2015 Fall

"Phase Transformation *in* Materials"

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Introduction

- **Web lecture assistance: http://etl.snu.ac.kr**
  - All materials will be posted at the webpage.
  - text message will be sent for the important and urgent notice.
- **Hand out copied materials or scanned materials in website**

Text: "Phase Transformations in Metals and Alloys",

D.A. Porter and K.E. Eastering, Chapman & Hall

Prerequisite coursework: Materials Science and Engineering, Thermodynamics

References: 1) "Diffusion in Solid," Paul G. Shewman, TMS (1989)

2) "Physical Metallurgy Principles," Reed-Hill, PWS–Kent (1992)

Additional reading materials will be provided.

Course Goals

This course presents a unified treatment of the thermodynamics and kinetics of phase transformations from phenomenological and atomistic viewpoints. Phase transformations in condensed metal and nonmetal systems will be discussed. This course begins with reviewing the principles of thermodynamics, phase equilibriums, diffusion, and crystal interfaces. The topics include absolute reaction rate theory, thermodynamics of irreversible processes, thermodynamics of surfaces and interfaces, chemical kinetics, nucleation and growth, spinodal decomposition, order-disorder transformations, diffusional transformations, martensitic transformations, coarsening, and glass transition. By the end of the semester, you will be able to understand key concepts, experimental techniques, and open questions in the transformation phenomena of various materials.

Schedule

week 1 Introduction to phase transformation
week 2 Equilibrium single component system/ Binary solutions
week 3 Binary phase diagram
week 4 Ternary phase diagram
week 5 Atomic mechanism of diffusion/ Interstitial diffusion
week 6 Substitutional diffusion/ Atomic mobility
week 7 Diffusion in alloy
week 8 Interfacial free energy/ Solid/vapor interfaces/ Mid-term exam
week 9 Boundaries in single-phase solids/ Interphase interfaces in solids
week 10 Interface migration/ Nucleation in pure metals
week 11 Growth a pure solid/ Alloy solidification
week 12 Solidification of ingots and casting
week 13 Nucleation/ Precipitate growth/ Precipitation in age-hardening alloys
week 14 Various diffusional transformation in solids
week 15 Diffusionless transformation – Martensite transformation
week 16 Team project presentation & Final exam

Contents of this course_Phase transformation

Background to understand phase transformation

- **(Ch1) Thermodynamics and Phase Diagrams**
- **(Ch2) Diffusion: Kinetics**
- **(Ch3) Crystal Interface and Microstructure**

Representative Phase transformation

- **(Ch4) Solidification: Liquid → Solid**
- **(Ch5) Diffusional Transformations in Solid: Solid → Solid**
- **(Ch6) Diffusionless Transformations: Solid → Solid**

Components of Your Grade:

1) Exams (midterm: 30% + final: 35%)

There will be two exams, each of which will take 2-3 hours. I will not use class time for the exams and instead will reserve separate time slots.. The exams will be conceptual and difficult.

2) Team project (15%)

Course participants will organize into small groups. Topics for phase transformation will be discussed, and each group will submit a proposal and reports as well as give a final presentation.

3) Quizzes (10%)

There will be two short quizzes between the major exams. These will take place in class and last for 20 minutes.

4) Homework (5%) (+Incentive Homework 5%) and Attendance (5%)

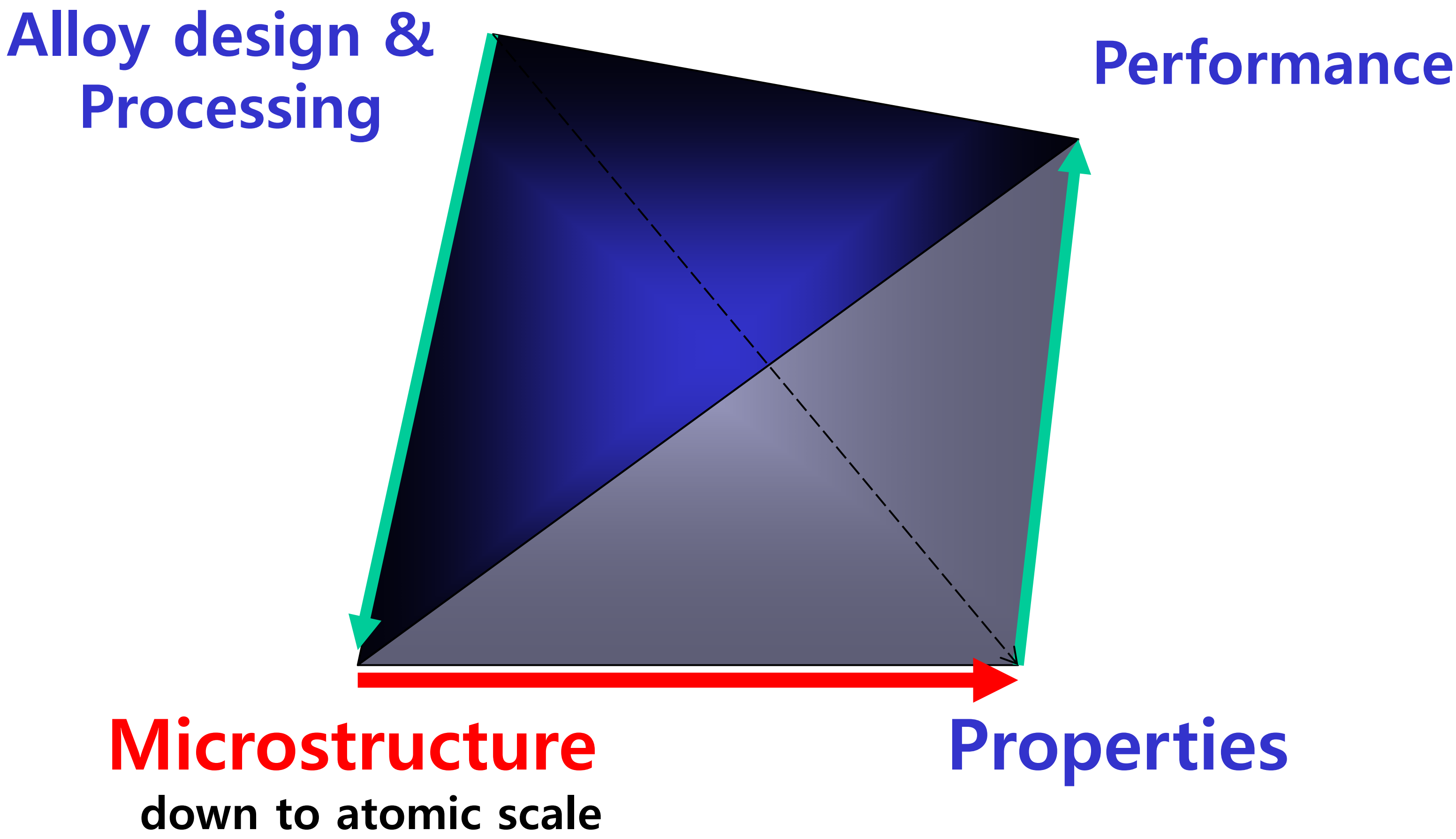
Assignments handed in after the start of class lose credit depending on the timing. If you wish, you may work together on homework assignments. But, you must hand in your own work, in your own words.

Remarks: 1) The weight of each component above could be adjusted up to 5% based on students' performance. 2) Student who retakes this course will have their final scores adjusted downward by 5% in order to ensure fairness with other students.

Policies and Procedures

- ***All homework are due by the start of class on the stated deadline.***
  - Late assignments go to my office. If I'm not around, slide it under my door and leave me an email so that I know when you turned it in.
  - You lose 20% of the full assignment value per day late. Since homework are due on **Wednesday,** you can get 80% credit if you turn it in on **Friday,** 50% on next **Wednesday**, nothing thereafter.
- ***If you wish, you may work together on homework assignments. BUT, you must hand in your own work, in <u>your own words.</u>***
- **IMPORTANT*: you MUST reference your sources appropriately, including texts, journals web sites, etc.***
  - Article authors, title, journal, volume, year, pages
  - Book authors, title, publisher, year, pages
  - Web address
  - etc.

Microstructure-Properties Relationships



"Tailor-made Materials Design"

Alloy design + Process control ➡

Microstructure Control of Materials

Better Material Properties

Q1: What is alloy design?

"Materials selection"

One of the Most Popular Structural Materials
; Iron-Carbon Alloy (or Steel)

Steel frame of building

Application of Iron-Carbon Alloy

K1 – main battle tank of Korea army

Need of the strongest materials

Dominant Material for Airplanes
; Aluminum Alloy

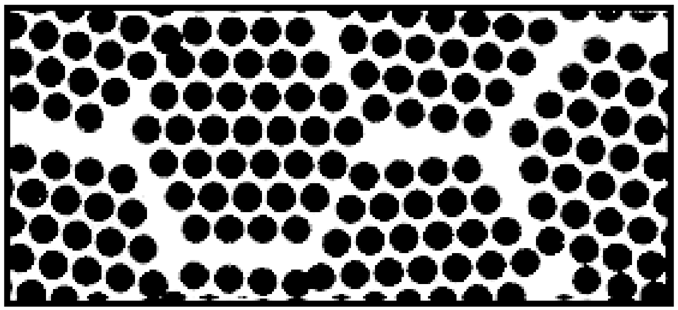
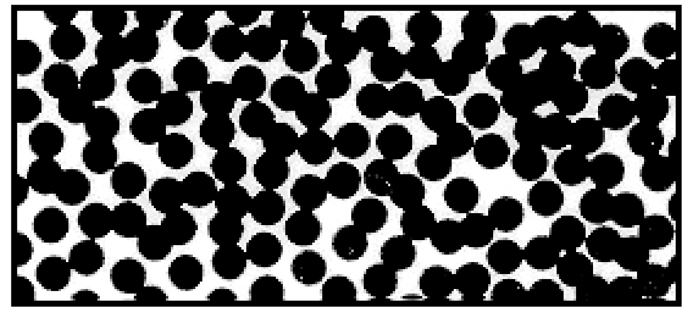
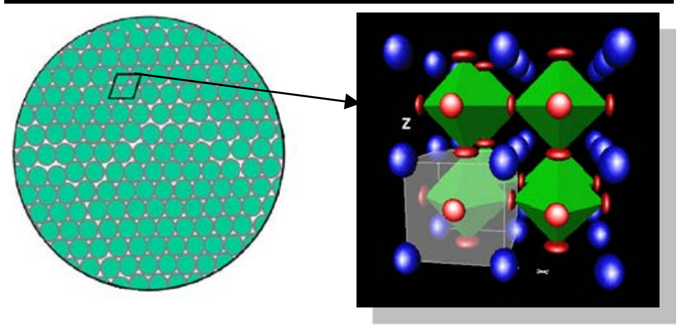
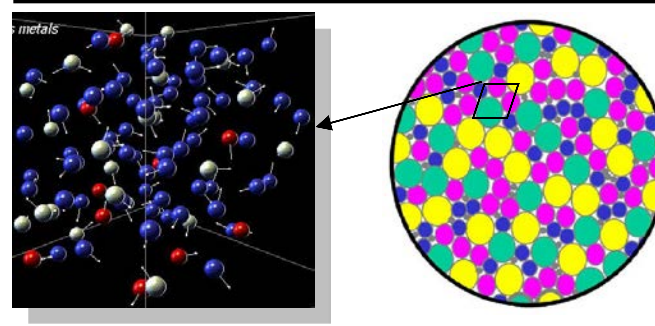
B737-800 of Korean Air

Need of light, strong and tough material

Q2: How to classify material depending on the structure?

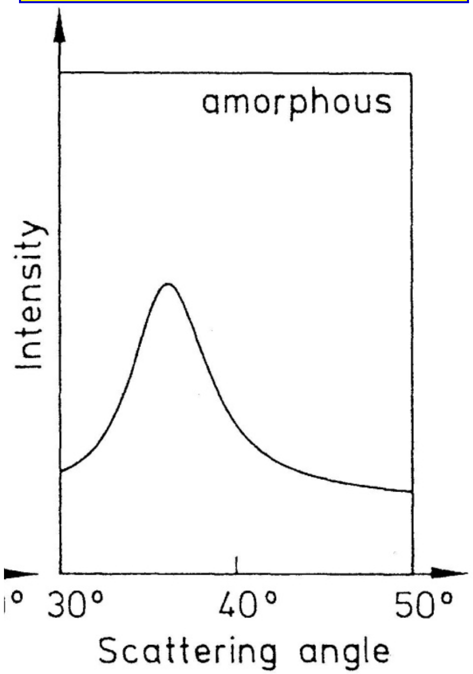
2) Classification of Material depending on the structure

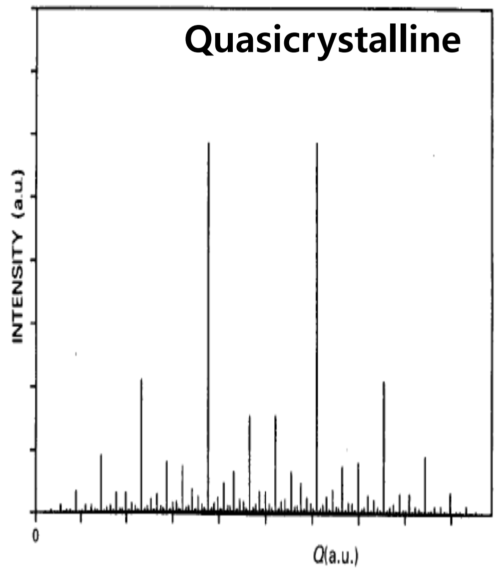
Structure *of crystals, liquids and glasses*

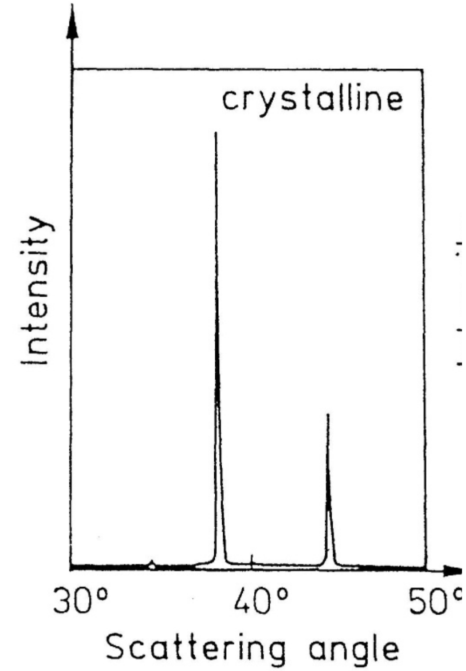
Crystals	***Liquids, glasses***
	
	
• **periodic** • **grain boundaries**	• **amorphous = non-periodic** • **no grain boundaries**

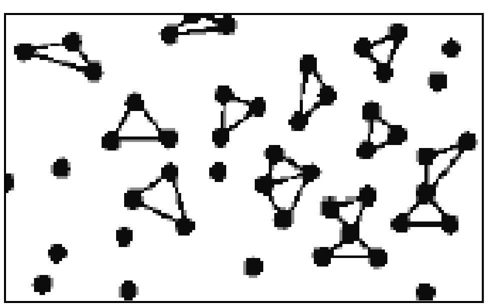
Atomic structure

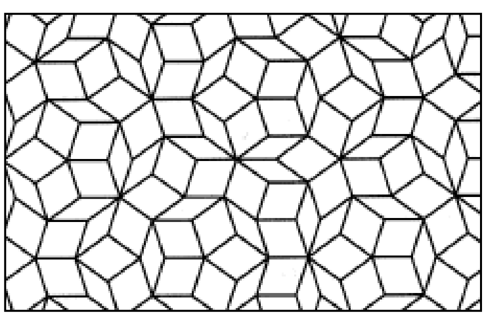
Short-range order ← **Quasi-periodic order** → **Periodic order**

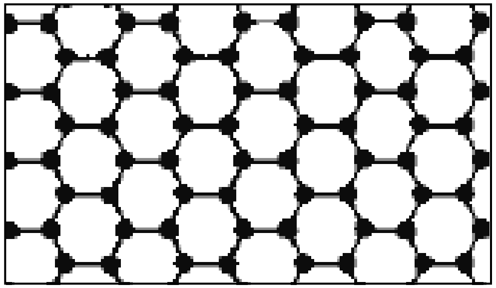












Q3: What are phase, phase diagram and phase transformation?

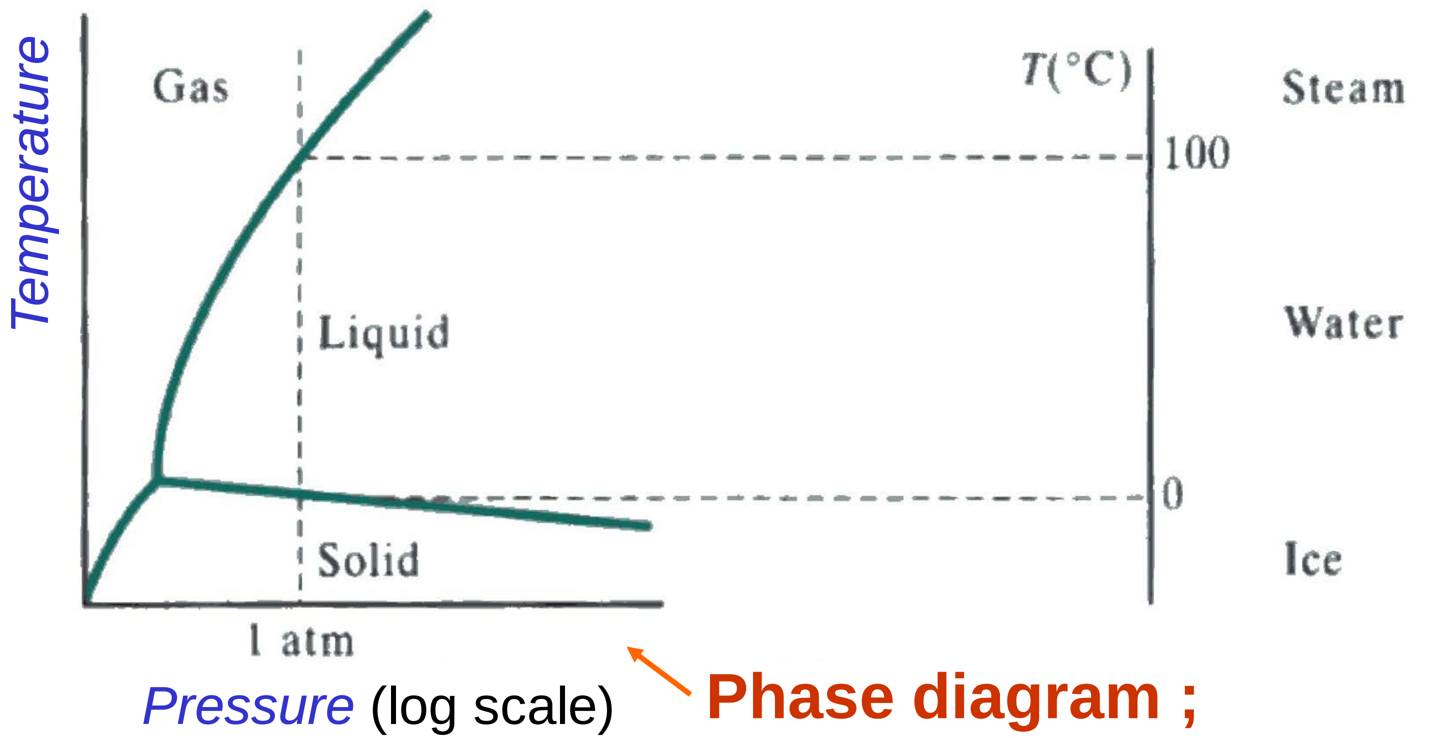
3) Microstructure control

: Equilibrium phase ➡ Only consider Thermodynamics

① What is *Phase*?

A phase is a chemically and structurally homogeneous portion of the microstructure.

(structure or composition or order)



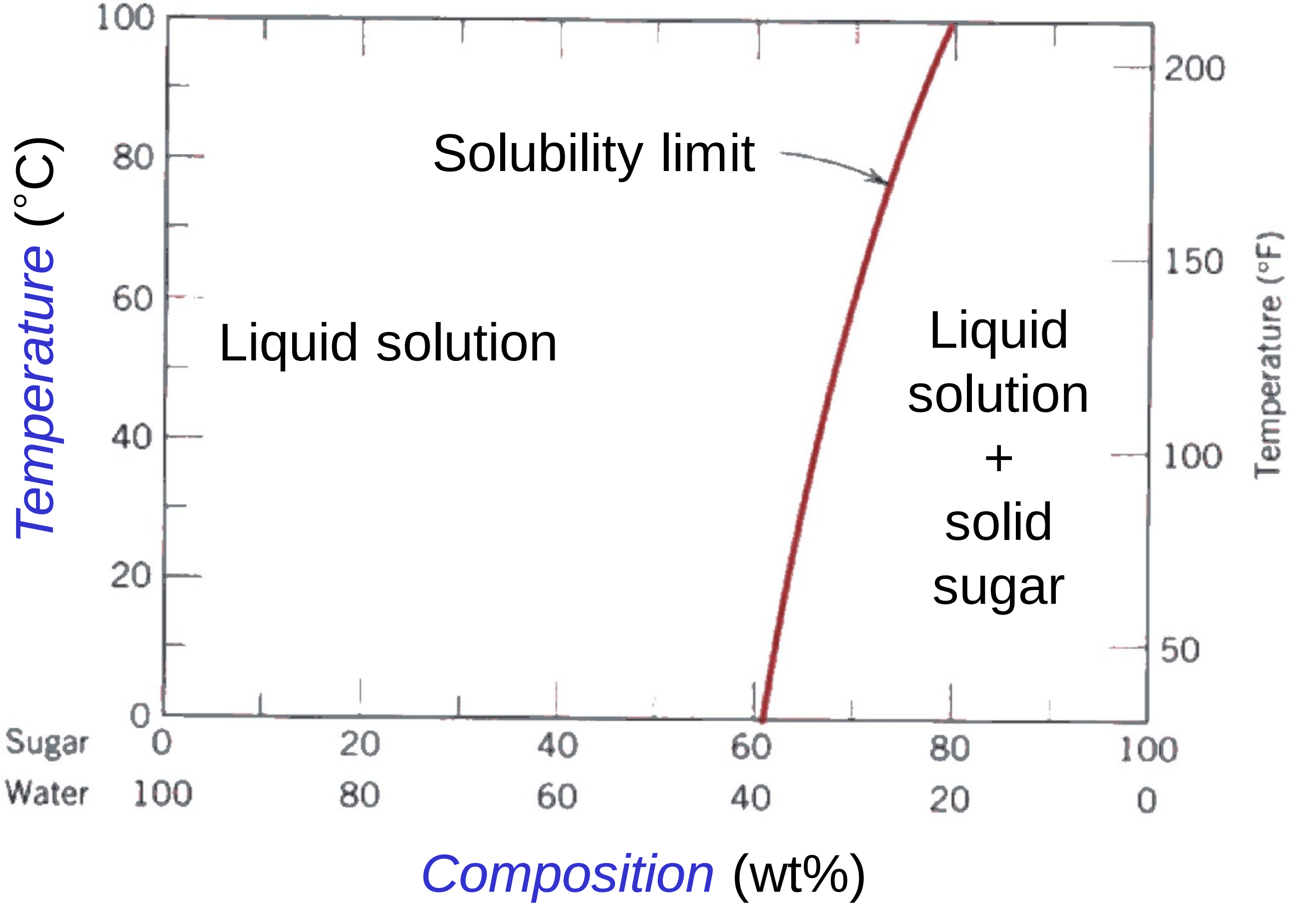
Phase diagram ;
<u>equilibrium phase</u> of material

Microstructure control

: Equilibrium phase ➡ Only consider Thermodynamics

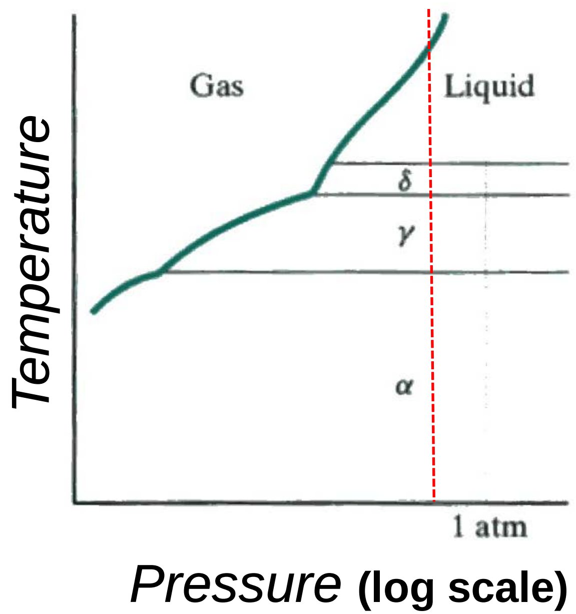
② ***Phase Diagram*** of Temperature – Composition ;

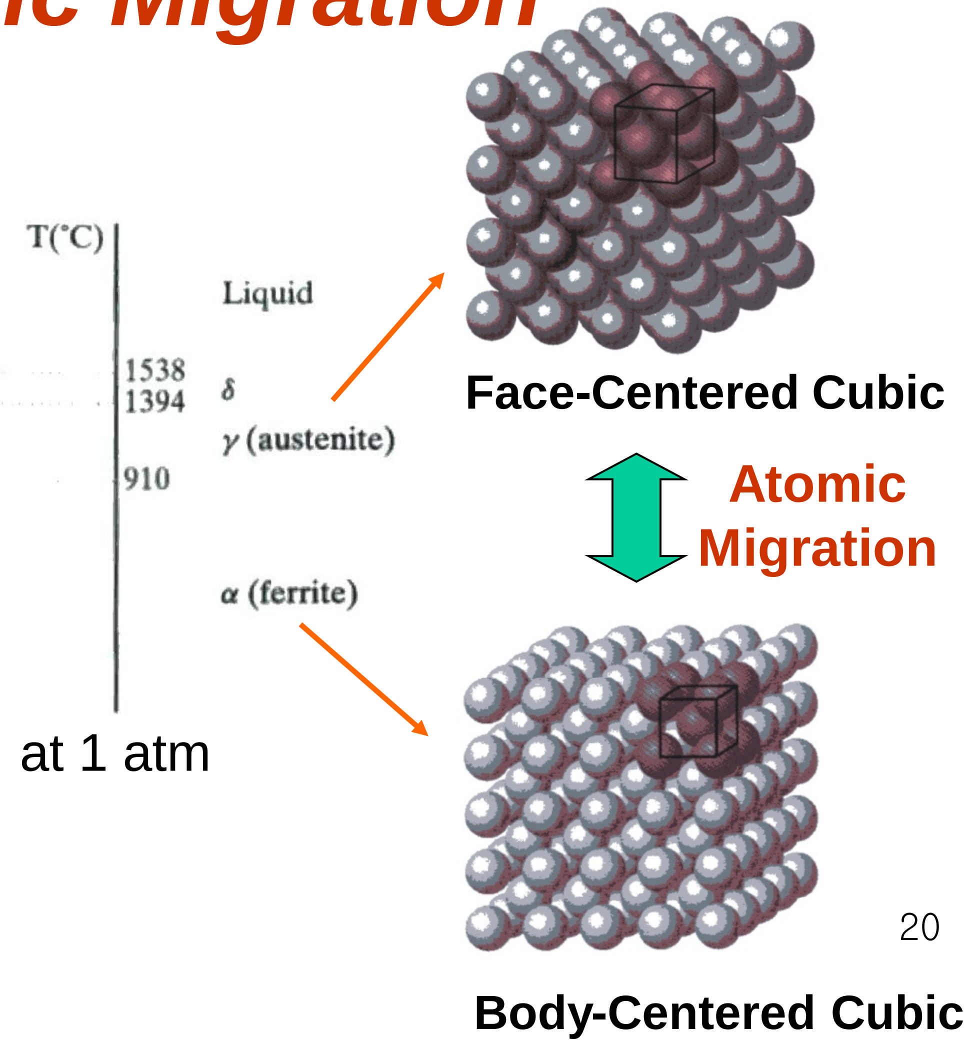
most useful in materials science & engineering



Microstructure control
: Phase transformation ➡ Atomic Migration

③ *Phase Transformation* of Iron and *Atomic Migration*





Q4: What is microstructure?

4) What is microstructure?

Microstructure originally meant the structure inside a material that could be observed with the aid of a microscope.

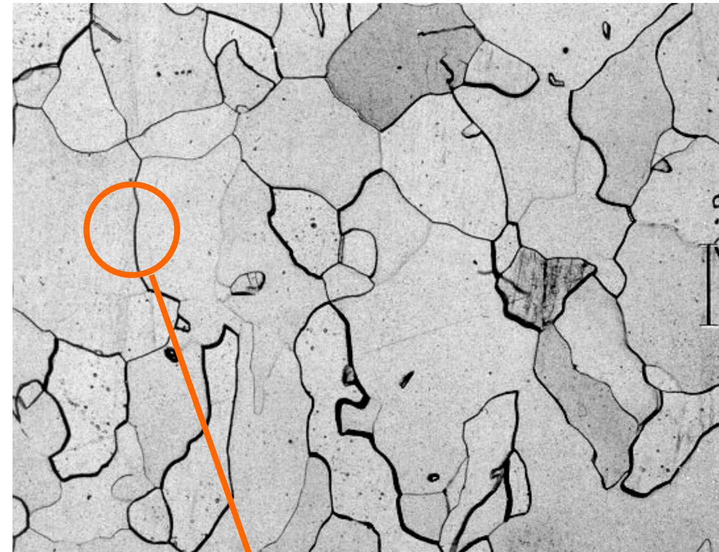
In contrast to the crystals that make up materials, which can be approximated as collections of atoms in specific packing arrangements (crystal structure), microstructure is the collection of defects in the materials.

What defects are we interested in?
Interfaces (both grain boundaries and interphase boundaries), which are planar defects,
Dislocations (and other line defects), and
Point defects (such as interstititals and vacancies as well as solute atoms in solution)

* *Imperfection:* Grain Boundaries

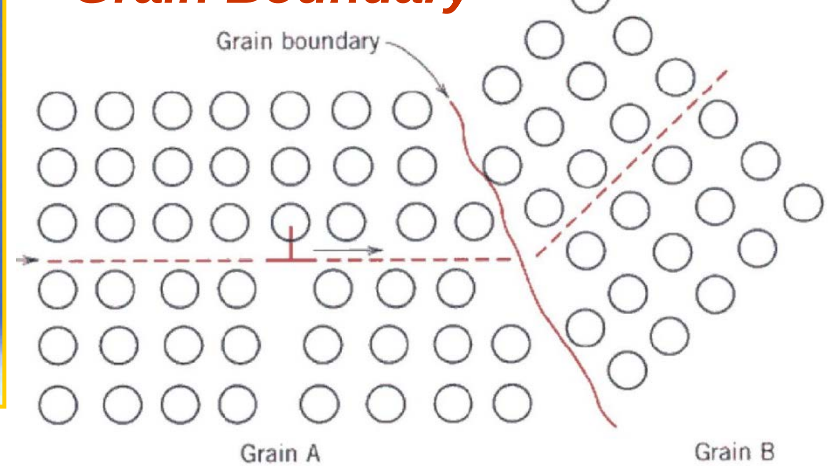
(Planer defect)

Low Carbon Steel



Optical Microscope

Grain Boundary

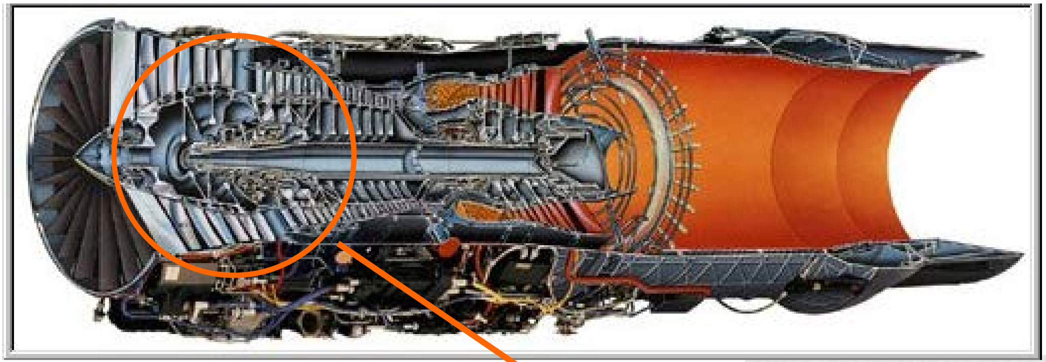


Q5: How to control the microstructure by process control?

5) Microstructure control

: process control after materials selection ➡ property optimization

A Example of ①<u>Grain Boundary Engineering</u> ;
Turbine blade in Aircraft Engine



F100-PW-229
in F-16 fighting falcon

Turbine Blade

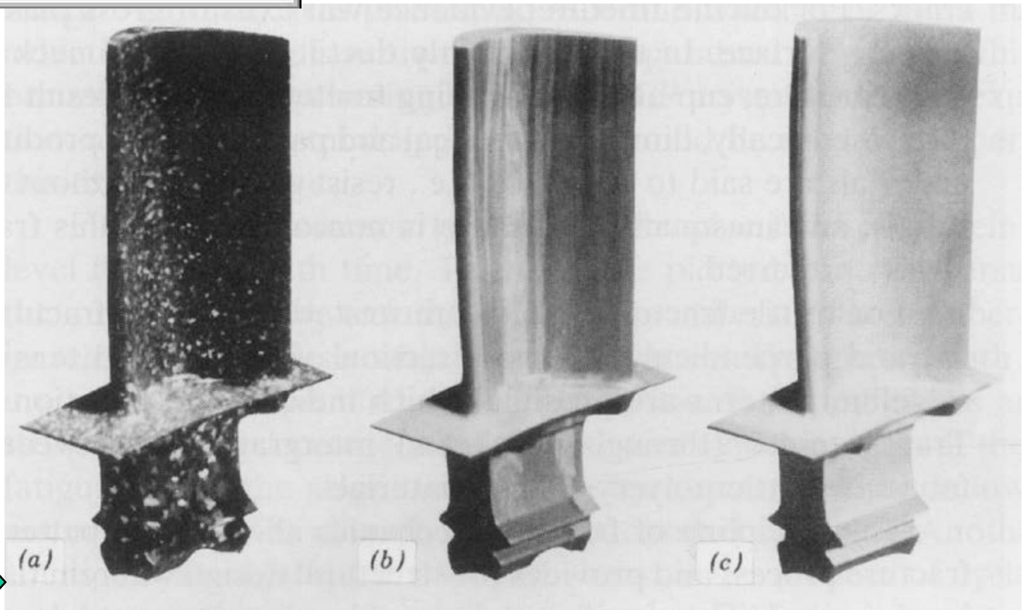
Grain boundaries
at high Temperature ;
Diffusion path of atoms

⬇

Creep

⬇

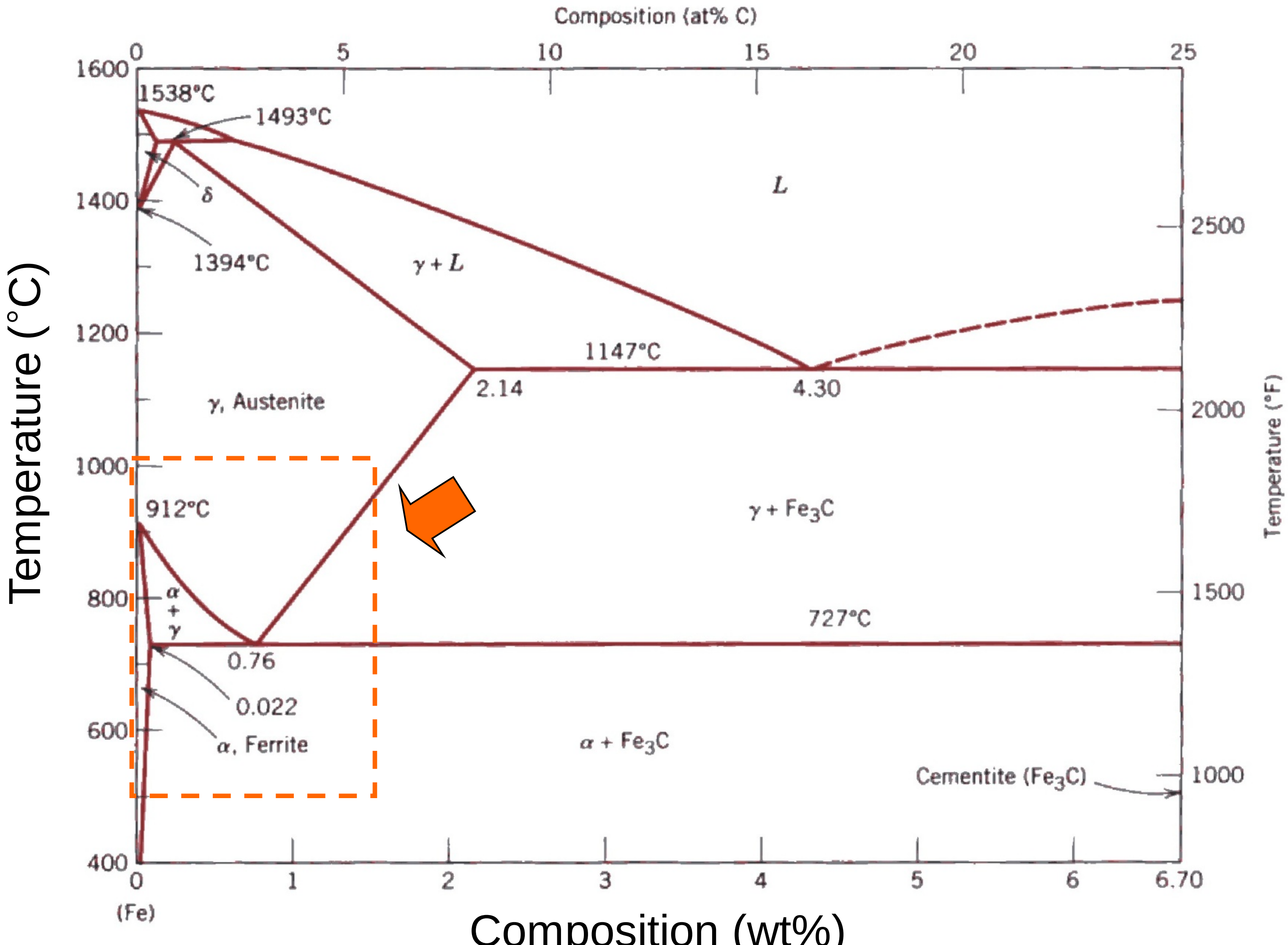
Reducing grain boundaries ➡



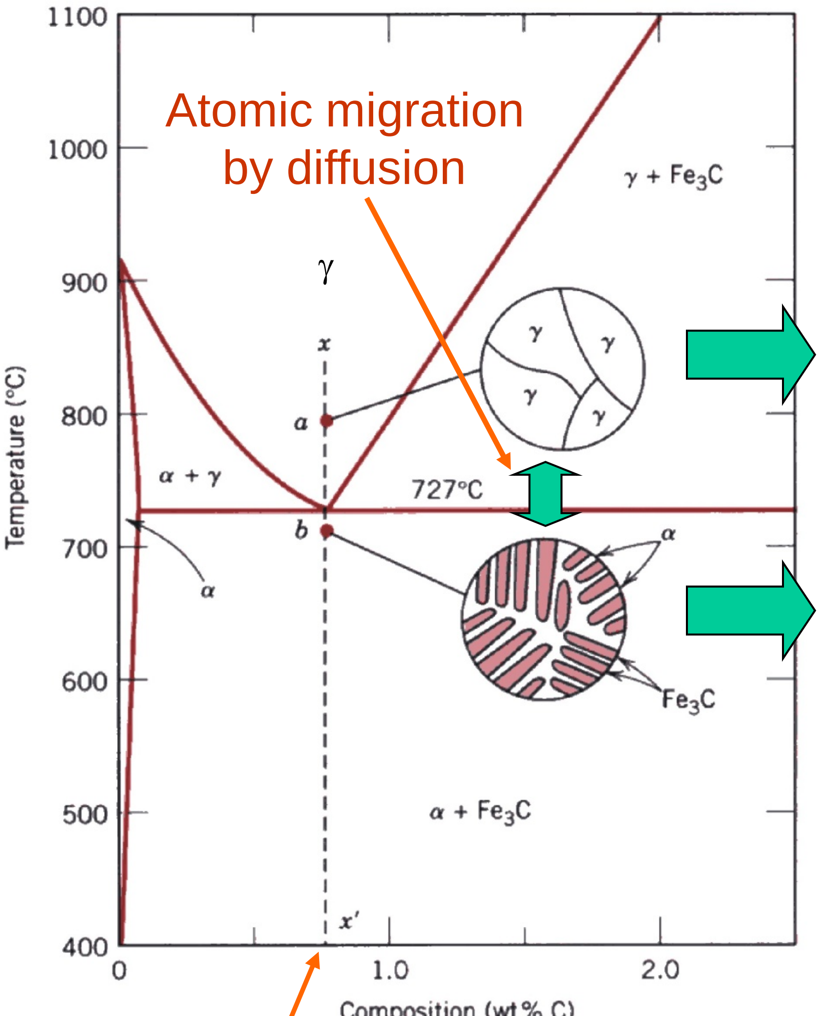
Conventional casting   Columnar grain   Single crystal

5) Microstructure control : ② Secondary phase control

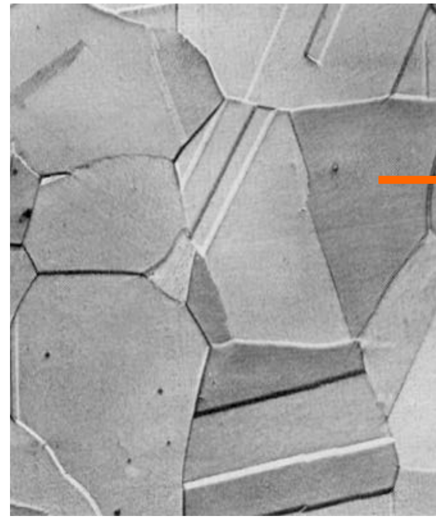
a. Phase Diagram of Iron–Carbon Alloy

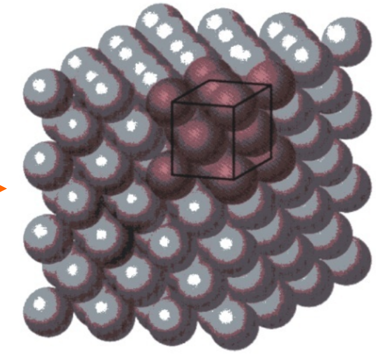


b. Equilibrium Phases of Iron-Carbon Alloy

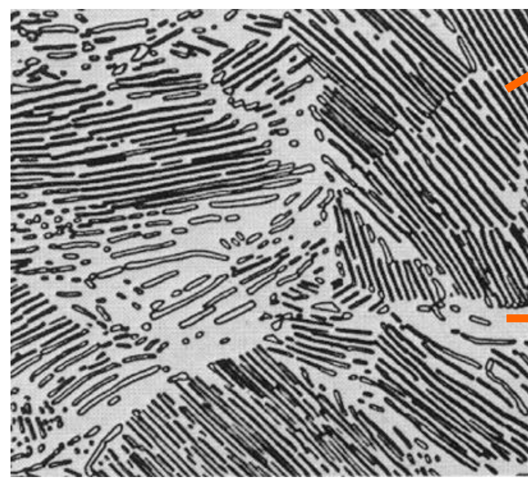


Eutectoid composition

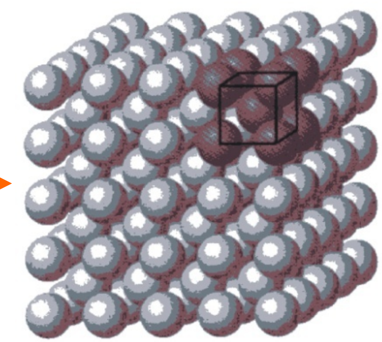




γ phase (FCC)



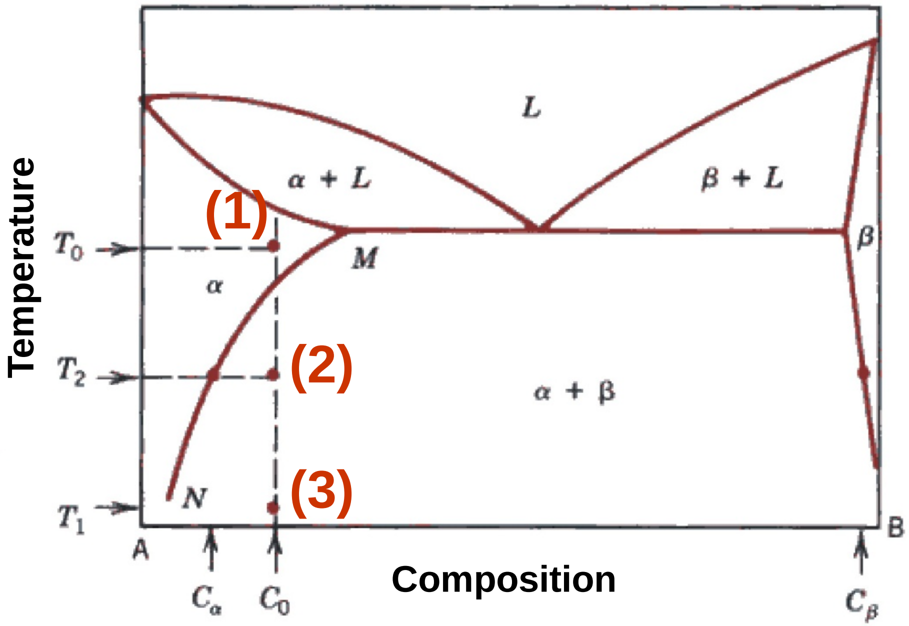
Fe_3C phase

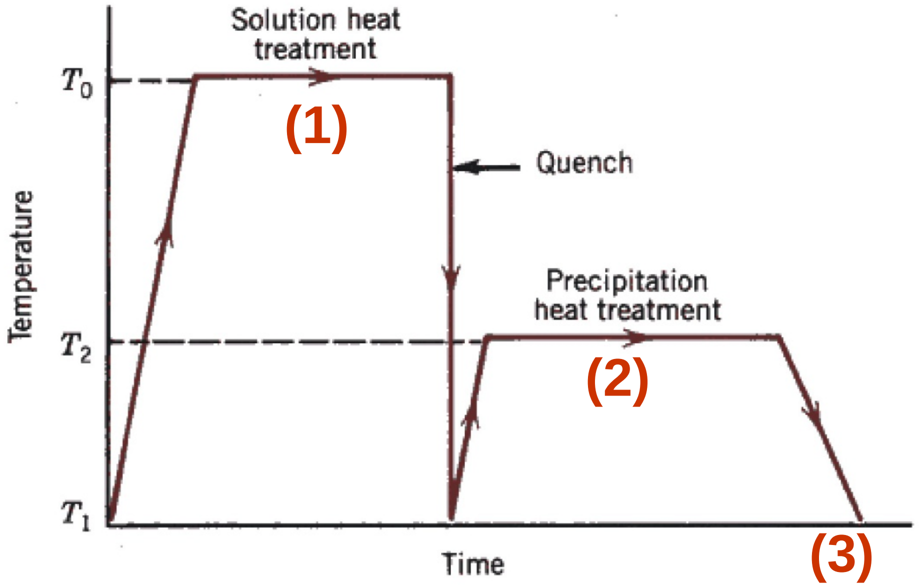


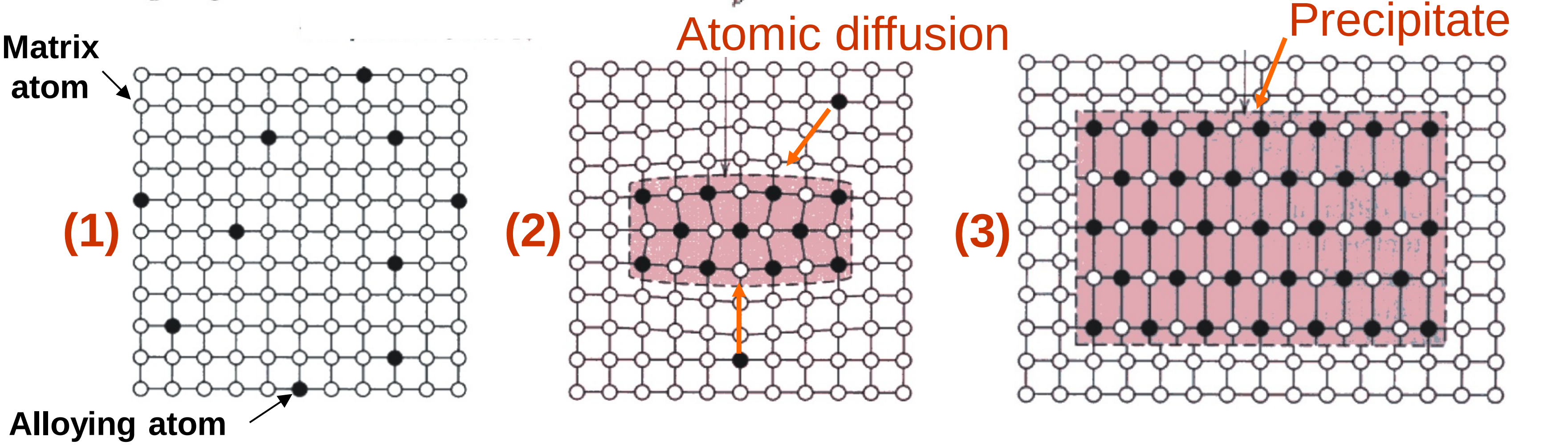
α phase (BCC)

5) Microstructure control : ② Secondary phase control

c. Mechanism of Precipitation







d. Effect of Second Phase Particle on Mechanical Property

Second phase particle in matrix material

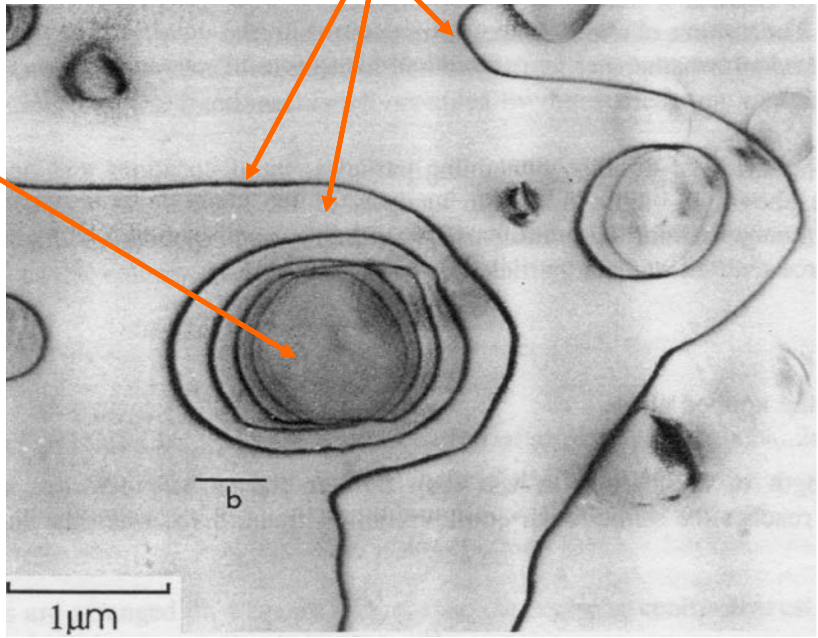
↓

Obstacle of dislocation slip & grain growth

↓

High strength

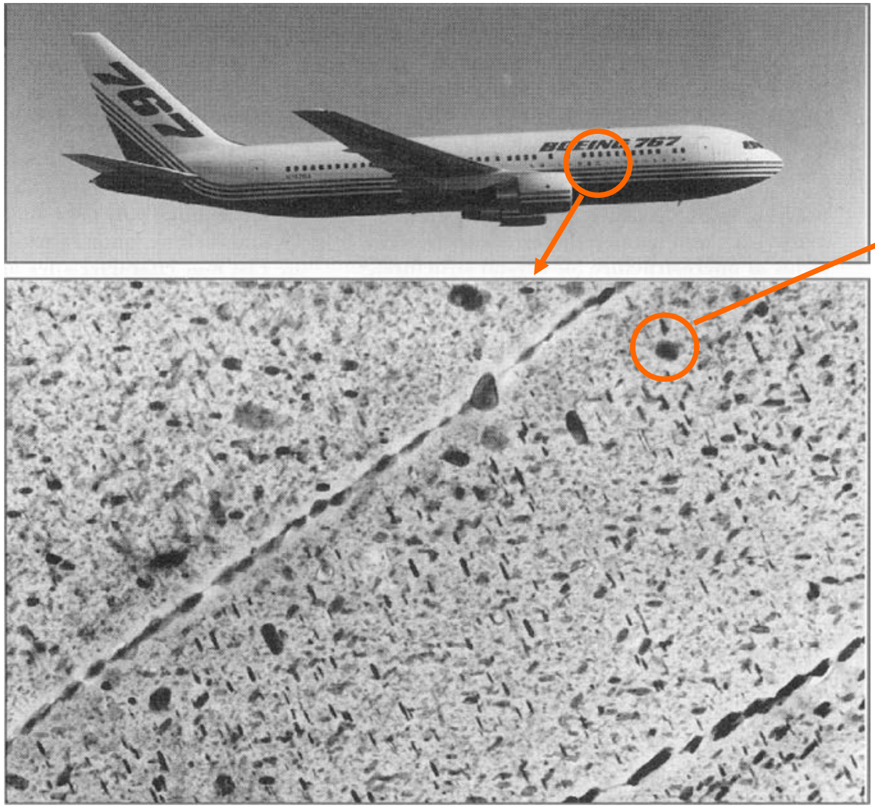
Dislocations



Ni_3Si particles in Ni-6%Si single crystal

e. Control of Microstructures by Precipitation Transformation in Aluminum Alloy

Boeing 767 by AA7150 T651 alloy



Precipitates in aluminum matrix

↓

Hindering dislocation slip

↓

High strength

Q6: How to optimize microstructure by process control?

6) Microstructure optimization by process control

① *Cold Work*_압력을 가해 성형하고 인성을 증가시키는 과정

김홍도 "Smithy_대장간"

Joseon Dynasty

Modern forging machine

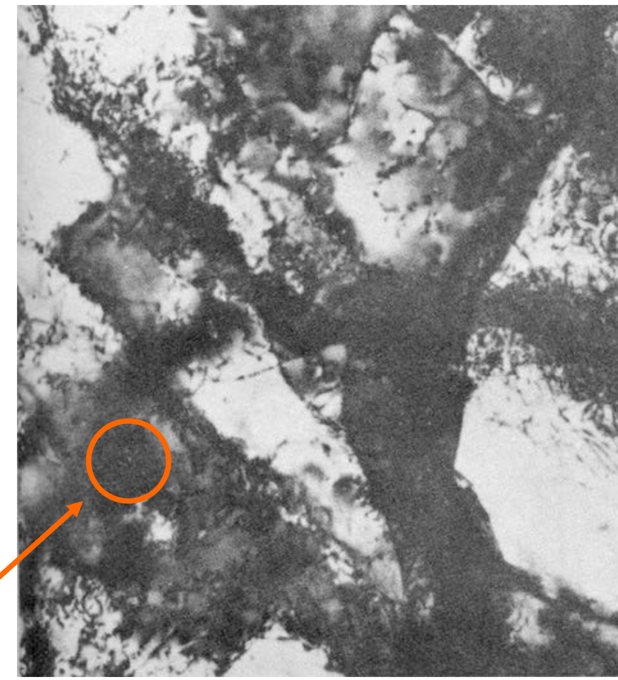
6) Microstructure optimization by process control

Hardening Mechanism by Cold Working

Before cold work

Deformation
or
Cold work

Aluminum alloy



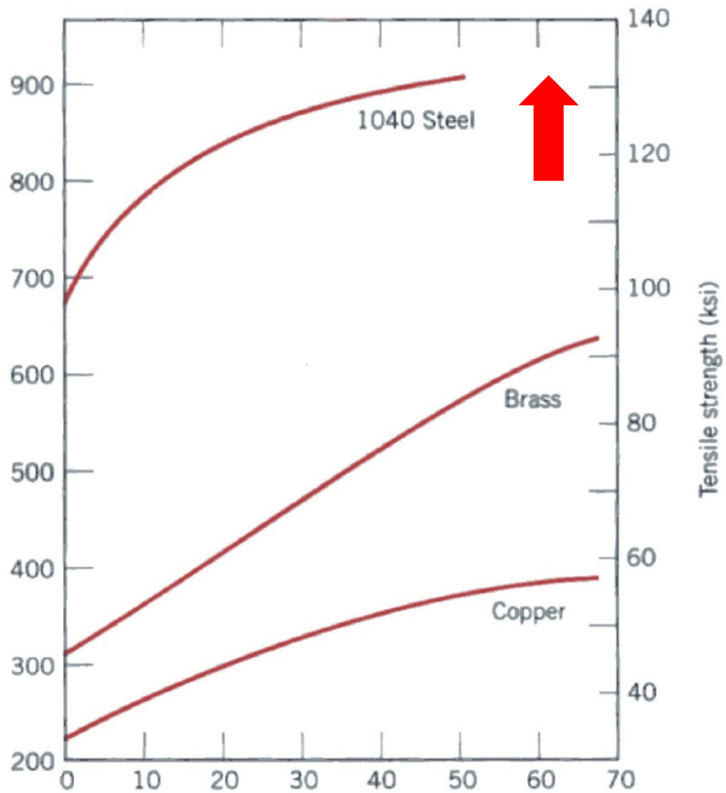
Accumulation of dislocations

Dislocation tangle

6) Microstructure optimization by process control

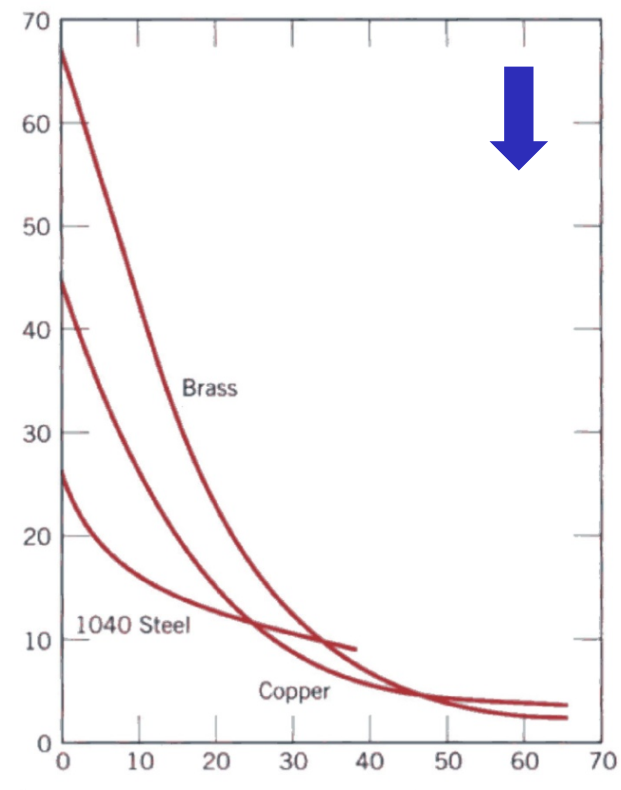
Changes of Strength and Ductility by Cold Working

Tensile strength



Percent cold work

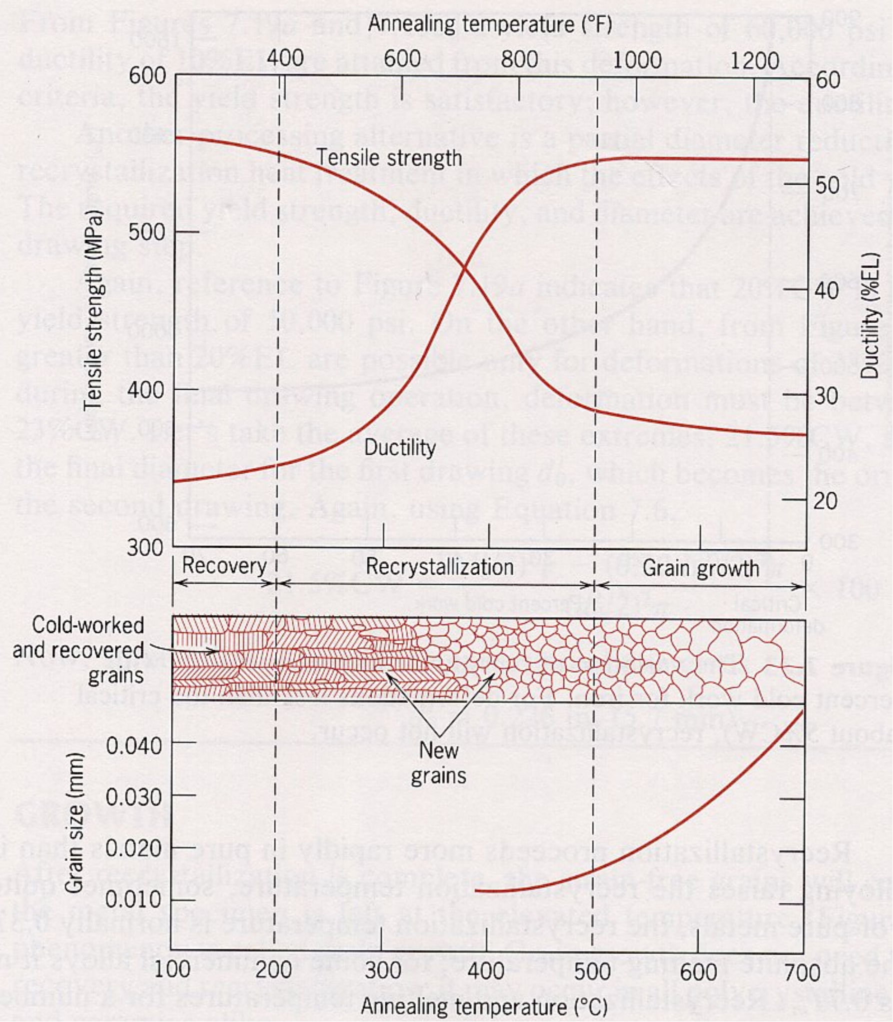
Ductility



Percent cold work

6) Microstructure optimization by process control

② Changes of Microstructure & Mechanical Properties during Annealing



Cold working → recovery → recrystallization → grain growth

내부 변형률 에너지 제거 낮은 전위밀도 (변형률이 없는) 결정립

Q7: How to optimize material property?

“Alloy design + Process control”

e.g. Production and Application of Electrical Steel

Hot rolling - cold rolling – 1st annealing – 2nd annealing

Coils

Stacked transformer core

Transformer
Motor
Etc.

Soft magnetization property

Microstructural Parameters vs Properties

Properties

- Strength
- Toughness
- Formability
- Conductivity
- Corrosion Resistance
- Piezoelectric strain
- Dielectric constant
- Magnetic Permeability

↔

Microstructural Parameters

- Grain size
- Grain shape
- Phase structure
- Composite structure
- Chemical composition (alloying)
- Crystal structure
- Defect structure (e.g. porosity)

Alloy design + Process control ➡
Microstructure Control of Materials

➡

Better Material Properties

Important!!!

8) *Understanding* and *Controlling*

Phase Transformation *of* Materials

Q8: How to control the phase transformation?

"Thermodynamics + Kinetics"

Phase Transformation

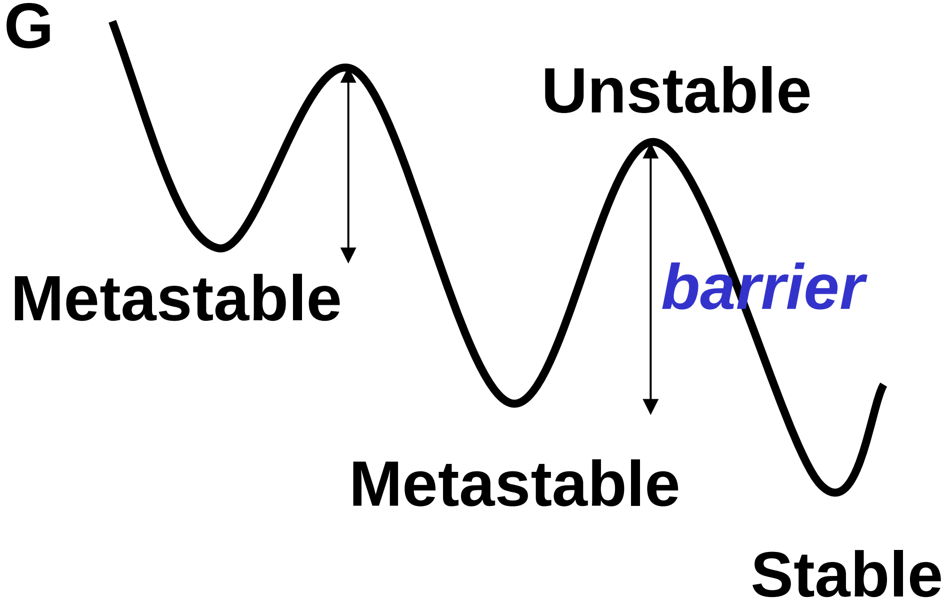
$$\Delta G = G_2 - G_1 < 0$$

Phase 1 → phase 2 ➡ **equilibrium state**

structure or **composition** or **order**

Lowest possible value of Gibb's Free Energy

No desire to change ad infinitum



$$dG = 0$$

How does thermodynamics different from kinetics?

Thermodynamics ➡ There is no time variable.

says which process is possible or not and never says how long it will take.

The existence of a thermodynamic driving force does not mean that the reaction will necessarily occur!!!

Allotrope (同質異像): any of two or more physical forms in which an element can exist

화학성분 같고 결정구조 다름

There is a driving force for diamond to convert to graphite but there is (huge) nucleation barrier.

How long it will take is the problem of kinetics.

The time variable is a key parameter.

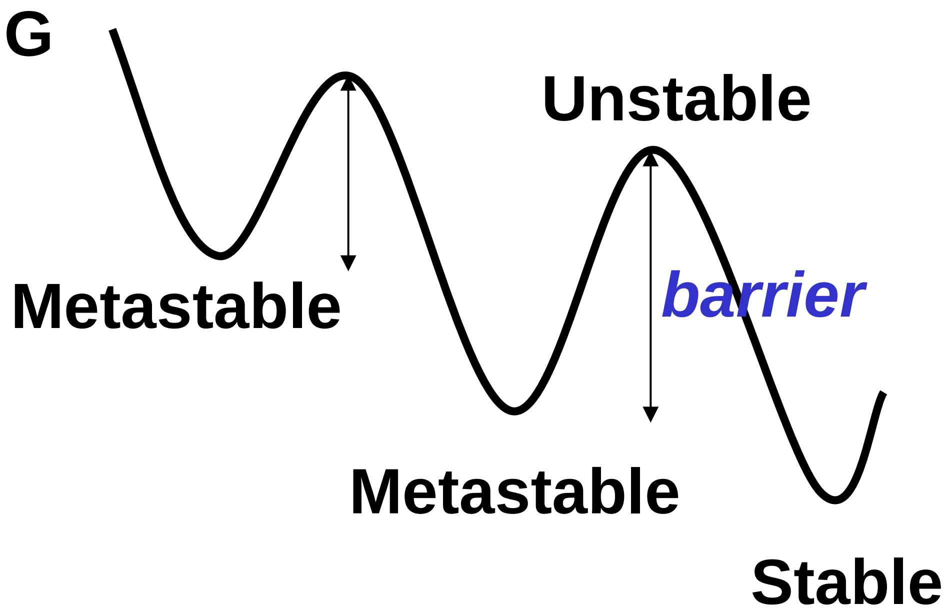
Phase Transformation

$$\Delta G = G_2 - G_1 < 0$$

Phase 1 → phase 2 ➡ **equilibrium state**

structure or **composition** or **order**

Lowest possible value of Gibb's Free Energy
No desire to change ad infinitum



$$dG = 0$$

➡ **Governed by Thermodynamics & Kinetics**

Q9: What are the representative PTs?

9) Representative Phase Transformation

- **Solidification: Liquid ⇨ Solid**

- **Phase transformation in Solids**

① Diffusion-controlled phase transformation ;

Generally long-distance atomic migration

- Precipitation transformation
- Eutectoid transformation (**S** ⇨ $\mathbf{S_1 + S_2}$)
- etc.

② Diffusionless transformation ;

Short-distance atomic migration

- Martensitic transformation

① Diffusion-controlled phase transformation

Diffusion- Controlled Phase Transformation
time dependency

↓

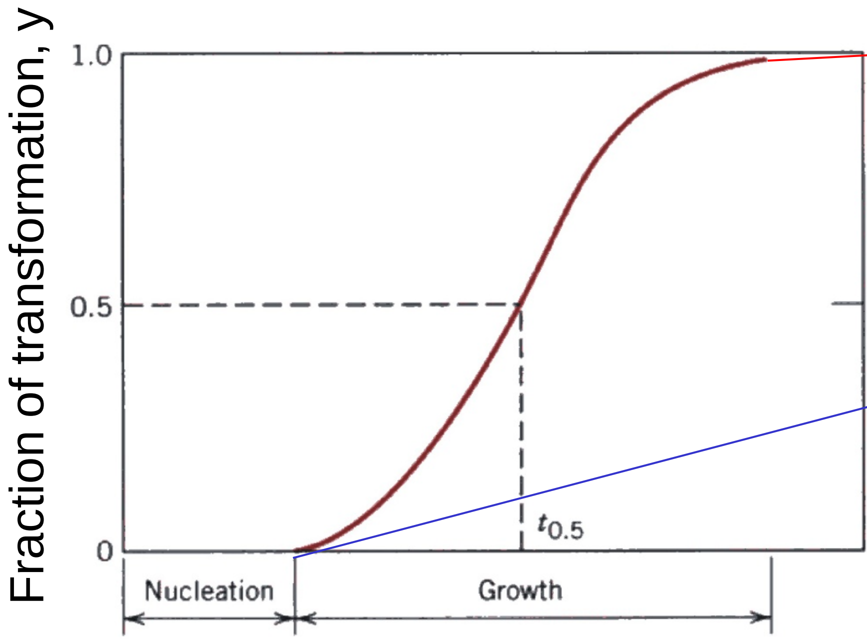
Non-Equilibrium Phases → Equilibrium phase

↓

a. Need of Controlling
not only *Temperature* & *Composition*
but *Process conditions* (Cooling Rate)

Transformation Kinetics :

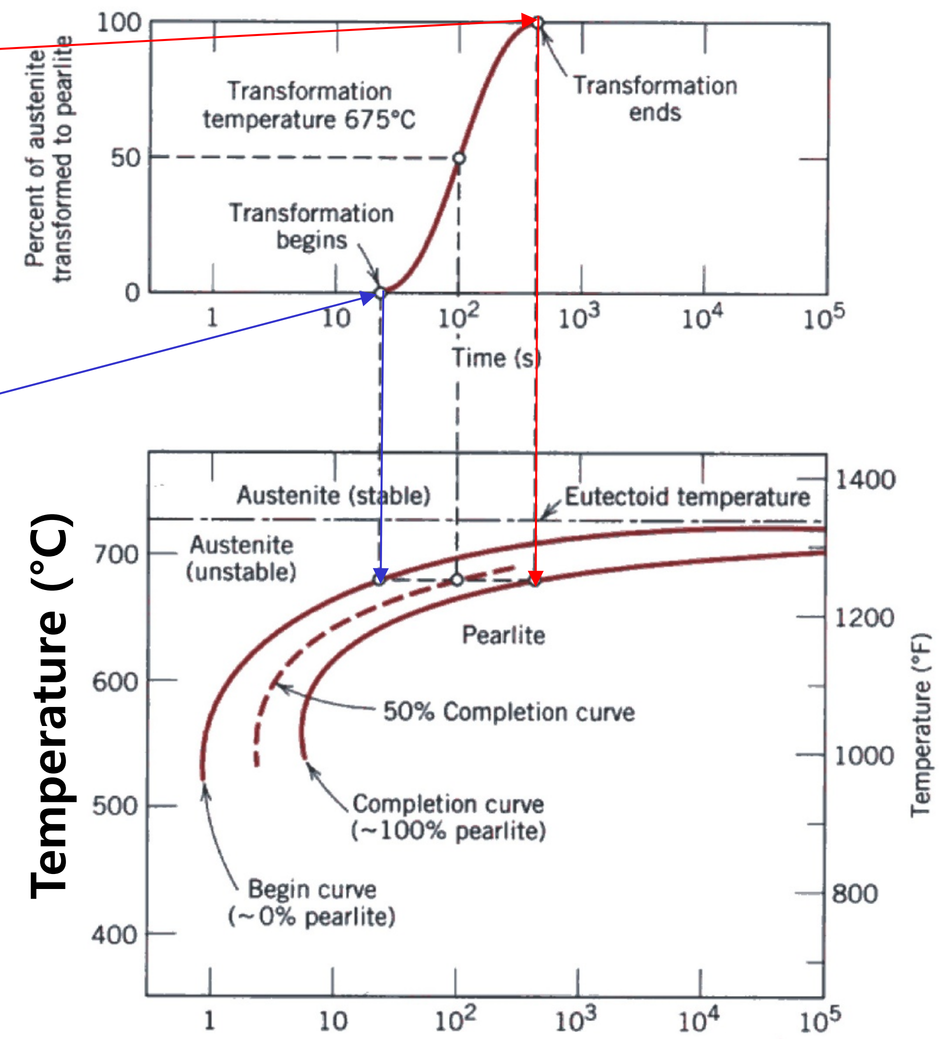
b. Isothermal Transformation Diagram



Logarithm of heating time, t

$$y = \exp(-kt^n)$$

Kinetics of diffusion-controlled solid-state transformation

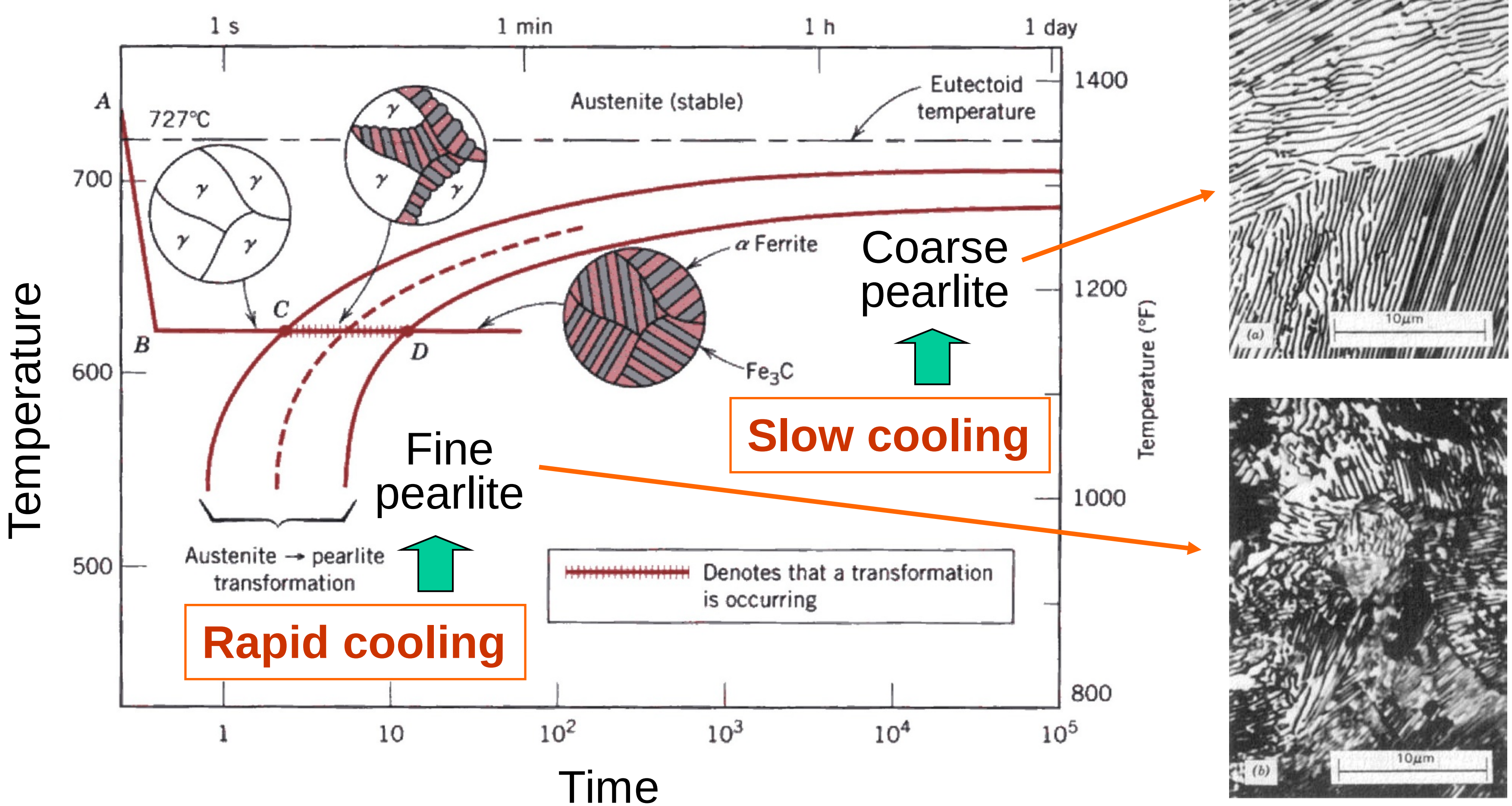


Time (s)

TTT diagram ➡ Isothermal transformation diagram

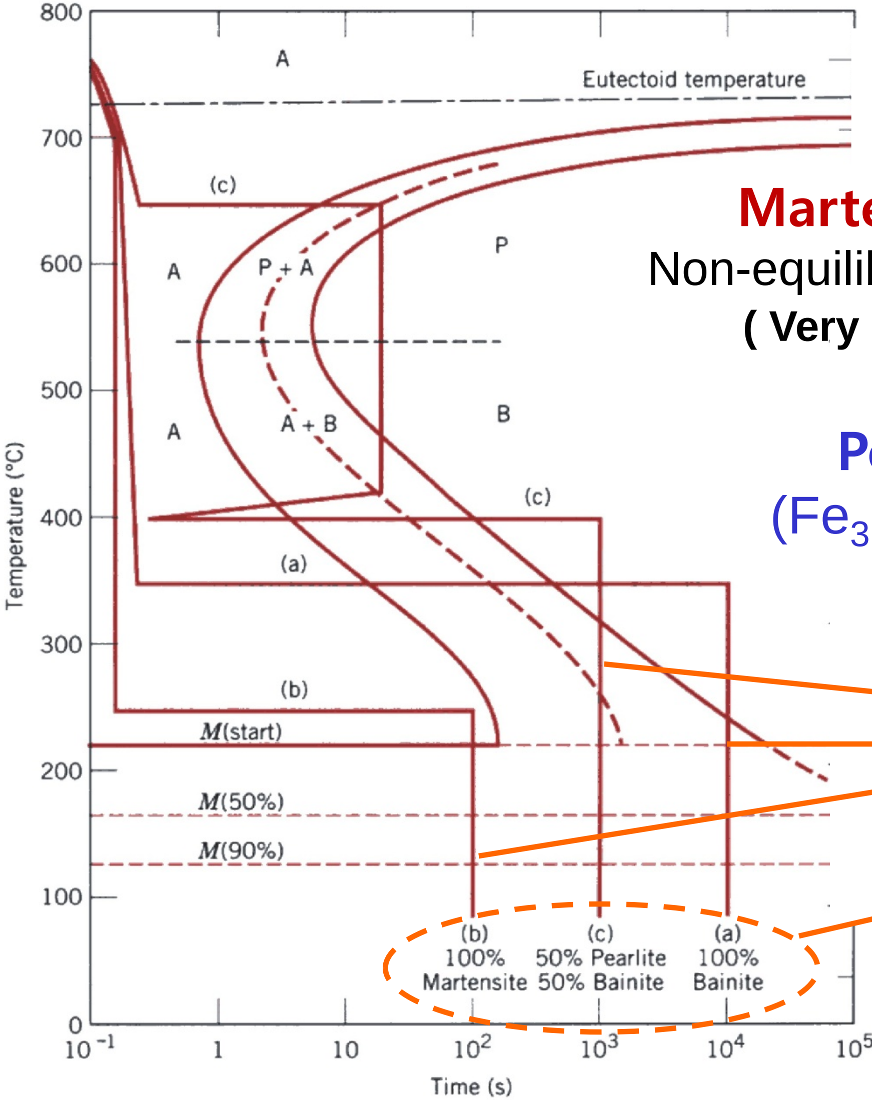
c. Isothermal Transformation Diagram of a Eutectoid Iron-Carbon Alloy

γ Austenite ⇒ α Ferrite + Fe_3C graphite



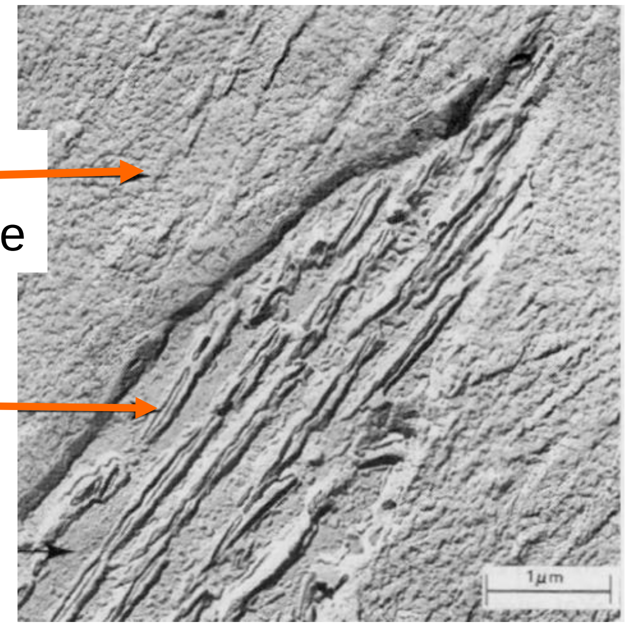
➡ **Microstructure control by phase transformation**

d. Control of Phases by Heat Treatment



Martensite ;
Non-equilibrium phase
(Very hard)

Pearlite
(Fe_3C+ferrite)



Heat Treatment

Process control

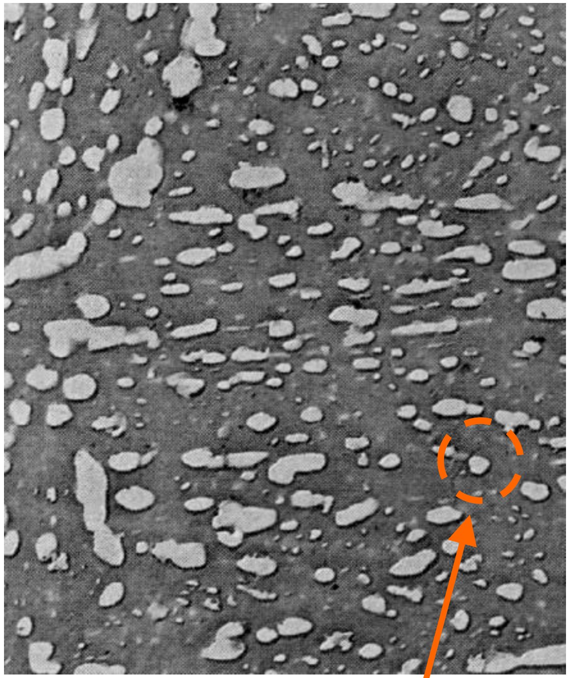
Phase & Microstructure

Properties of Material

e. Control of Mechanical Properties by Proper Heat Treatment in Iron-Carbon Alloy

Process control

Proper heat treatment (tempering)



Martensite

Tip of needle shape grain

Nucleation site of fracture

Brittle

Tempered martensite

Very small & spherical shape grain

Good strength, ductility, toughness

② Diffusionless Transformation

Individual atomic movements are less than one interatomic spacing.

e.g. a Martensitic transformation in iron-carbon alloy

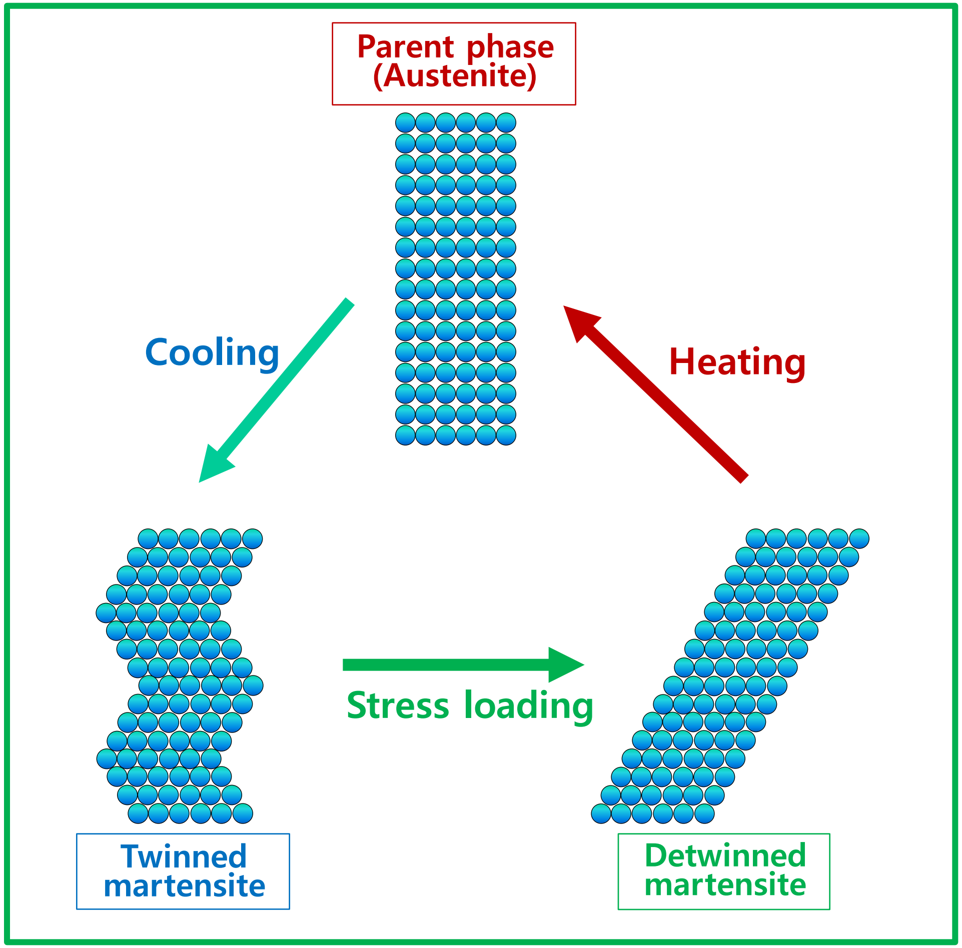
e.g. b Martensitic transformation in Ni-Ti alloy ;

55~55.5 wt%Ni - 44.5~45 wt%Ti ("Nitinol")

↓

Ex) Shape memory alloy

Principles - Shape memory process



1. A_f 이상의 온도로 열처리를 통해 Austenite 상에서 형상 기억

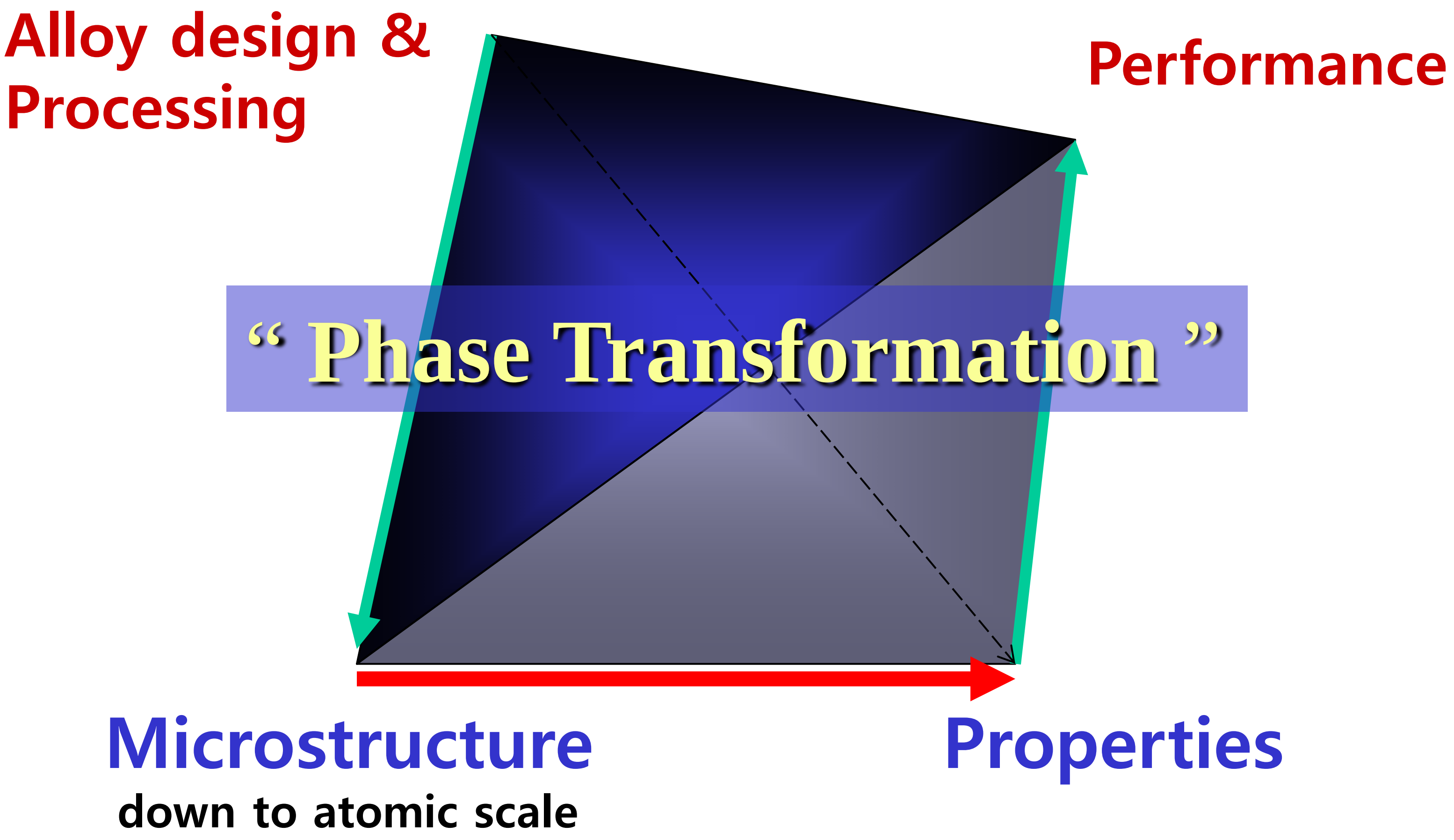
2. M_s 이하의 온도로 냉각시 Twinned martensite 생성

3. 항복강도 이상의 응력을 가하면 Twin boundary의 이동에 의한 소성 변형

4. A_f 이상으로 가열해주면 martensite 에서 다시 Austenite로 변태
➡ 기억된 형상으로 회복

" $\gamma \leftrightarrow$ M transformation: Short-distance atomic migration "

Microstructure-Properties Relationships



“Tailor-made Materials Design”

Q10: What are the contents of this course?

10) Contents of this course_Phase transformation

Background to understand phase transformation

- (Ch1) Thermodynamics and Phase Diagrams
- (Ch2) Diffusion: Kinetics
- (Ch3) Crystal Interface and Microstructure

Representative Phase transformation

- (Ch4) Solidification: Liquid → Solid
- (Ch5) Diffusional Transformations in Solid: Solid → Solid
- (Ch6) Diffusionless Transformations: Solid → Solid