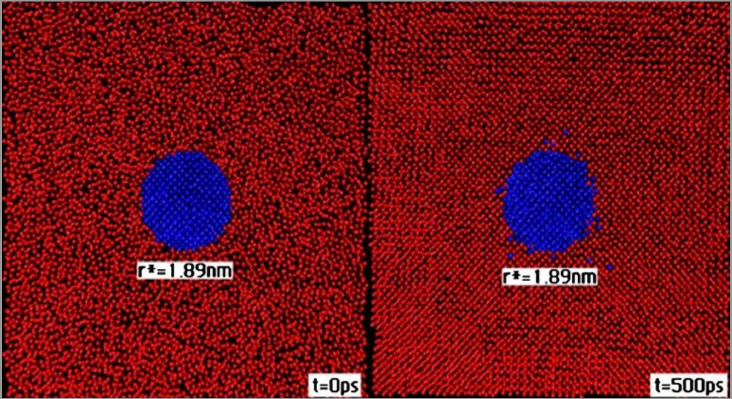


- Free Gibbs energy : $G - G_0 = -\Delta G_V \frac{4\pi}{3} r^3 + 4\pi r^2 \gamma$
- Minimum nucleation size : $r_{\text{min}} = \frac{2\gamma}{\Delta G_V}$

Surface energy

Nucleation size

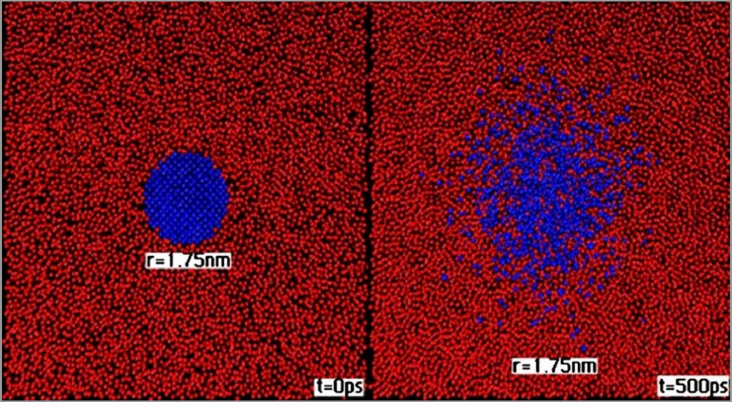
Liu et al. 2013



Surface energy

Nucleation size

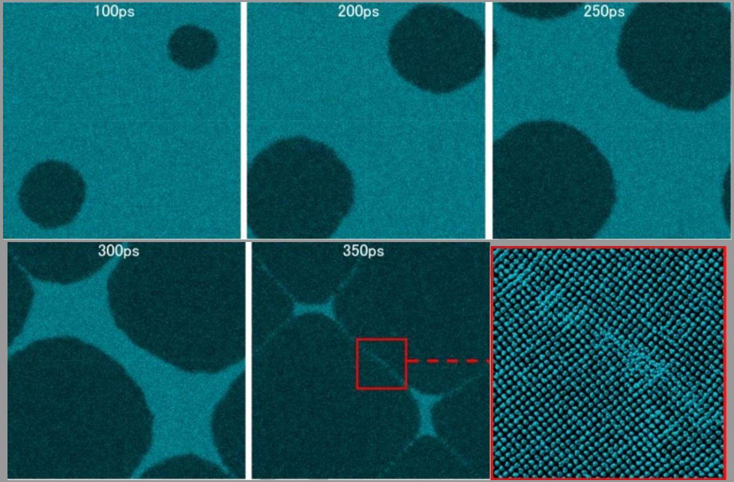
Liu et al. 2013



Surface energy

Polycrystals

Shibuta et al. 2014



Grain growth during solidification

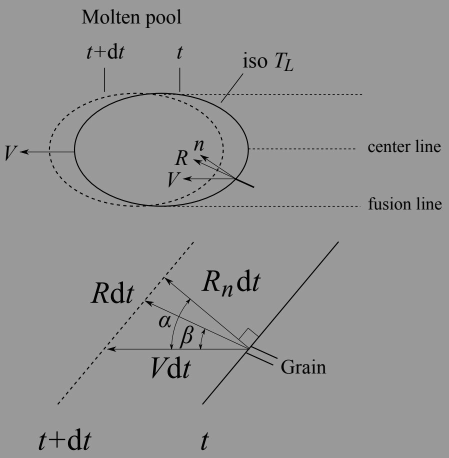
- Basic thermodynamics
- Surface energy
- Growth rate
- Grain morphology

Growth rate

Phenomenological approach

- $\underline{V}$: welding/laser speed
- $V = \|\underline{V}\|$ speed norm
- T : temperature
- $\underline{\nabla T}$: temperature gradient
- $\|\underline{\nabla T}\|$ gradient norm
- $\underline{R}$: growth speed
- $R = \|\underline{R}\|$ growth rate
- α : angle between $\underline{V}$ and $\underline{n}$
- β : angle between $\underline{V}$ and $\underline{R}$

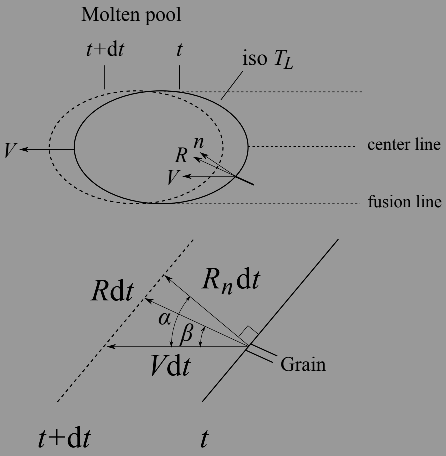
Kou 2003



Growth rate

Phenomenological approach

Kou 2003



- Increment dt

$$V \mathrm{d}t \, \cos(\alpha) = R \mathrm{d}t \, \cos(\alpha - \beta)$$

- Hence

$$R = \frac{V \cos(\alpha)}{\cos(\alpha - \beta)}$$

- Observation

$$\underline{R} \sim \underline{\nabla} T$$

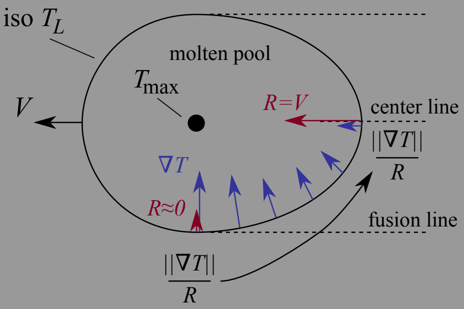
- Hence

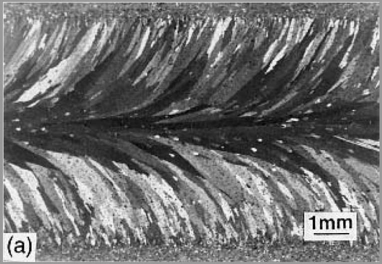
$$\cos(\beta) = \frac{-\frac{\partial T}{\partial x}}{\|\underline{\nabla} T\|}$$

Growth rate

Phenomenological approach

Kou 2003

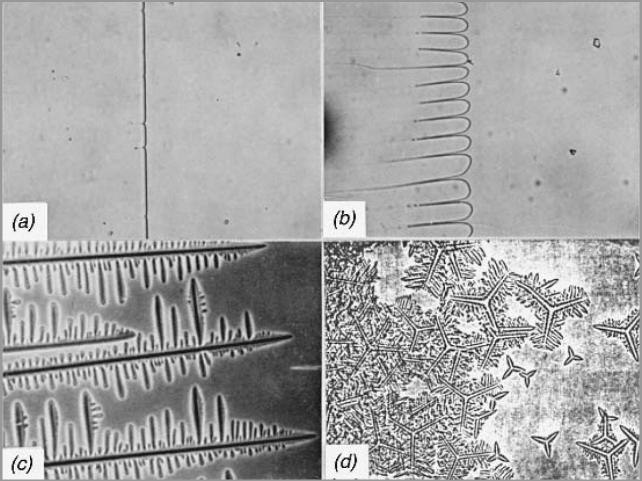




Grain growth during solidification

- Basic thermodynamics
- Surface energy
- Growth rate
- Grain morphology

Grain morphology
Jackson 1971

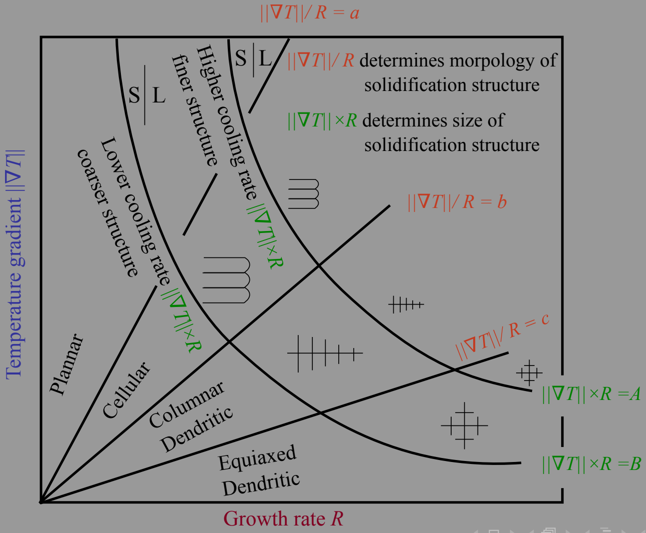


a) Front b) Cellular c) Dendritic d) Equiaxed

Grain morphology

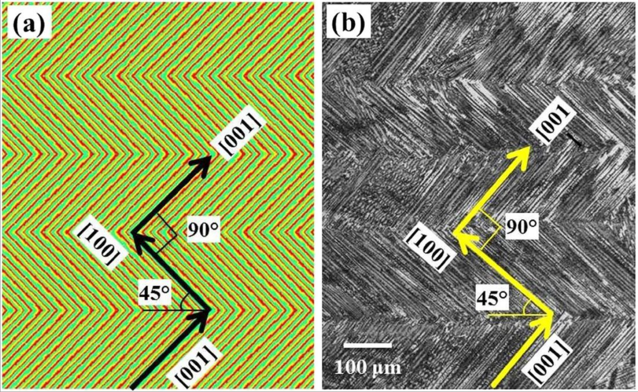
Kou 2003

$||\underline{\nabla} T|| \times R$: cooling rate, $||\underline{\nabla} T|| \;/\; R$: morphology indicator



Grain morphology

Wei et al. 2015



Lecture outline

Grain growth during annealing

- Atomic interactions and energy
- Crystal
- Disorientation energy
- Classic evolution laws
- Classic models
- Energetic approach

Atomic interactions and energy

Inter-atomic potentials

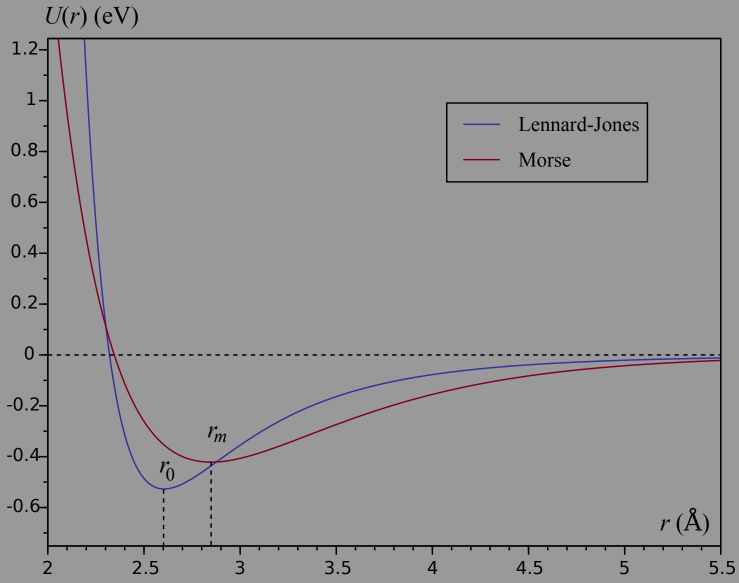
- Simplified physical approach
- Energy as a function of the inter-atomic distance
- Lennard-Jones

$$U(r_{ij}) = \epsilon \left[\left(\frac{r_0}{r_{ij}} \right)^{12} - 2 \left(\frac{r_0}{r_{ij}} \right)^{6} \right]$$

- Morse

$$U(r_{ij}) = D_0 \left[\exp(-2\alpha(r - r_m)) - 2 \exp(-\alpha(r - r_m)) \right]$$

Atomic interactions and energy



Grain growth during annealing

- Atomic interactions and energy
- Crystal
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Crystal

- Total potential energy of N atoms

$$E_{\text{tot}} = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i} U(r_{ij})$$

- Periodic lattice : energy per atom

$$E_{\text{atom}} = \frac{1}{2}\sum_{j\neq 0} U(r_{0j})$$

- Infinite sum => cube of 1 μm^3.
- Crystal lattice : minimum of E_{atom}
- Default stack energy

Grain growth during annealing

- Atomic interactions and energy
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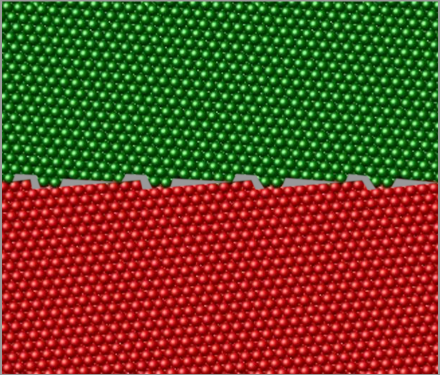
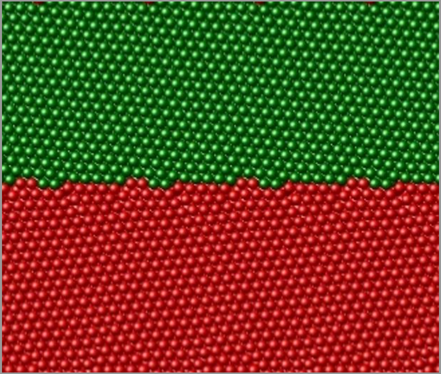
Disorientation energy

Before minimization of E_{atom}



After minimization of E_{atom}



- Additional energy with respect to the default stack energy
- Disorientation energy γ
- Surface energy

Disorientation energy

Classic molecular dynamics

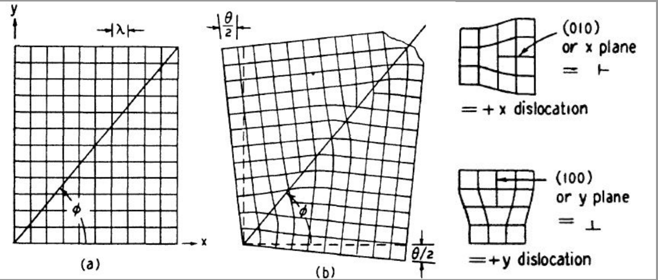
- Dynamic equation
- Energy minimization

Disorientation energy

Simplest model : Read & Shockley (1950)

- Dislocation theory
- Analytic solution
- Assumptions : low disorientation angles,plane, cubic

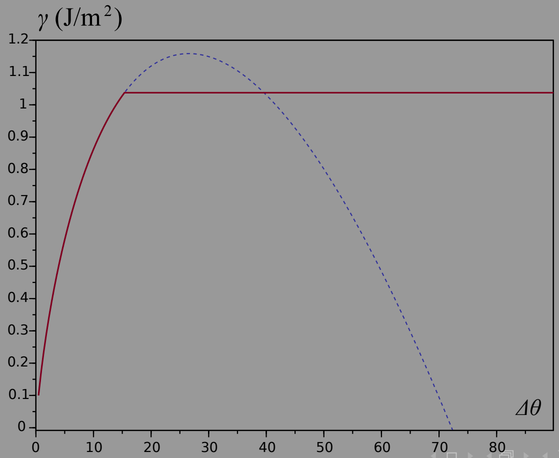
$$\gamma = \gamma_0 \Delta\theta (A - \ln(\Delta\theta))$$



Disorientation energy

Simplest model : Read & Shockley (1950)

- R & S : $0 \leq \Delta\theta \leq 15$
- Constant value $\Delta\theta \geq 15$



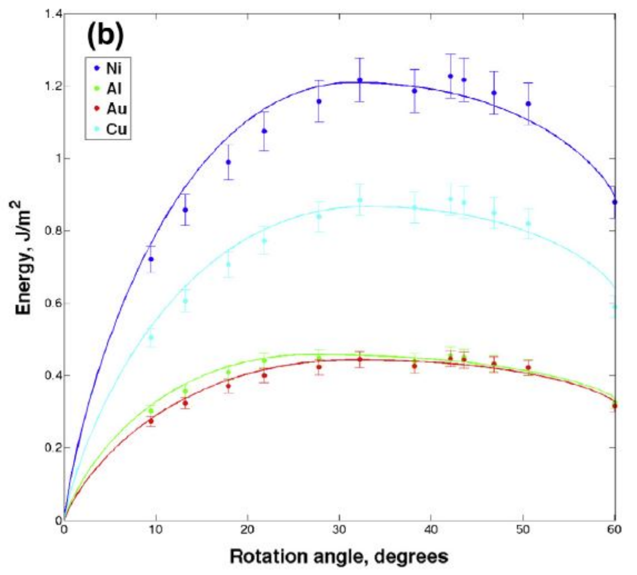
Disorientation energy

Simplest model : Wolf (1989)

- Large disorientation angles
- Phenomenological adaptation of R & S

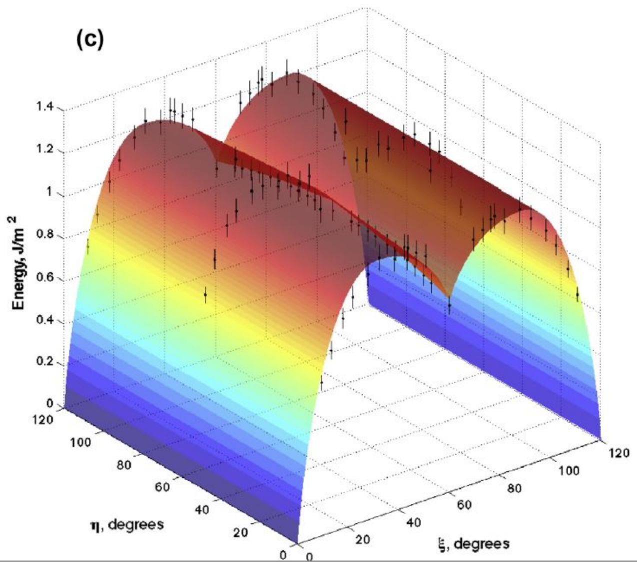
$$\begin{cases} \gamma = \gamma_0 \sin\left(\frac{\pi}{2}\frac{\Delta\theta - \Delta\theta_m}{\Delta\theta_M - \Delta\theta_m}\right)\left[1 - a\ln\left(\sin\left(\frac{\pi}{2}\frac{\Delta\theta - \Delta\theta_m}{\Delta\theta_M - \Delta\theta_m}\right)\right)\right] \\ (\Delta\theta_m \leq \Delta\theta \leq \Delta\theta_M) \end{cases}$$

Disorientation energy
Bulatov et al. 2014



Disorientation energy

Bulatov et al. 2014



Grain growth during annealing

- Atomic interactions and energy
- Crystal
- Disorientation energy
- Classic evolution laws
- Classic models
- Energetic approach

Classic evolution laws

Curvature driven evolution

- Spherical inclusion
- S : grain boundary surface
- E : grain boundary energy $E = S\gamma$
- State variable : volume V
- Viscous evolution law

$$v = -m\frac{\partial E}{\partial V}$$

- v : outward speed of the grain boundary
- $F = -\partial E/\partial V$: driving force
- m : grain boundary mobility $(T, \Delta\theta, \varphi)$

Classic evolution laws

Curvature driven evolution

- Spherical inclusion (radius r)
- $V = \frac{4\pi}{3} r^3$
- $S = 4\pi r^2$
- $E = S\gamma$

$$E = S\gamma = 4\pi r^2 \gamma$$

- Driving force

$$\frac{\partial E}{\partial V} = \frac{\partial r}{\partial V}\frac{\partial E}{\partial r} = \frac{8\pi r\gamma}{\frac{\partial V}{\partial r}} = \frac{2\gamma}{r}$$

- Evolution law

$$v = -m\frac{2\gamma}{r}$$

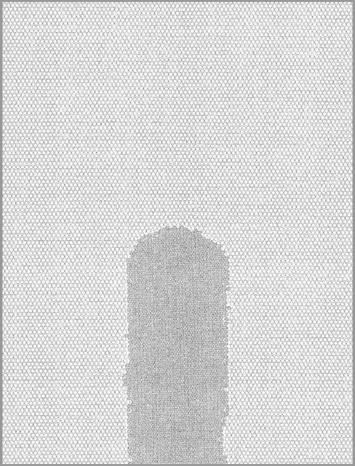
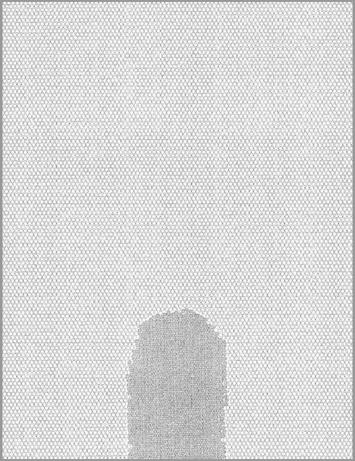
- Extension

$$v = -m\gamma\left(\frac{1}{r_I} + \frac{1}{r_{II}}\right)$$

Classic evolution laws

Curvature driven evolution

Upmanyu et al. 1999

Grain growth during annealing

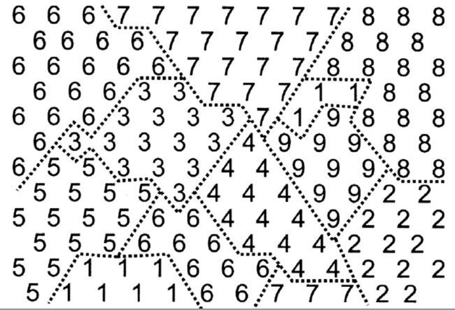
Classic models

- Potts models
- Moving Finite Element
- Level Set function
- Phase field
- Molecular dynamics

Classic models

Potts models : Monte Carlo based

- Image based method : pixels
- Each pixel has attributes
  - Crystal orientation
  - Stored energy
  - ...
- Pixels of same orientation share the same ID



Classic models

Potts models : Monte Carlo based

- Grain boundary energy
  - Grain boundaries are implicit
  - Interaction energy E_I between pairs (e.g., $6/7, 7/8$)
  - Range of interaction : first, second, third nearest neighboring pixels
- Bulk energy H (e.g., stored energy of deformation)
- Total energy

$$E_{\text{tot}} = \frac{1}{2} \sum_{i=1}^{N_{\text{pix}}} \sum_{j=1}^{N_{\text{nei}}} E_I(s_i, \widetilde{s}_j^i) + \sum_{i=1}^{N_{\text{pix}}} H(s_i)$$

- N_{pix} : total number of pixels
- N_{nei} : number of considered neighbors
- s_i : ID of pixel i
- $\widetilde{s}_j^i$: ID of the j-th neighboring pixel of i

Classic models

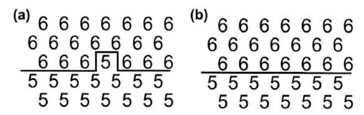
Potts models : Monte Carlo based

- Evolution : mimic

$$v = -m\frac{\partial E}{\partial V} = -m\frac{2\gamma}{r}$$

- Random substitution of pixels ID
- Acceptance probability

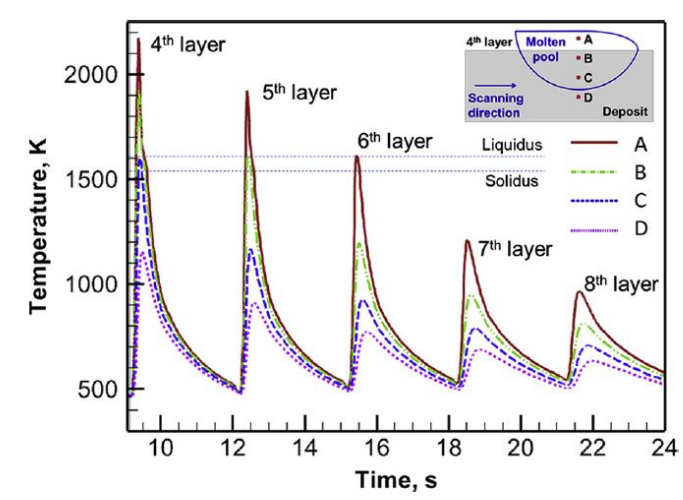
$$P = \begin{cases} \dfrac{E_I(s_i, \widetilde{s}_j^i)}{\max(E_I)} \dfrac{m(s_i, \widetilde{s}_j^i)}{\max(m)} & \Delta E_{\text{tot}} \leq 0 \\ \dfrac{E_I(s_i, \widetilde{s}_j^i)}{\max(E_I)} \dfrac{m(s_i, \widetilde{s}_j^i)}{\max(m)} \exp\left(-\dfrac{\Delta E_{\text{tot}}}{\max(E_I)\, k\, T}\right) & \Delta E_{\text{tot}} > 0 \end{cases}$$



Classic models

Application to additive manufacturing

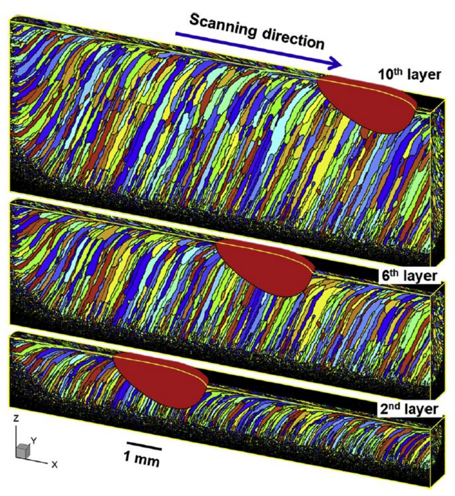
Wei et al. 2019



Classic models

Application to additive manufacturing

Wei et al. 2019



Grain growth during annealing

- Atomic interactions and energy
- Crystal
- Disorientation energy
- Classic evolution laws
- Classic models
- Energetic approach

Energetic approach

Most common approach

- Describe the energy
  - Surface energy
  - Default stack energy
- Define state variables and driving forces
- Postulate the evolution law

$$v = -m\frac{\partial E}{\partial V}$$

- Dissipated power

$$D = -v\,\frac{\partial E}{\partial V} \geq 0$$

Energetic approach

Dissipative mechanism

- Describe the energy
  - Surface energy
  - Default stack energy
- Define state variables and driving forces
- Find a physical resistive mechanism
  - Crystal plasticity
  - Dissipated power within any virtual motion
- Infer the evolution law
- Balance equation for all possible evolutions

$$\boxed{\underline{\underline{\sigma}} : \underline{\underline{d}} - \rho \left(\dot{\Psi} + \dot{T} s \right) - \frac{\underline{q}.\underline{\nabla T}}{T} = D}$$

- Automatically verifies thermodynamic laws

Energetic approach

Simple example for grain growth

- Grain boundary energy (Wolf)

$$\begin{cases} \gamma(\Delta\theta) = \gamma_{\frac{\pi}{6}} \sin\left(3\Delta\theta\right)\left[1 - a_1 \ln\left(\sin\left(3\Delta\theta\right)\right)\right] \\ \left(0 \leq \Delta\theta \leq \dfrac{\pi}{6}\right) \\ \gamma(\Delta\theta) = \gamma_{\frac{\pi}{6}} \sin\left(\pi - 3\Delta\theta\right)\left[1 - a_2 \ln\left(\sin\left(\pi - 3\Delta\theta\right)\right)\right] \\ \left(\dfrac{\pi}{6} \leq \Delta\theta \leq \dfrac{\pi}{3}\right) \end{cases}$$

- Dissipation by crystal plasticity

$$D(T, \Delta\theta, v^*) = \frac{X(\Delta\theta)}{m}\left[v^*\right]^2$$

$$X(\Delta\theta) = \frac{6}{\pi}\left(\frac{\pi}{3} + 2\sqrt{3}\ln\left(\frac{\sqrt{3}}{2}\right)\right) \min\left\{\Delta\theta, \frac{\pi}{3} - \Delta\theta\right\}$$

Energetic approach

Lecture outline

Solid-state phase transitions

- Example
- Multiscale problem
- Evolution law
- Carbon diffusion
- Macroscopic model
- Application to additive manufacturing

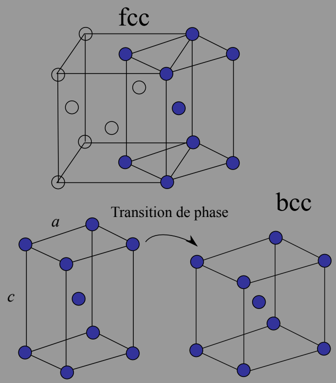
Example

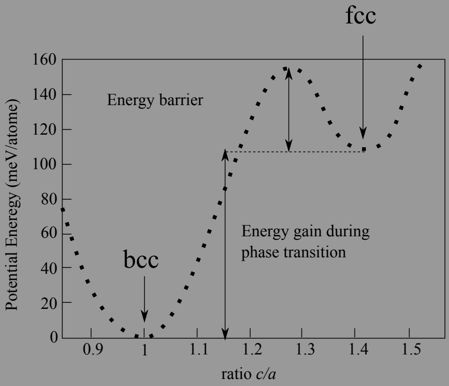
Solid-state phase transitions

Multiscale problem

Atomic scale

Muller et al. 2004

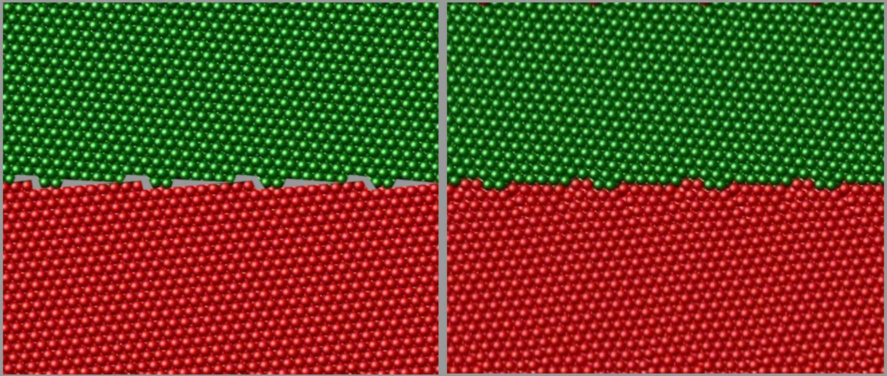




- Energy per unit volume : E_{phase}

Multiscale problem

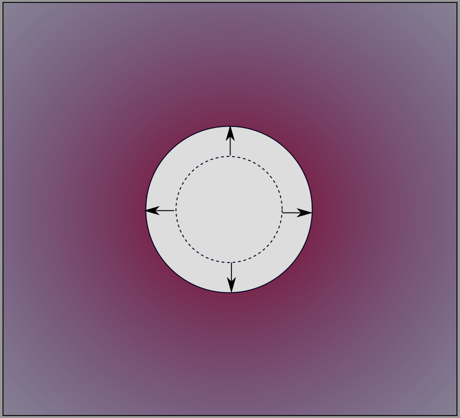
Microscopic scale



- Energy per unit area : γ

Multiscale problem

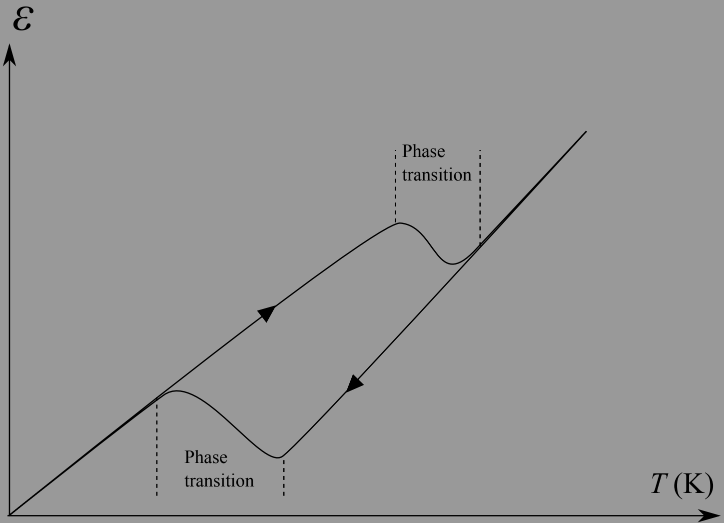
Mesoscopic scale



- Stored elastic energy E_e

Multiscale problem

Macroscopic scale



Solid-state phase transitions

- Example
- Multiscale problem
- Evolution law
- Carbon diffusion
- Macroscopic model
- Application to additive manufacturing

Evolution law

Mesoscopic evolution

- Define a microstructure
- Define nucleation points (defects)
- Define state variables $\underline{\phi} = (\phi_1, \cdots, \phi_n)$
  - Volume of each phase
  - Phase field
  - $\cdots$
- Define the total energy $E_{\text{tot}} = \int_V E_{\text{phase}} \mathrm{d}V + \int_S \gamma \mathrm{d}S + E_e$
- Define a simple evolution law

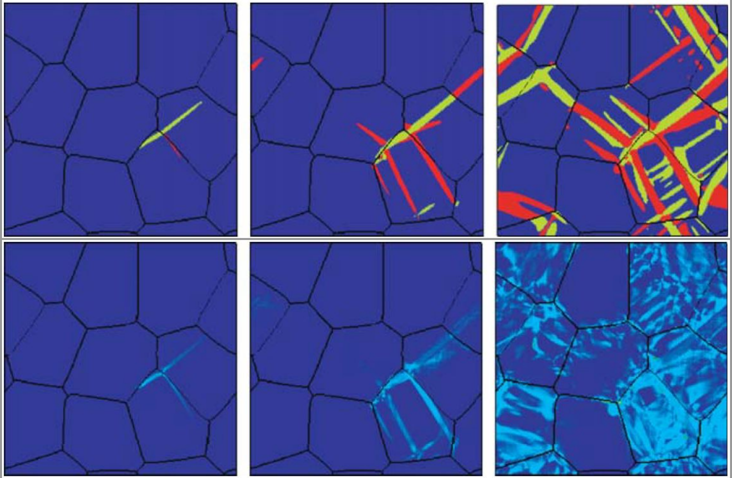
$$\dot{\underline{\phi}} = -\underline{\underline{M}}.\frac{\partial E_{\text{tot}}}{\partial \underline{\phi}}$$

- Find a numerical approach to compute this problem
  - Phase field
  - $\cdots$

Evolution law

Mesoscopic phase field model

Yamanaka et al. 2010



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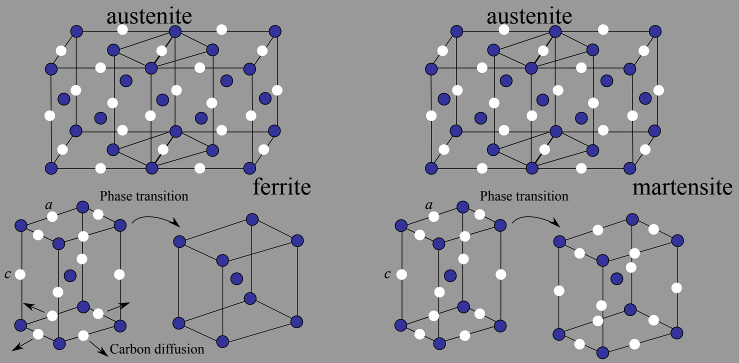
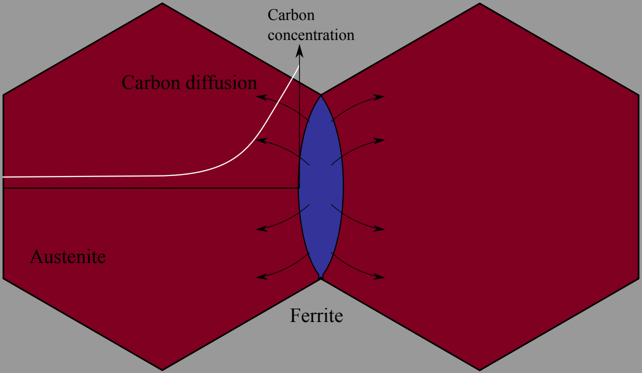
Carbon diffusion



- Austenite fcc
- Ferrite bcc
- Martensite : deformed bcc with carbon
- Carbide precipitates : F_3C

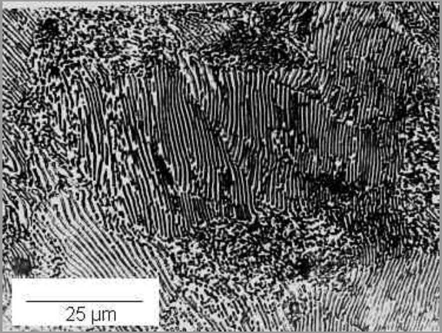
Carbon diffusion



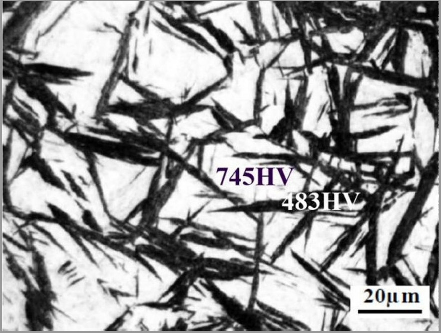
- Good carbon solubility in austenite
- Carbon almost not soluble in ferrite
- Precipitation Fe_3C
- Various patterns : Pearlite, Bainite

Carbon diffusion

Lamellar pearlite



Lower bainite



The list is long like cryptozoology

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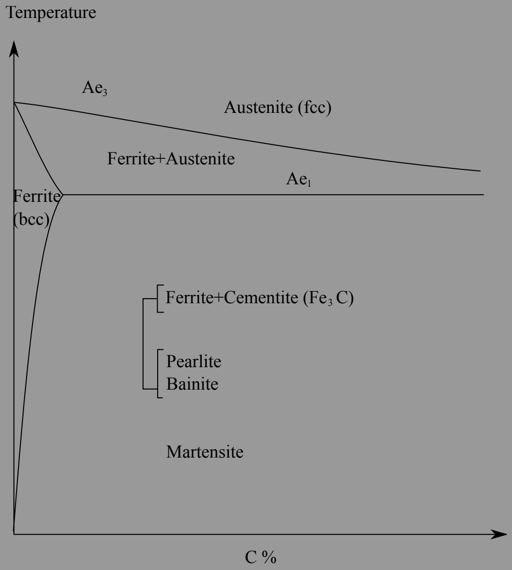
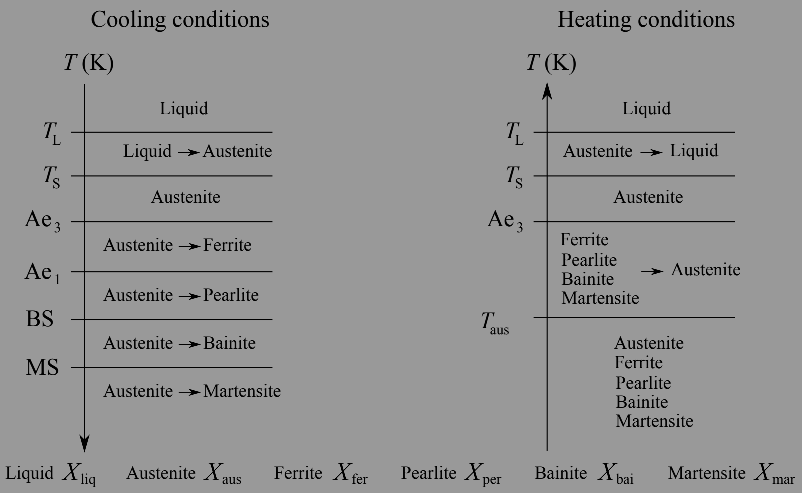
Macroscopic model

Phase diagram : equilibrium



Macroscopic model



Macroscopic model

Diffusive phase transitions

- Depends on temperature rate
- Avrami equation

$$\Delta X_\phi = X_{\text{aus}} \left[1 - \exp\left(-k_\phi \left(t - t_\phi \right)^{n_\phi} \right) \right]$$

- ϕ =fer, per, bai or aus
- k_ϕ and n_ϕ to be identified experimentally for each grade

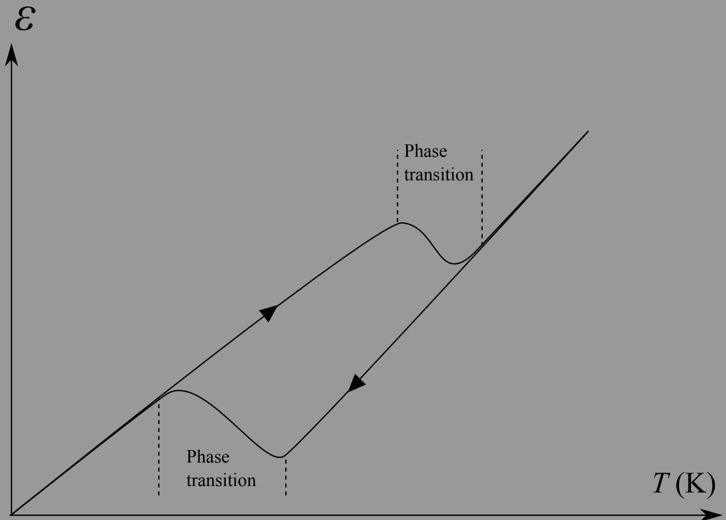
Martensite

- High cooling rates
- Koistinen-Marburger equation

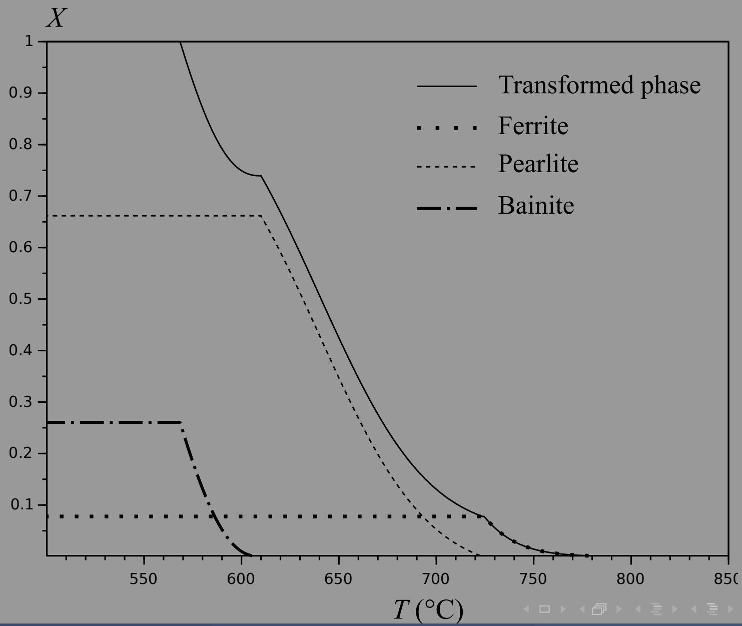
$$\Delta X_{\text{mar}} = X_{\text{aus}} \left[1 - \exp\left(\alpha_{\text{MS}} \left(T - \text{MS} \right) \right) \right]$$

Macroscopic model

Experimental identification : dilatometric test



Macroscopic model



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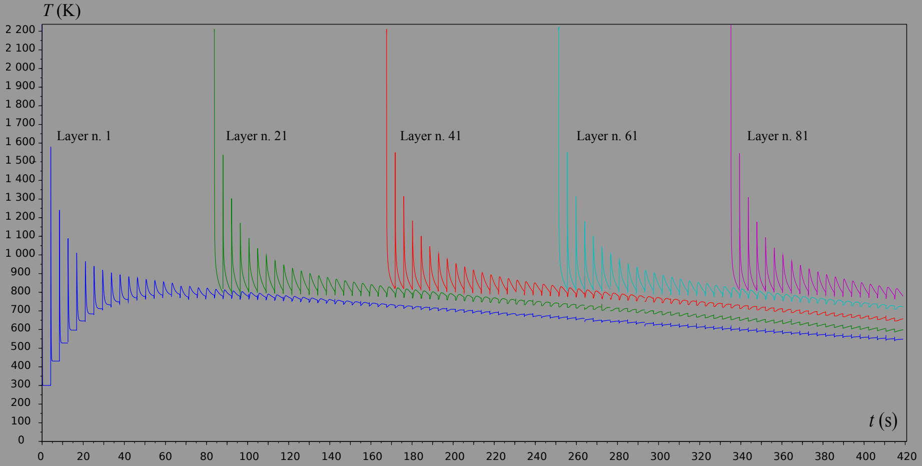
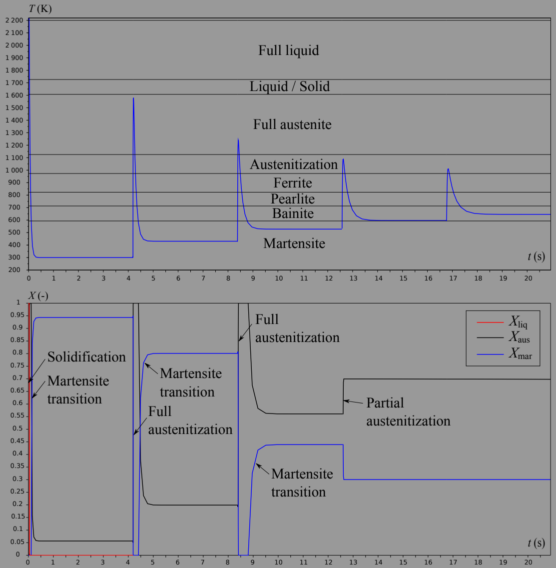
Application to additive manufacturing

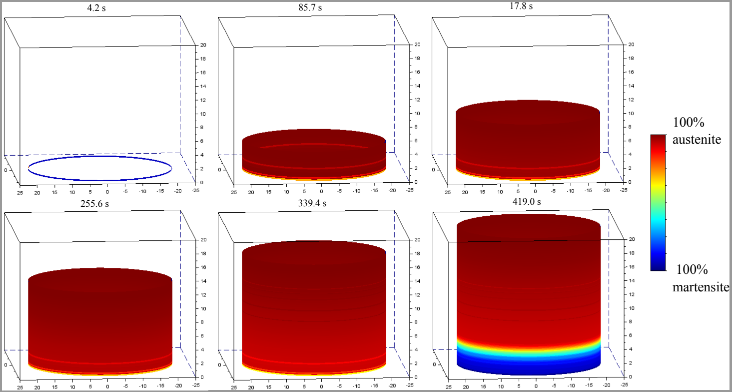


Application to additive manufacturing

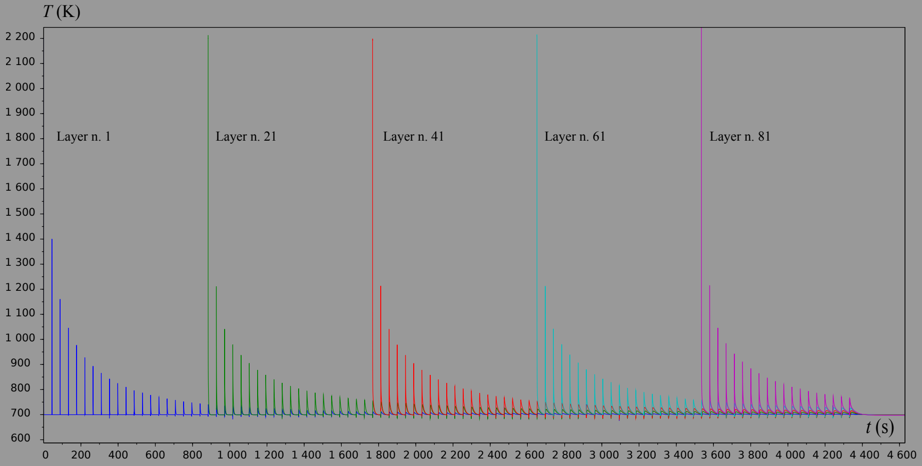


Application to additive manufacturing

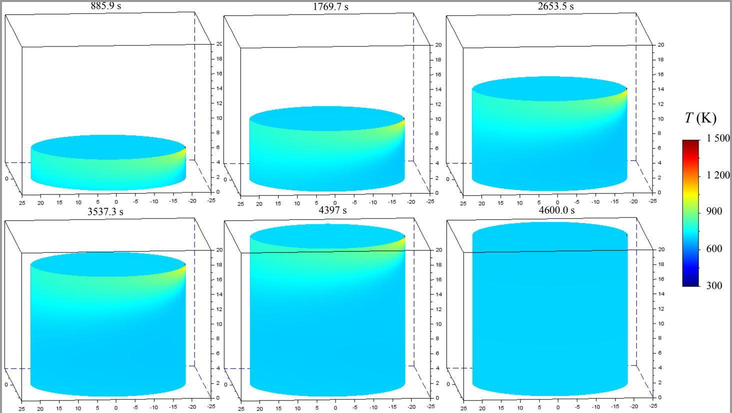
Application to additive manufacturing



Application to additive manufacturing



Application to additive manufacturing



Application to additive manufacturing