

2018 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 equilibria, 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/ Diffusion in alloy, **1st Exam**
- week 7** Interfacial free energy/ Solid/vapor interfaces
- week 8** Boundaries in single-phase solids/ Interphase interfaces in solids
- week 9** Interface migration
- week 10** Nucleation in pure metals
- week 11** Growth a pure solid/ Alloy solidification
- week 12** Solidification of ingots and casting, **2nd Exam**
- 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 \rightarrow Solid

(Ch5) Diffusional Transformations in Solid: Solid \rightarrow Solid

(Ch6) Diffusionless Transformations: Solid \rightarrow Solid

Components of Your Grade:

1) Exams (1st: 25%; 2nd 25%; final: 25%)

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) 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.

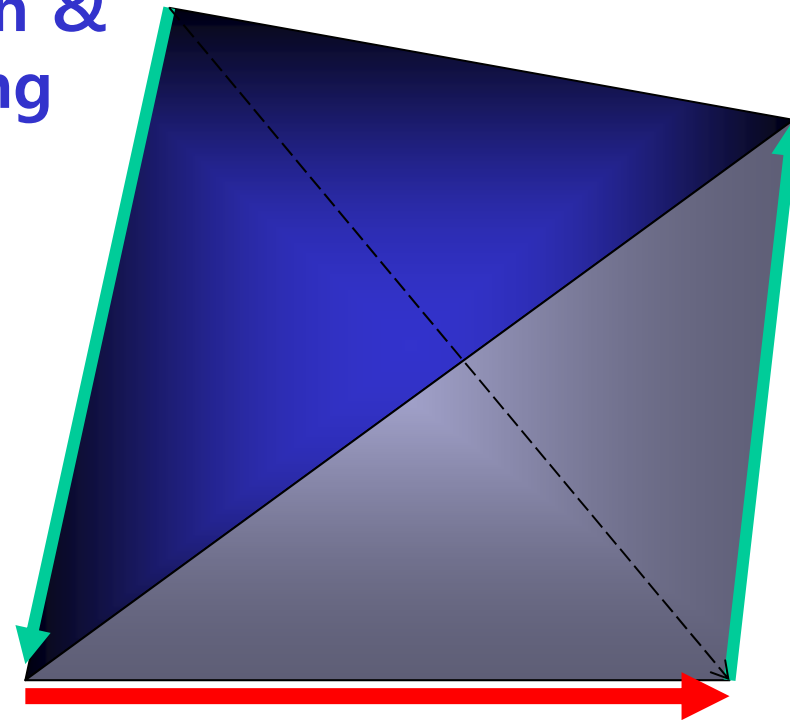
Policies and Procedures

- ***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 your own words.***
- **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

Alloy design &
Processing

Performance



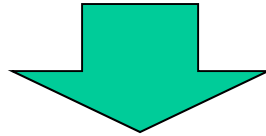
Microstructure
down to atomic scale

Properties

“Tailor-made Materials Design”

Alloy design + Process control →

Microstructure Control of Materials



Better Material Properties

Q1: What is alloy design?

“Materials selection”

1) Alloy design: a. Materials selection

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



Steel frame of building

1) Alloy design: Materials selection ➔ b. Change of alloy compositions

Application of **Iron-Carbon Alloy**

K1 – main battle tank of Korea army

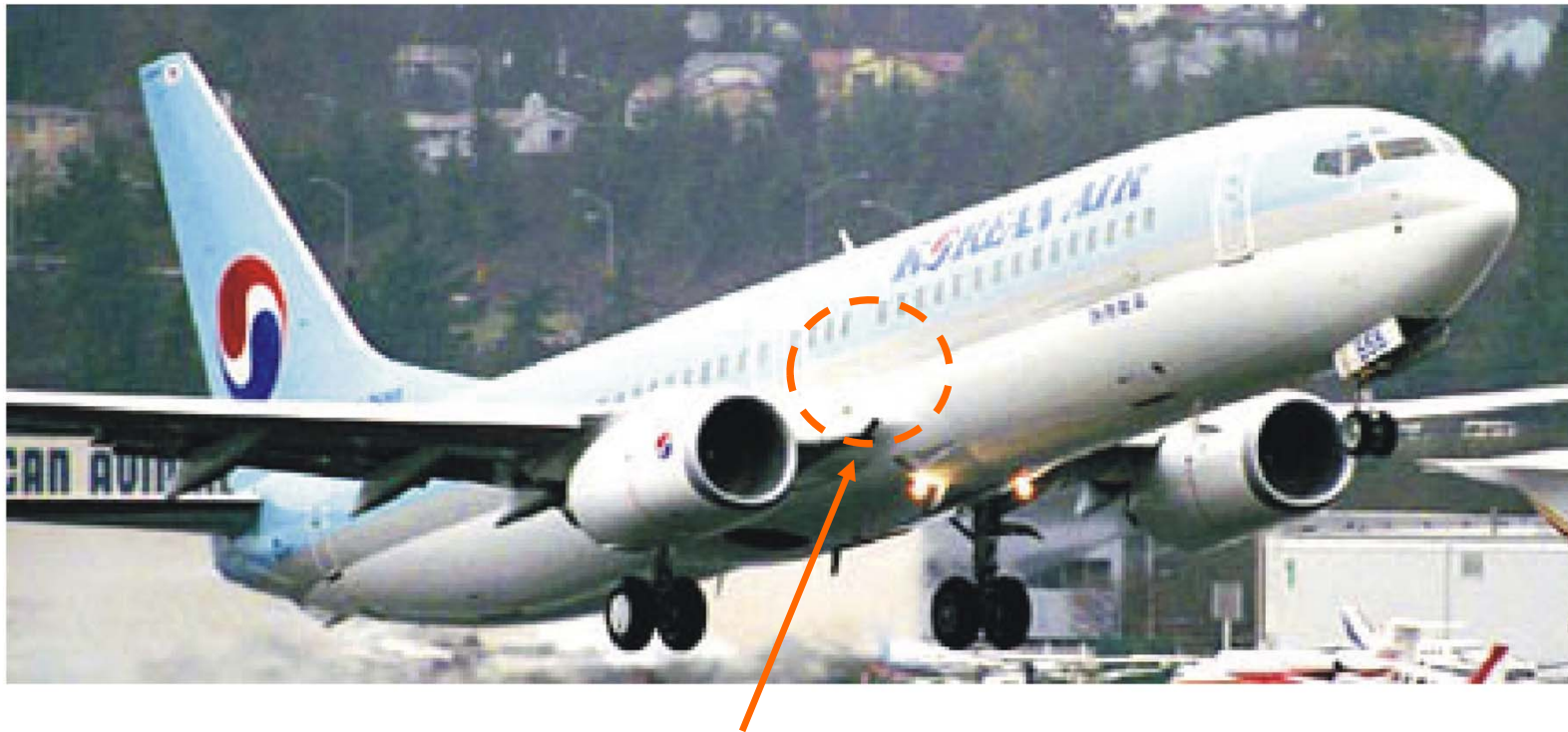


Need of the strongest materials

1) Alloy design: Materials selection ➔ c. Change of alloy system

Dominant Material for Airplanes ; **Aluminum Alloy**

B737-800 of Korean Air



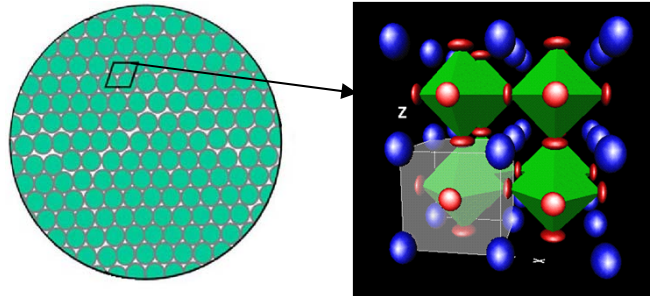
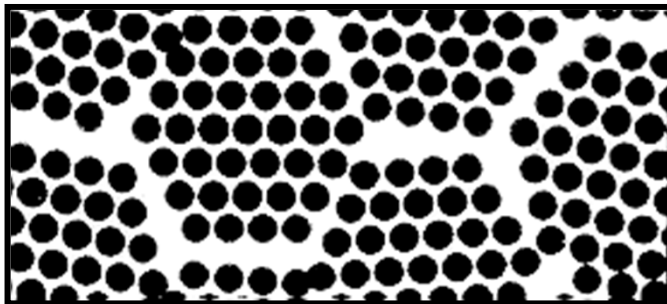
Need of light, strong and tough material

**Q2: How to classify material
depending on the structure?**

2) Classification of Material depending on the structure

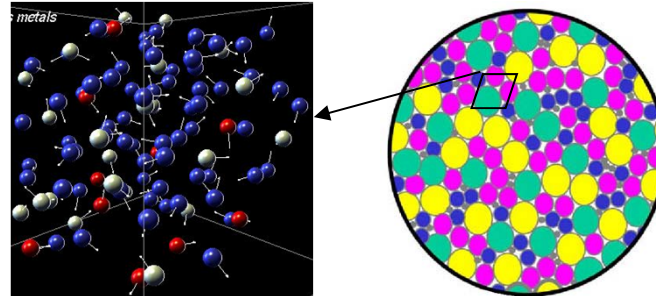
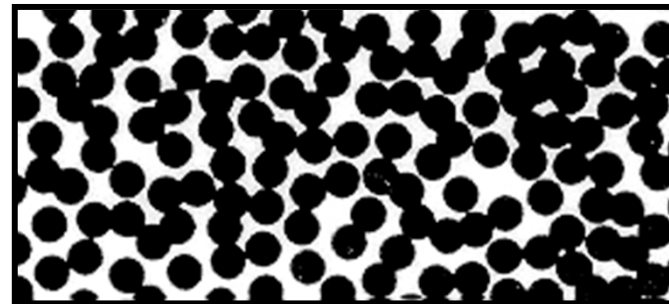
Structure of crystals, liquids and glasses

Crystals



- periodic
- grain boundaries

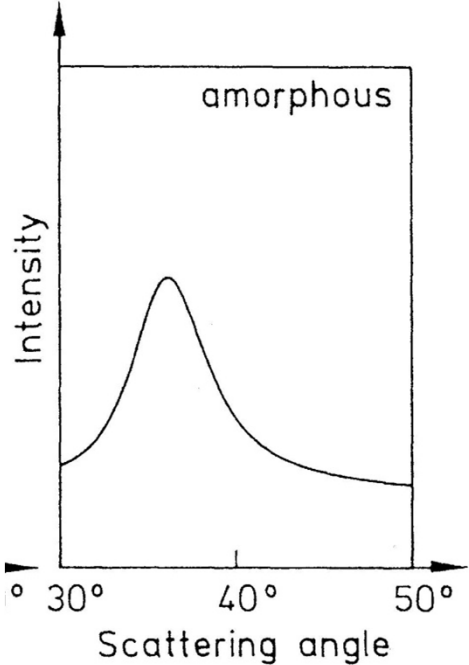
Liquids, glasses



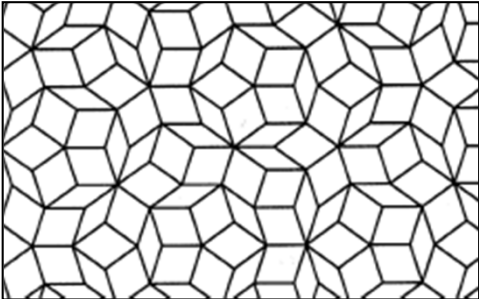
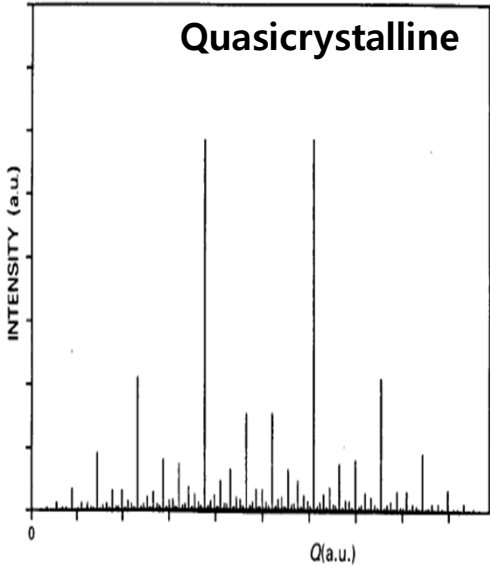
- amorphous = non-periodic
- no grain boundaries

Atomic structure

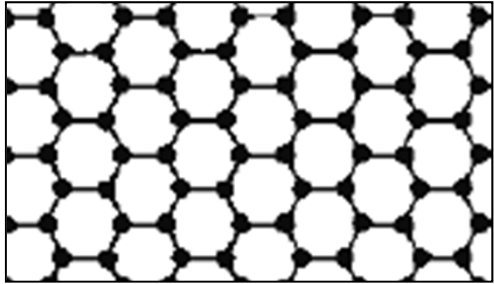
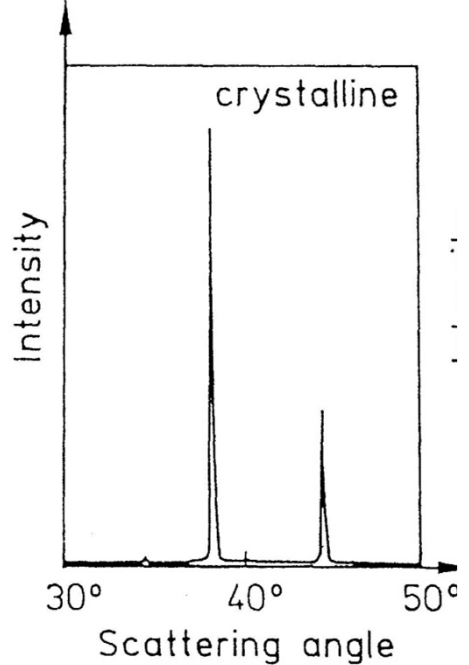
Short-range order



Quasi-periodic order



Periodic order



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

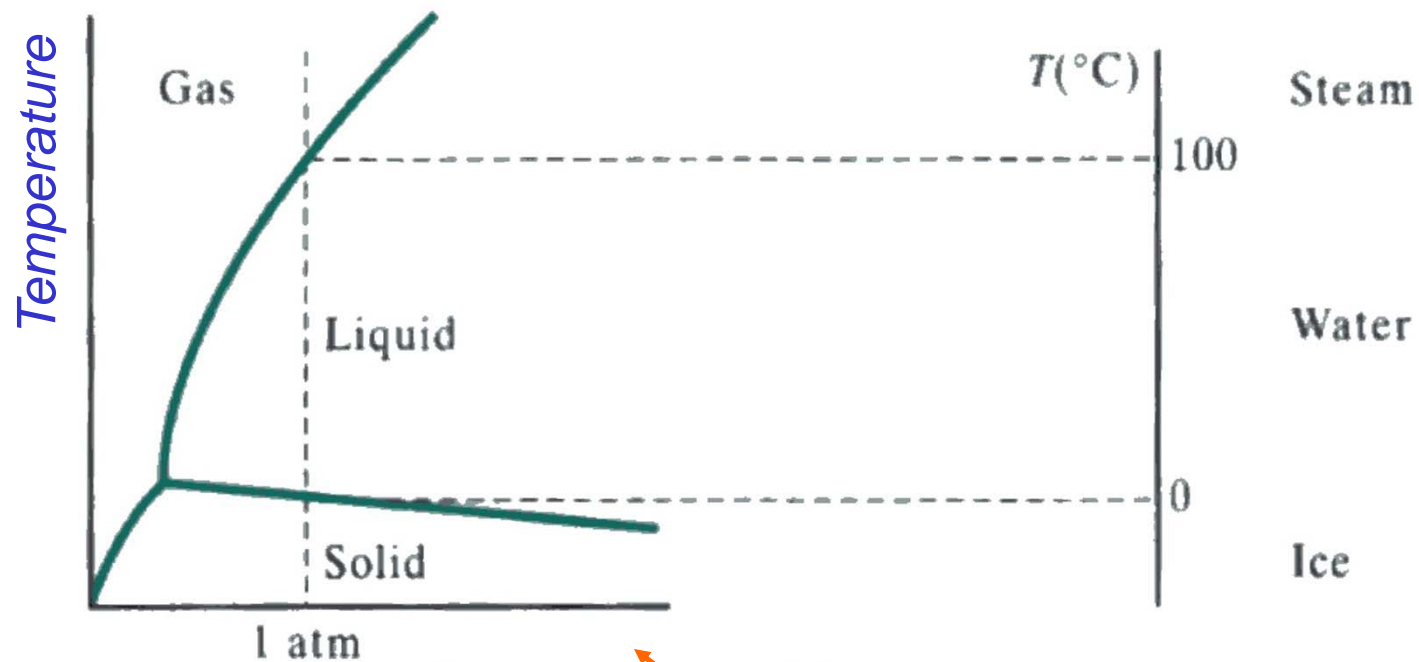
3) Microstructure control

: 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)



Pressure (log scale)

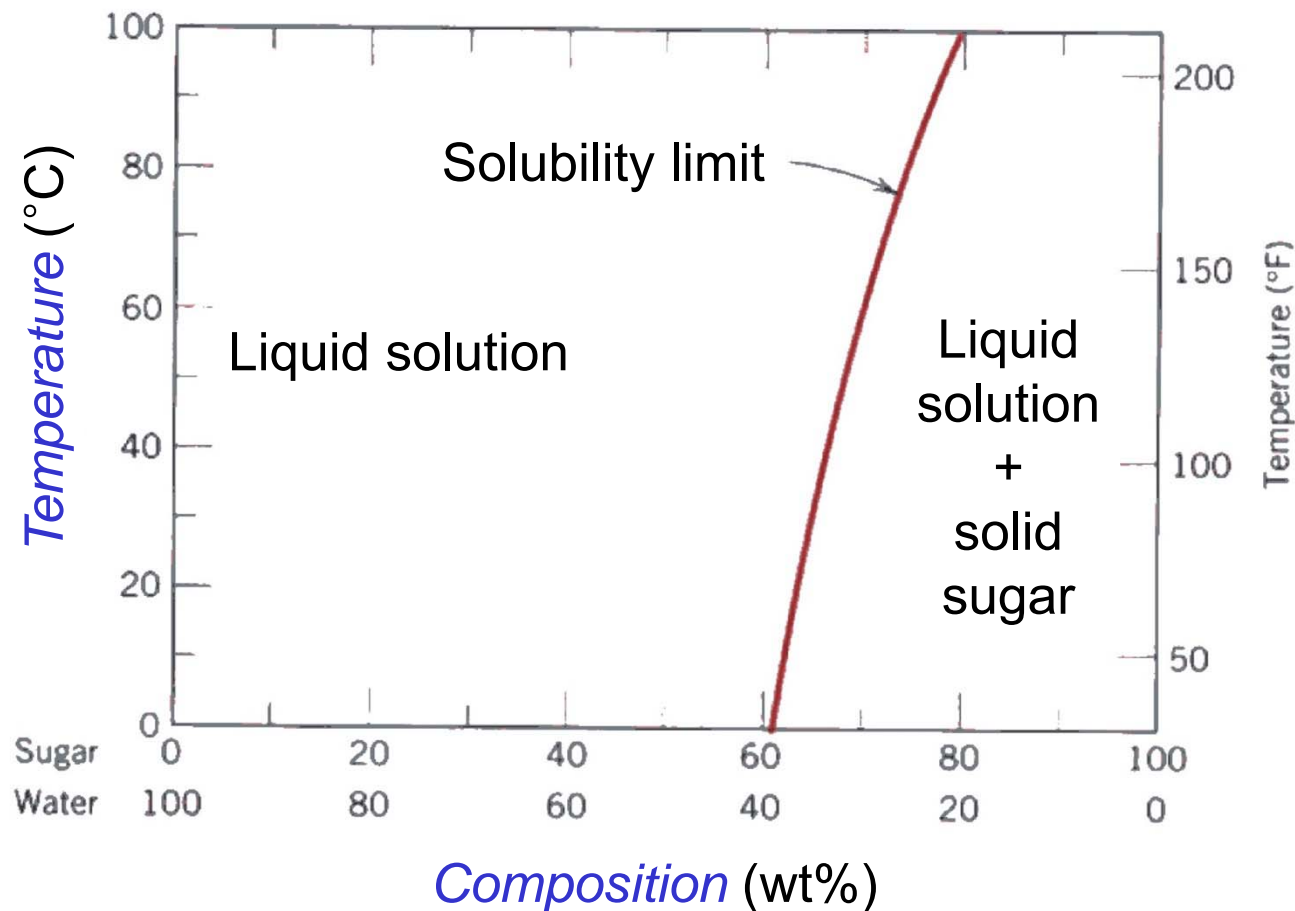
Phase diagram ;
equilibrium phase of material

Microstructure control

: Equilibrium phase → Only consider Thermodynamics

② *Phase Diagram* of Temperature – Composition ;

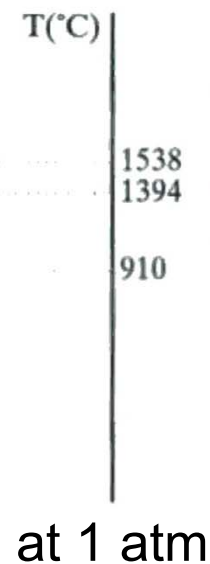
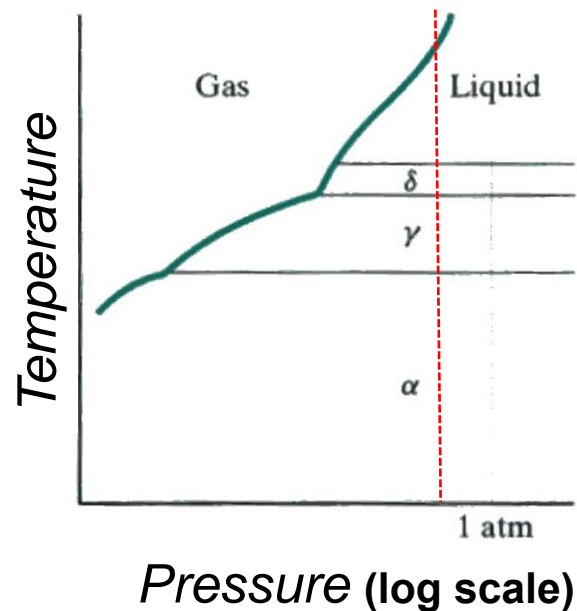
most useful in materials science & engineering



Microstructure control

: Phase transformation → Atomic Migration

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

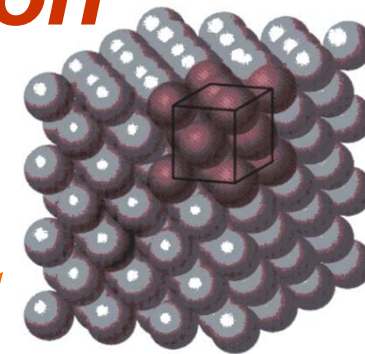


Liquid

δ

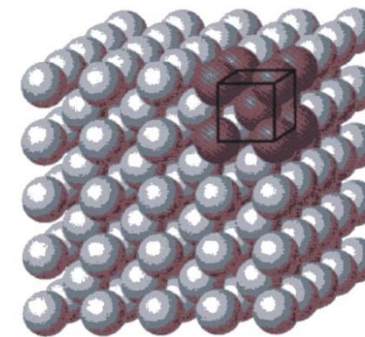
γ (austenite)

α (ferrite)



Face-Centered Cubic

↕ Atomic Migration ↕



Body-Centered Cubic

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,

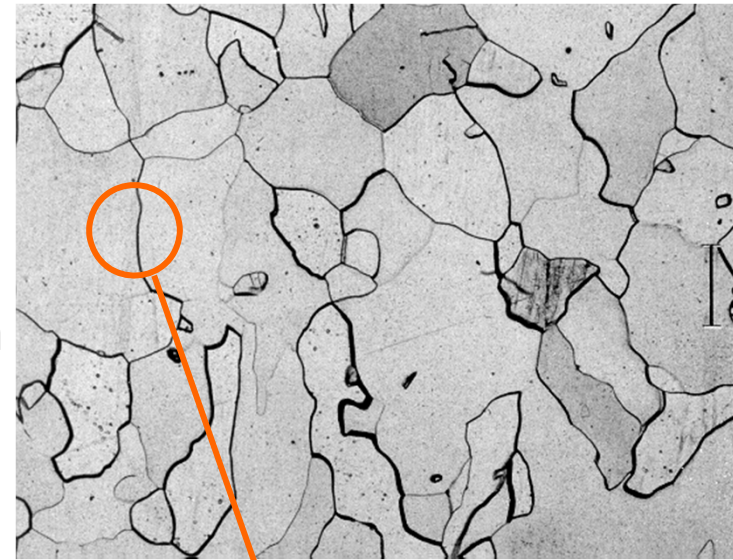
Dislocations (and other line defects), and

Point defects (such as interstitials and vacancies as well as solute atoms in solution)

* Imperfection: Grain Boundaries (Planer defect)



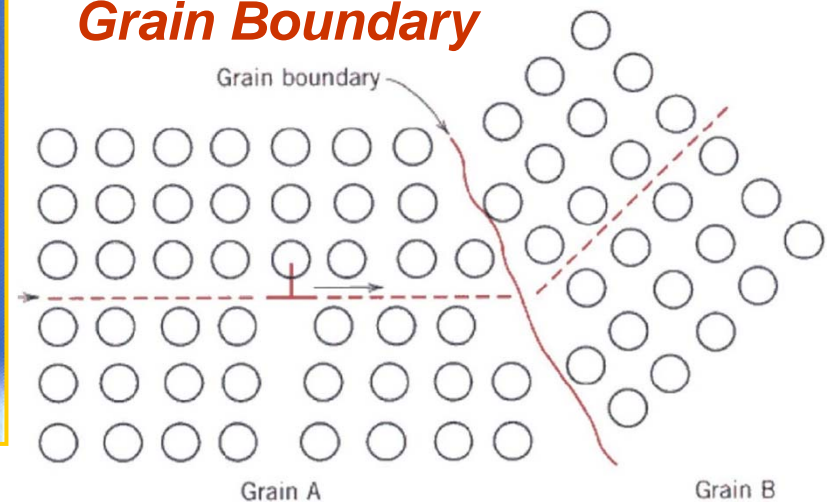
Low Carbon Steel



Optical
Microscope



Grain Boundary

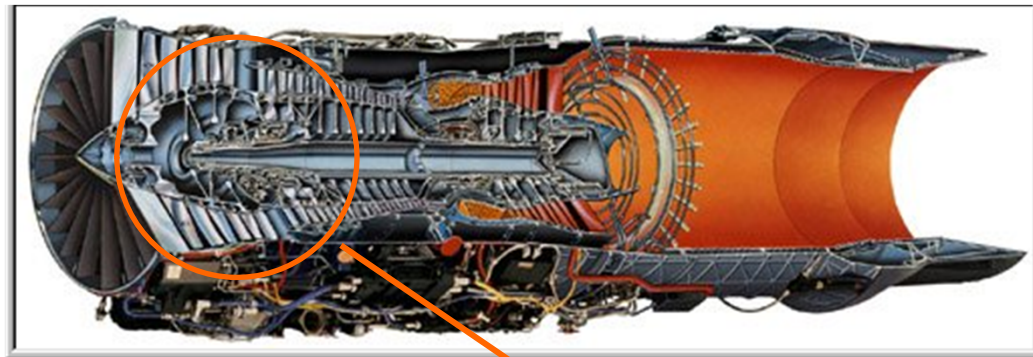


**Q5: How to control the microstructure
by process control?**

5) Microstructure control

: process control after materials selection → property optimization

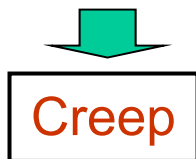
A Example of ① Grain Boundary Engineering ; Turbine blade in Aircraft Engine



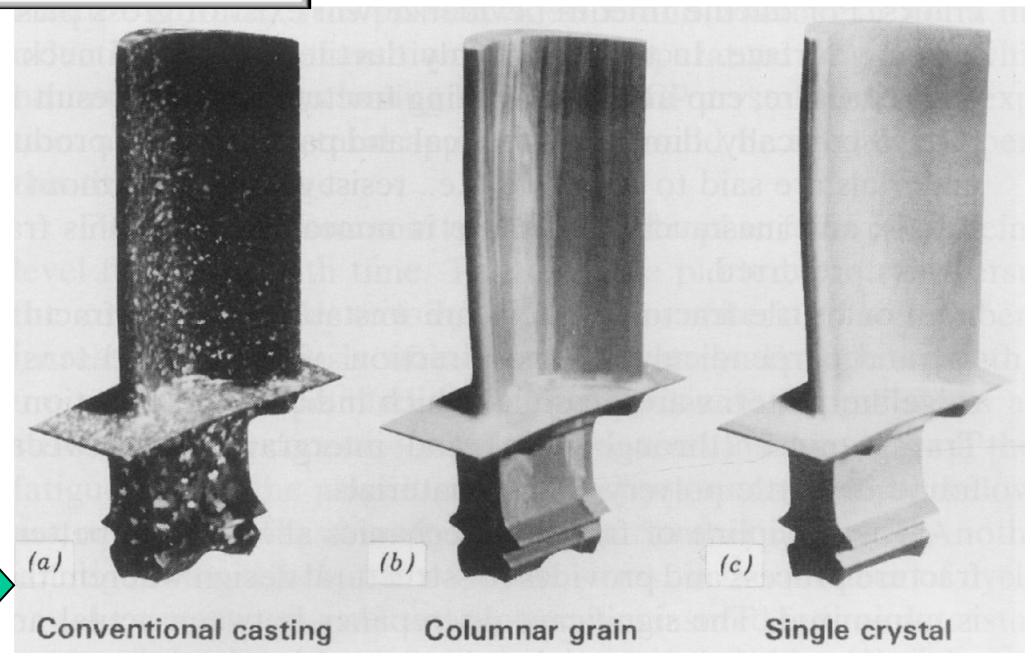
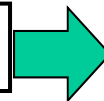
F100-PW-229
in F-16 fighting falcon

Turbine Blade

Grain boundaries
at high Temperature ;
Diffusion path of atoms

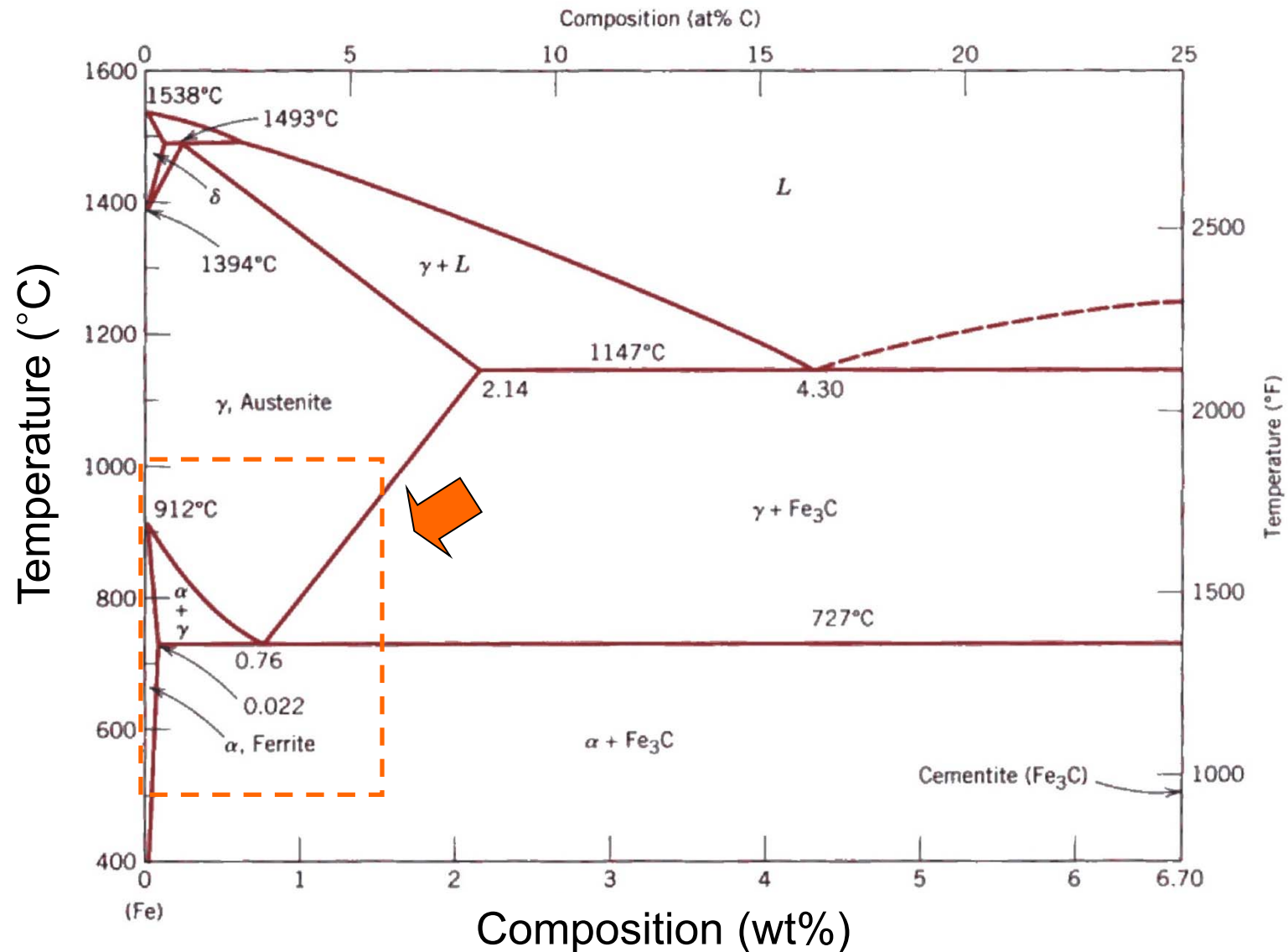


Reducing grain boundaries



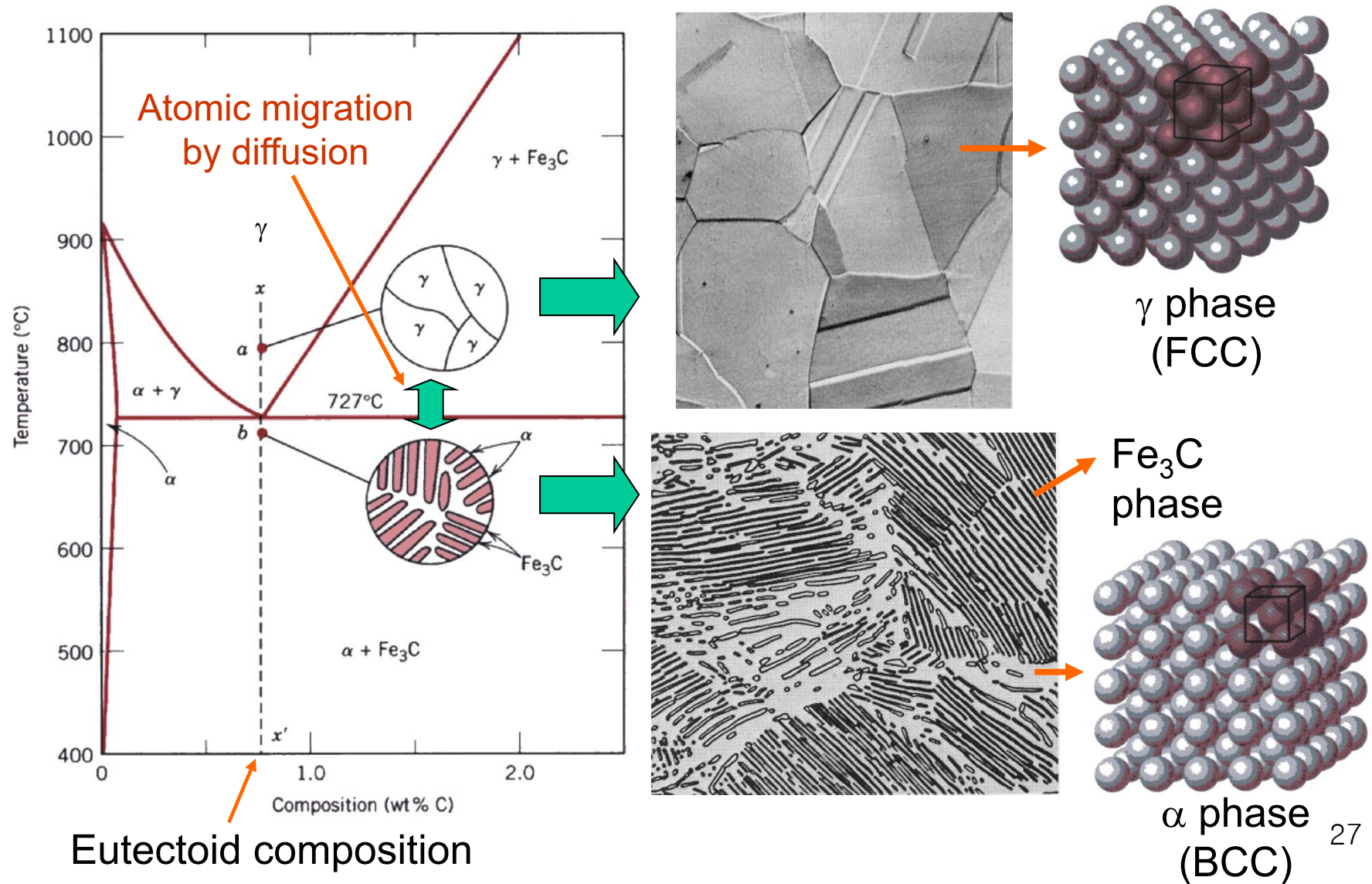
5) Microstructure control : ② Secondary phase control

a. Phase Diagram of Iron–Carbon Alloy



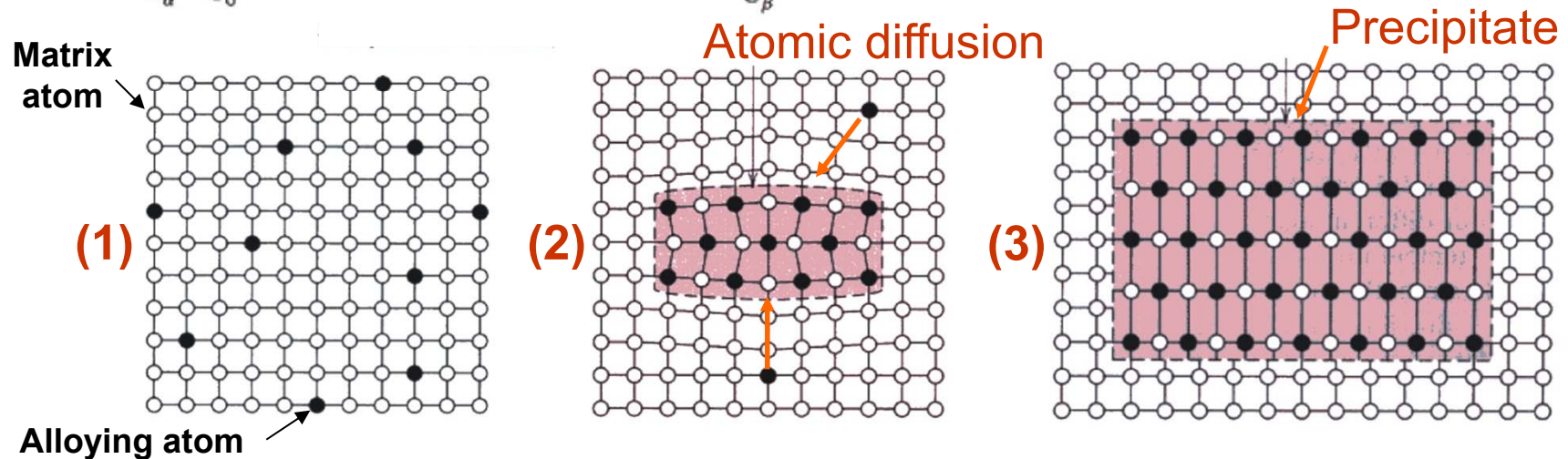
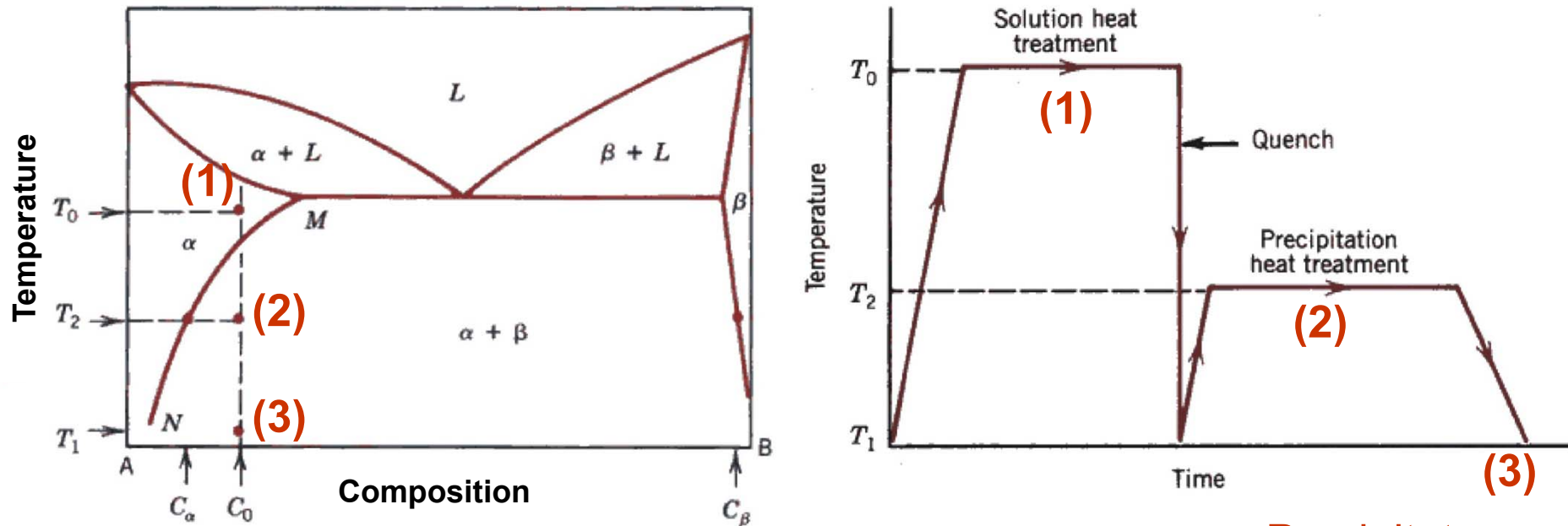
5) Microstructure control : ② Secondary phase control

b. Equilibrium Phases of Iron-Carbon Alloy



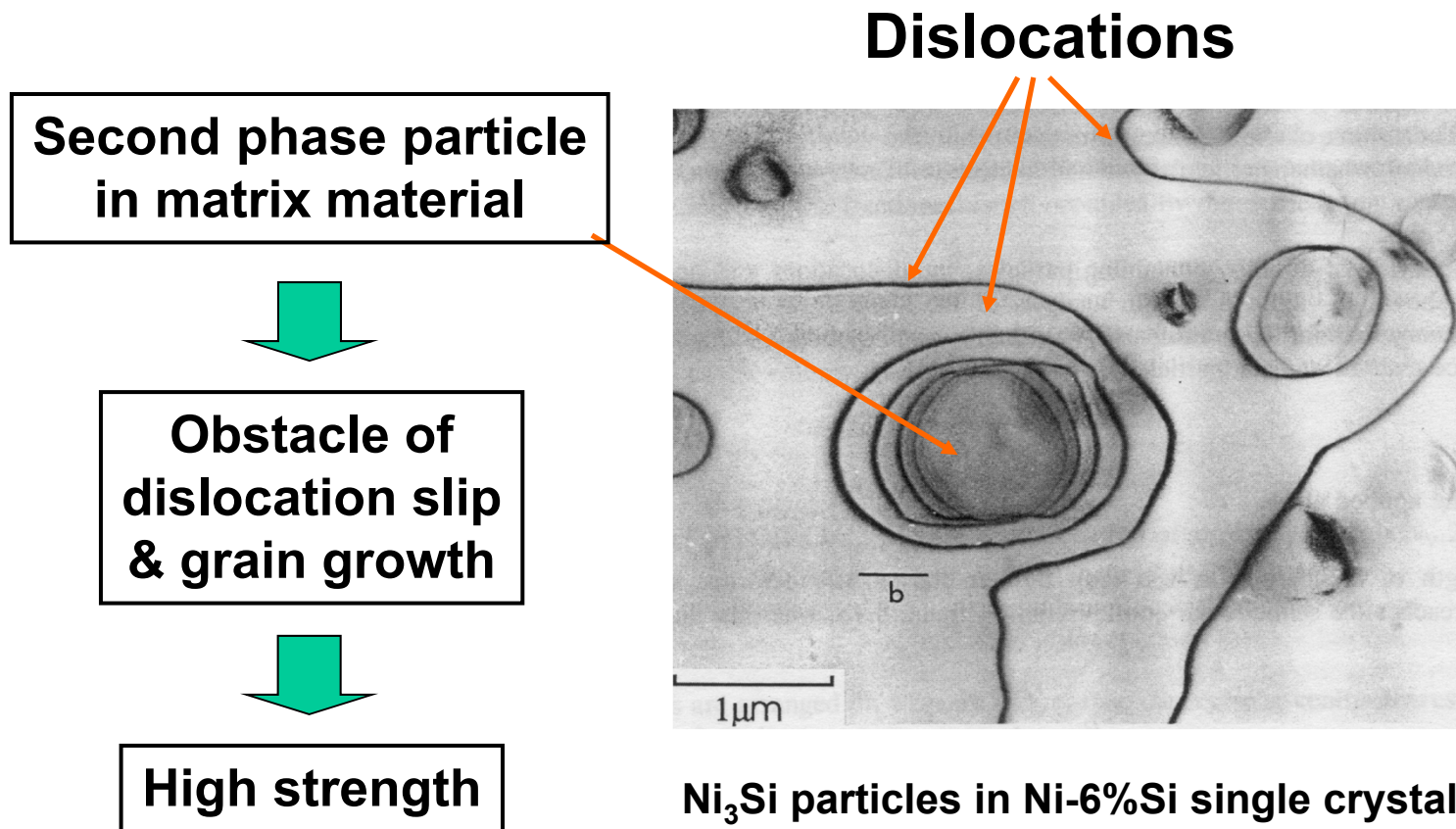
5) Microstructure control : ② Secondary phase control

c. Mechanism of Precipitation



5) Microstructure control : ② Secondary phase control

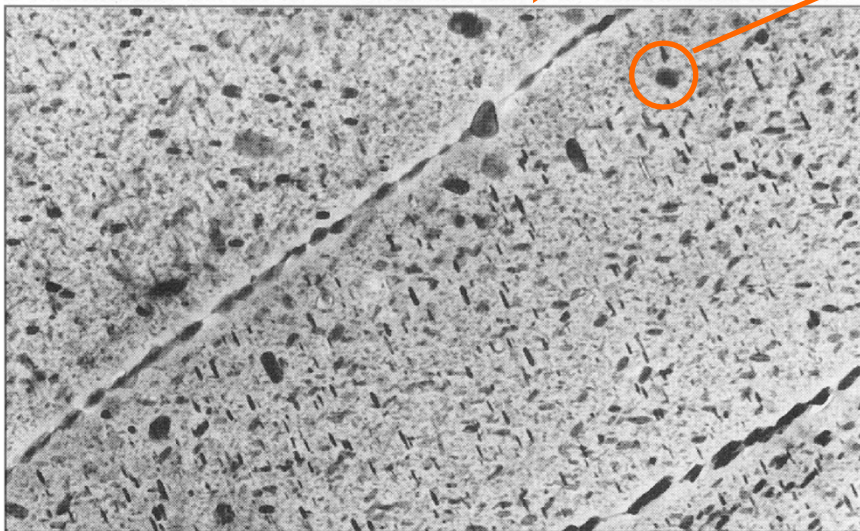
d. Effect of Second Phase Particle on Mechanical Property



5) Microstructure control : ② Secondary phase control

e. Control of Microstructures by Precipitation Transformation in Aluminum Alloy

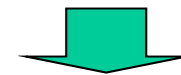
Boeing 767 by AA7150 T651 alloy



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

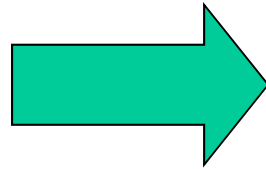
6) Microstructure optimization by process control

Hardening Mechanism by Cold Working



Before cold work

Deformation
or
Cold work



Aluminum alloy

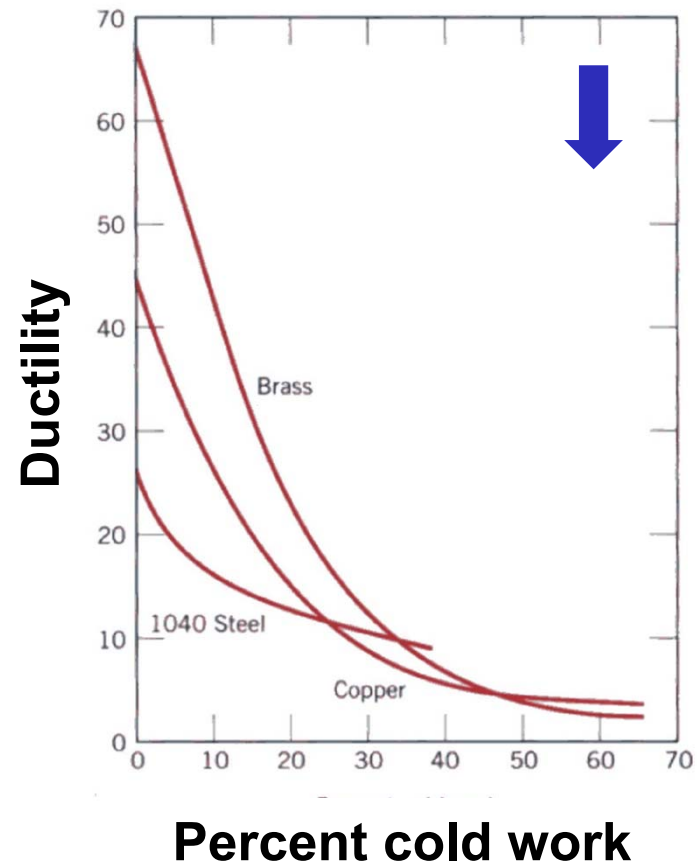
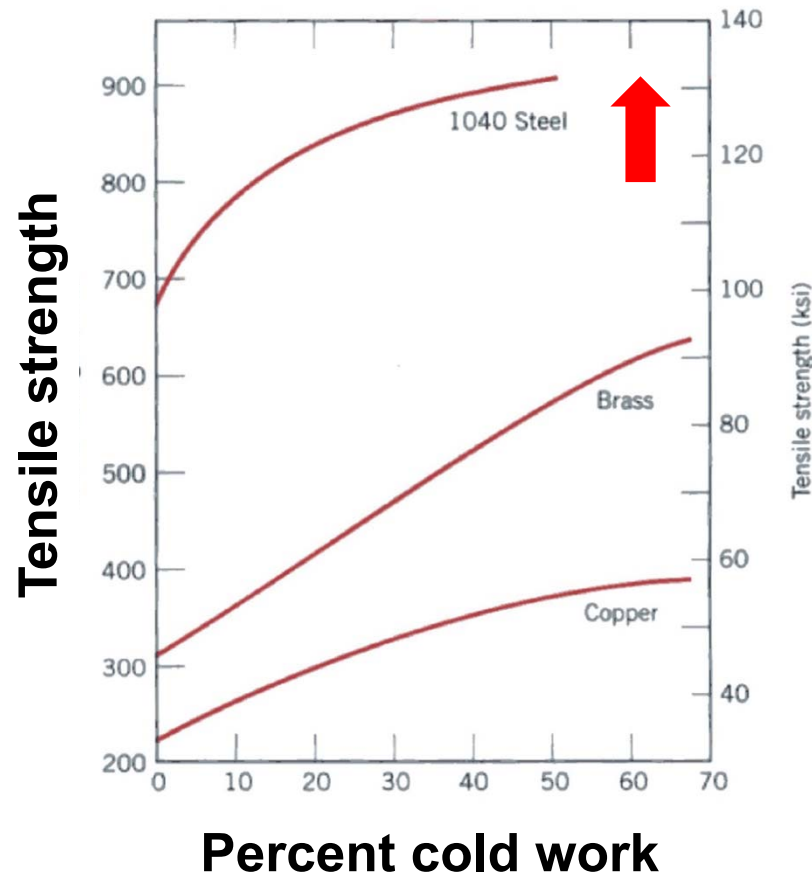


Accumulation
of dislocations

Dislocation tangle

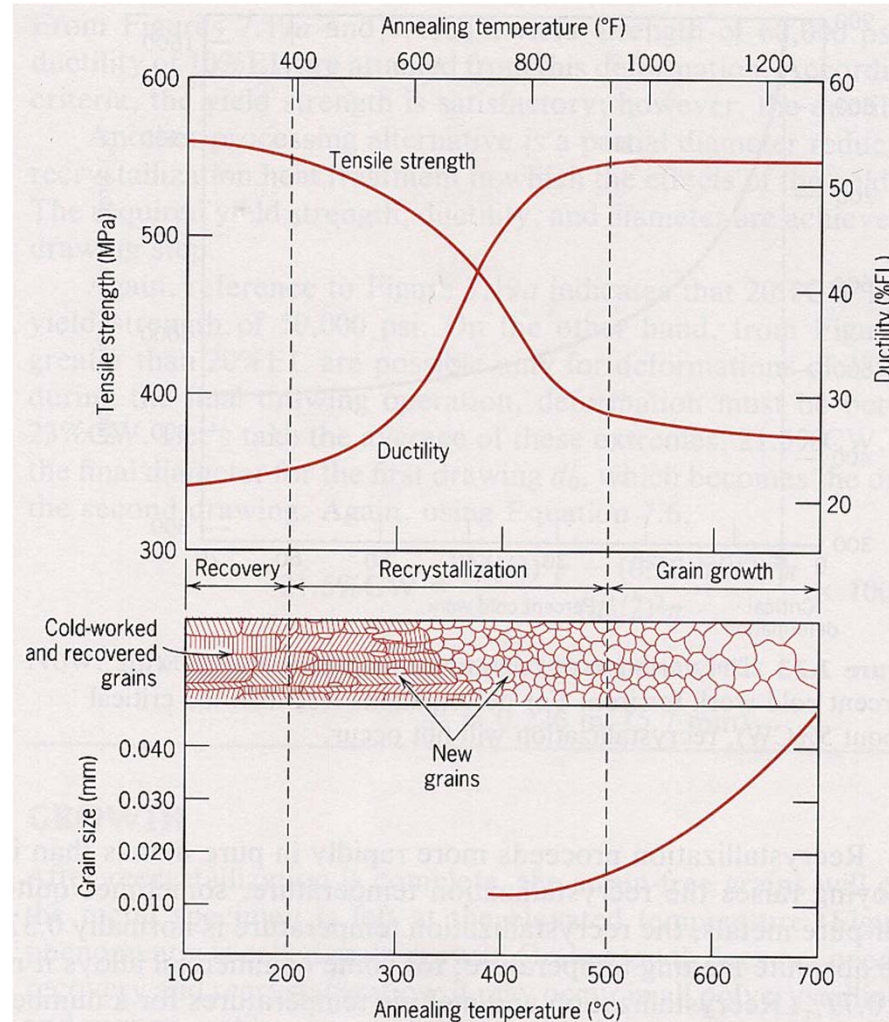
6) Microstructure optimization by process control

Changes of Strength and Ductility by Cold Working



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”

7) Alloy design + Process control → Property optimization

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

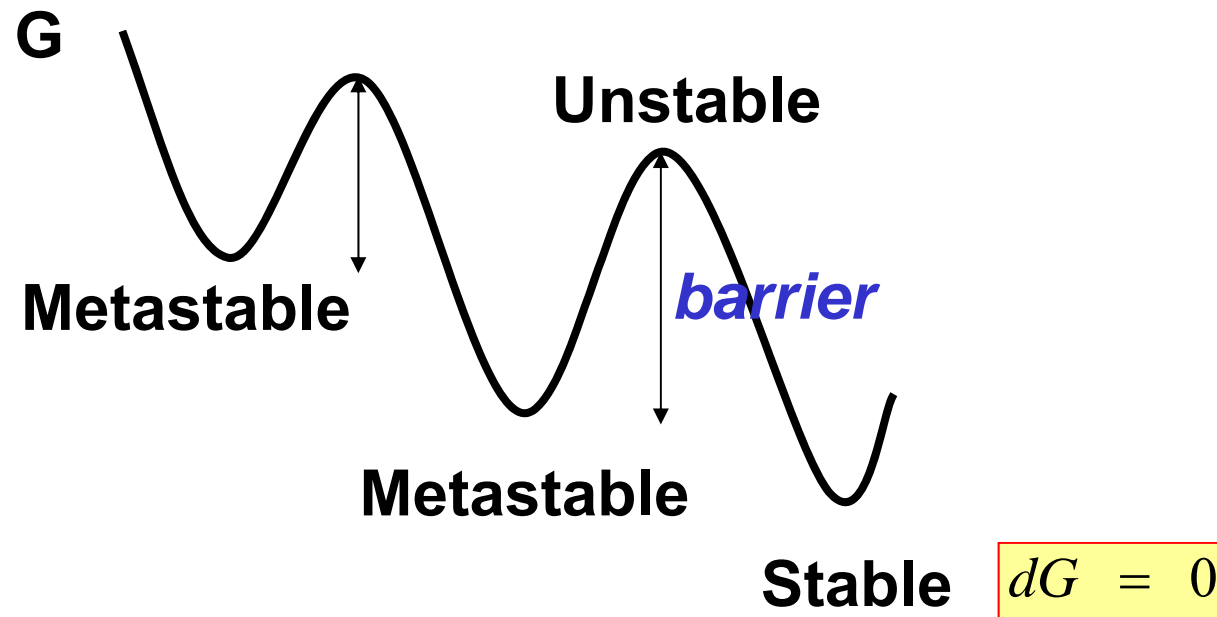
$$\Delta G = G_2 - G_1 < 0$$

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



How does thermodynamics differ 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

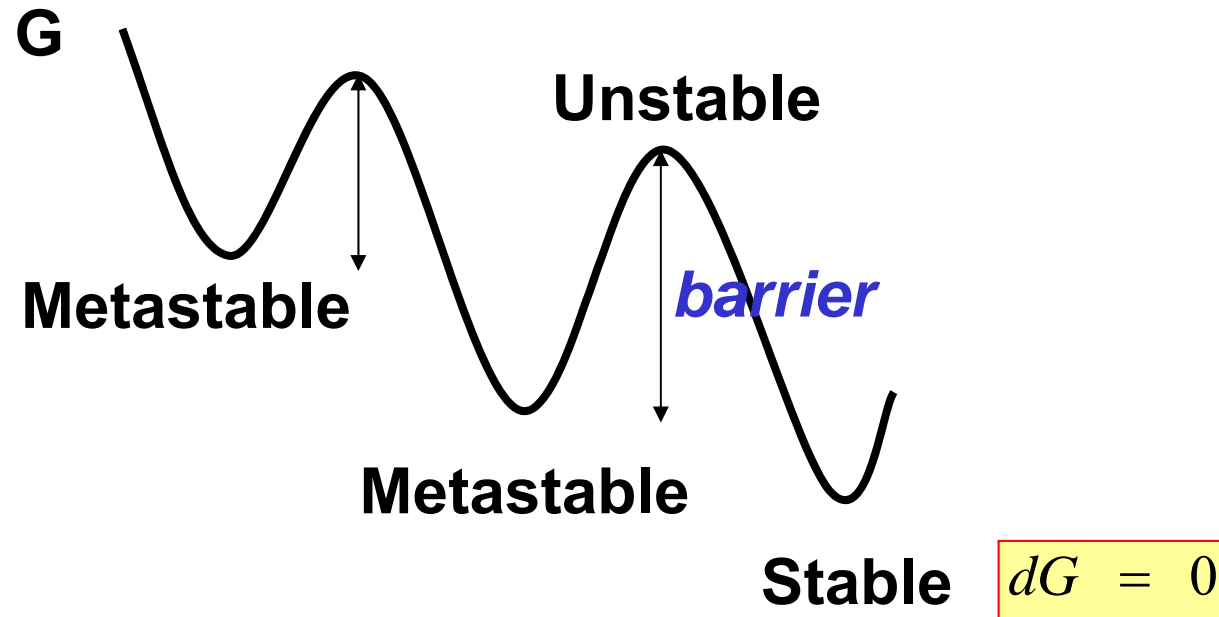
$$\Delta G = G_2 - G_1 < 0$$

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



→ Governed by Thermodynamics & Kinetics

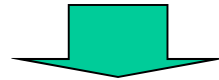
Q9: What are the representative PTs?

9) Representative Phase Transformation

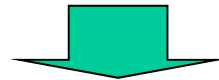
- **Solidification: Liquid \rightarrow Solid**
- **Phase transformation in Solids**
 - ① **Diffusion-controlled phase transformation ;**
Generally long-distance atomic migration
 - Precipitation transformation
 - Eutectoid transformation (**S \rightarrow S₁ + S₂**)
 - etc.
 - ② **Diffusionless transformation ;**
Short-distance atomic migration
 - Martensitic transformation

① Diffusion-controlled phase transformation

Diffusion- Controlled Phase Transformation
time dependency



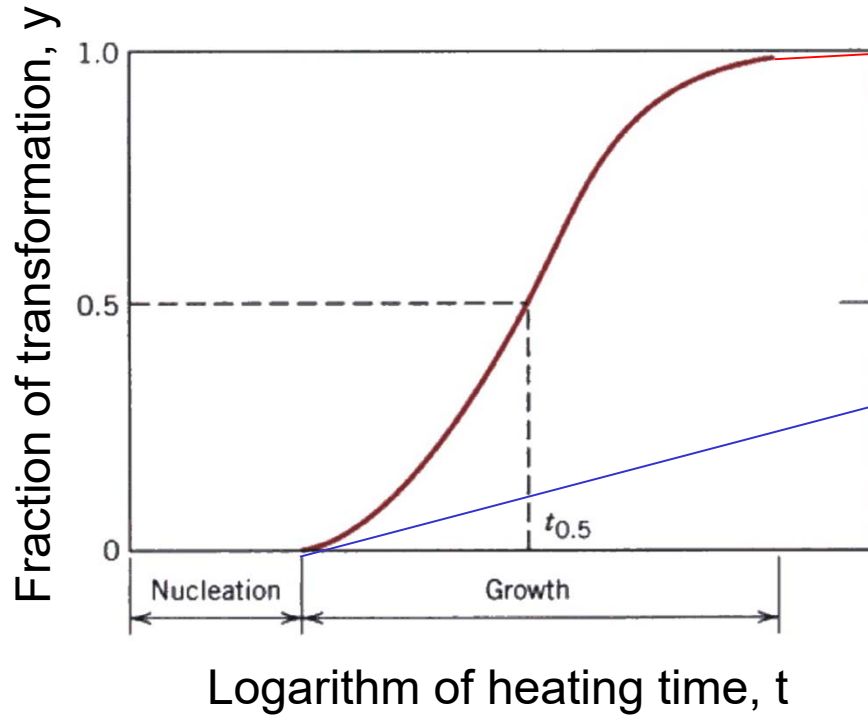
Non-Equilibrium Phases → Equilibrium phase



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

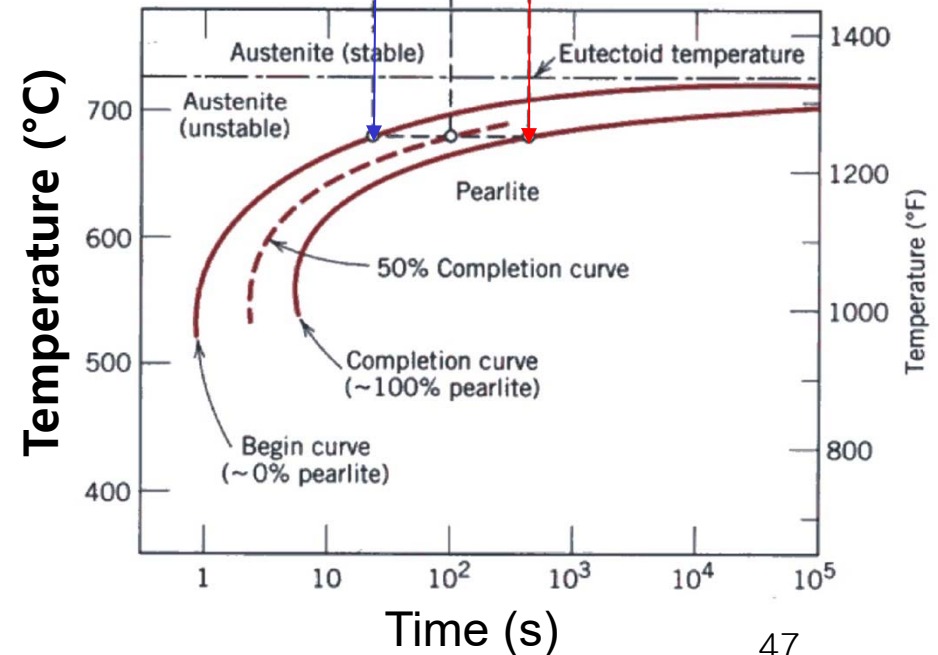
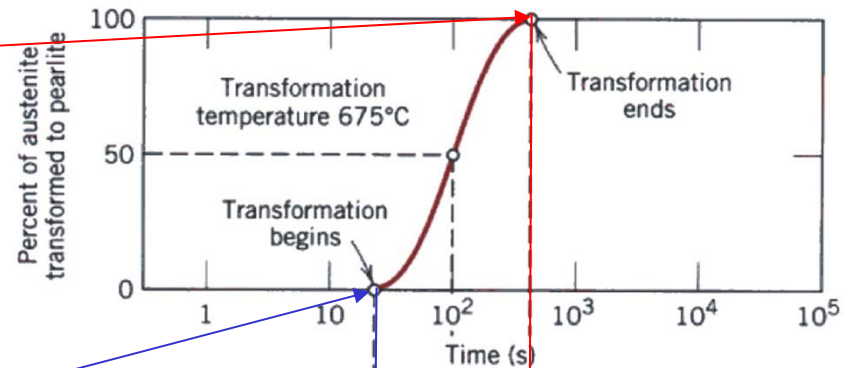
Transformation Kinetics :

b. Isothermal Transformation Diagram



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

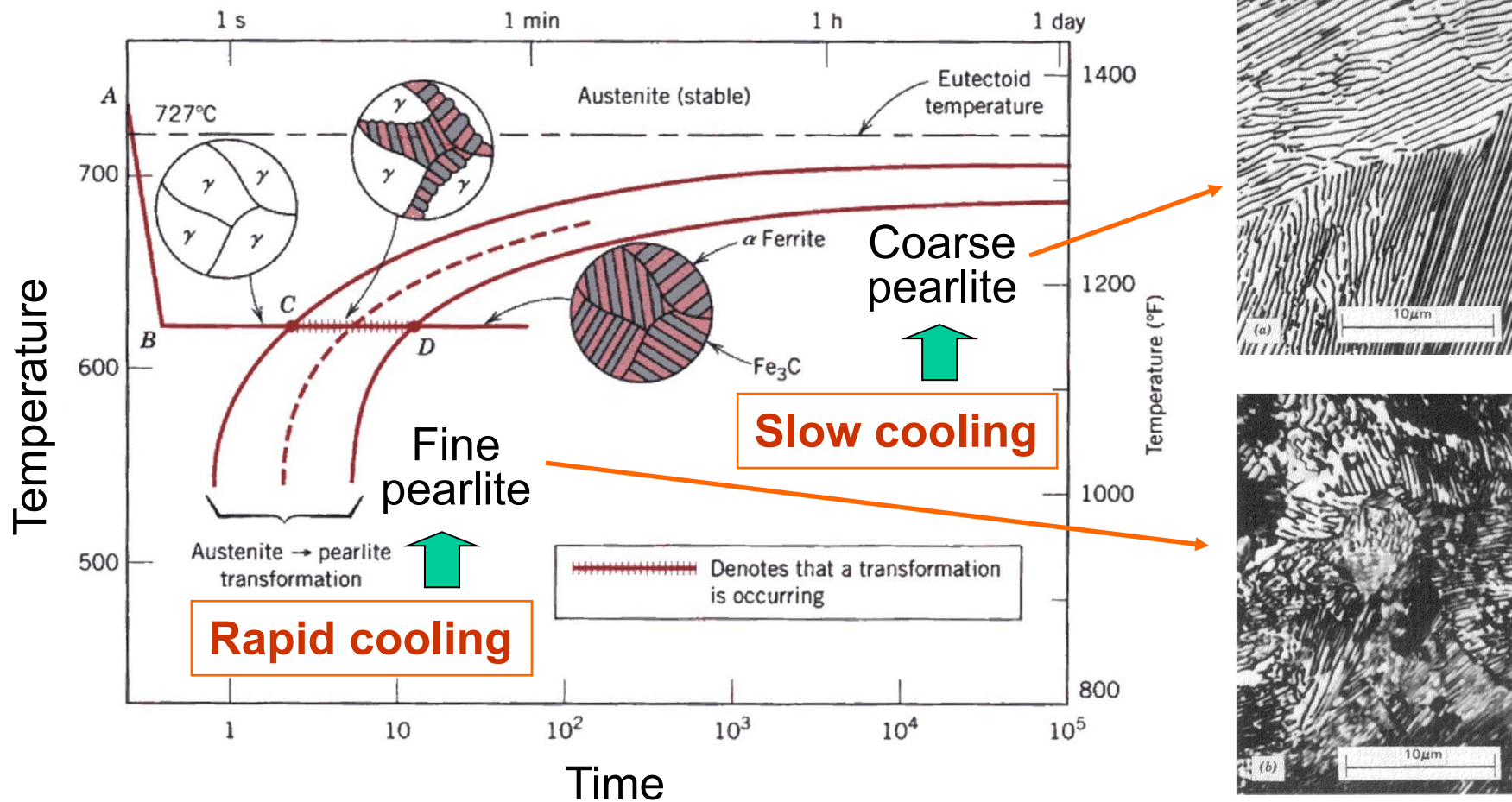
Kinetics of diffusion-controlled solid-state transformation



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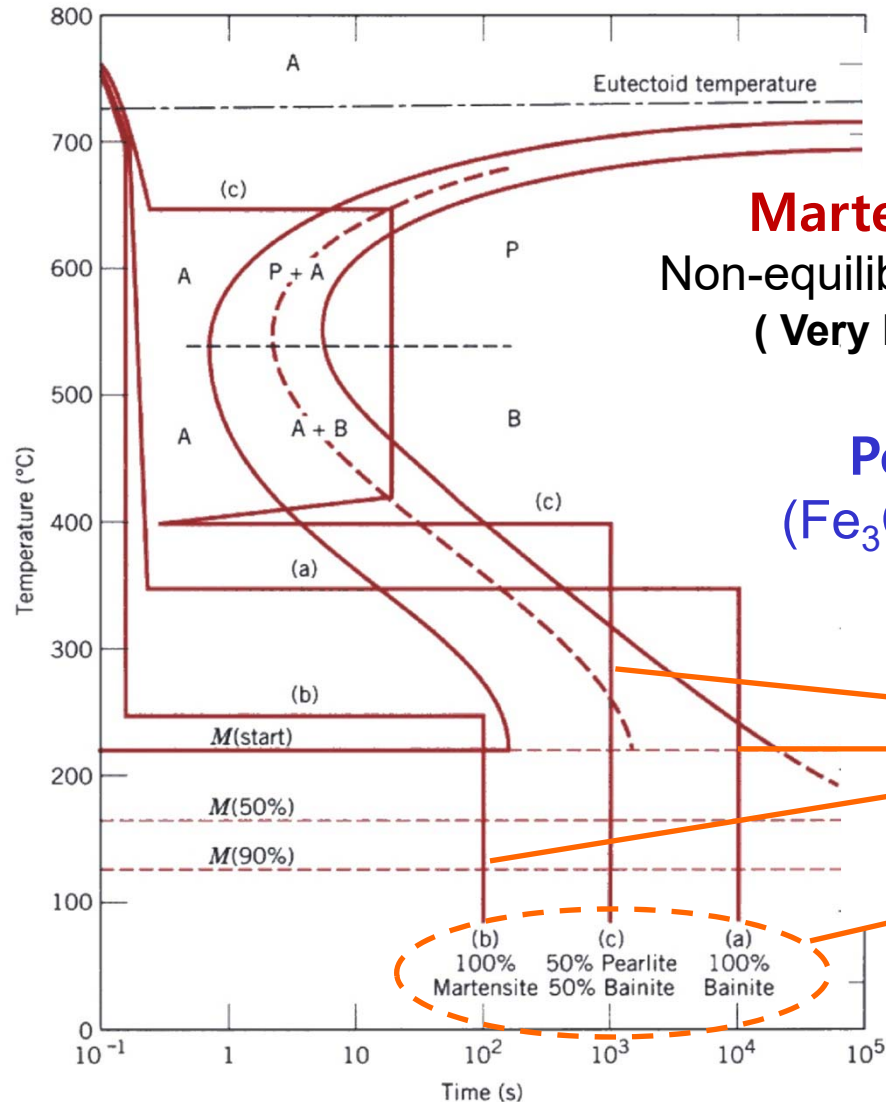
TTT diagram → Isothermal transformation diagram

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



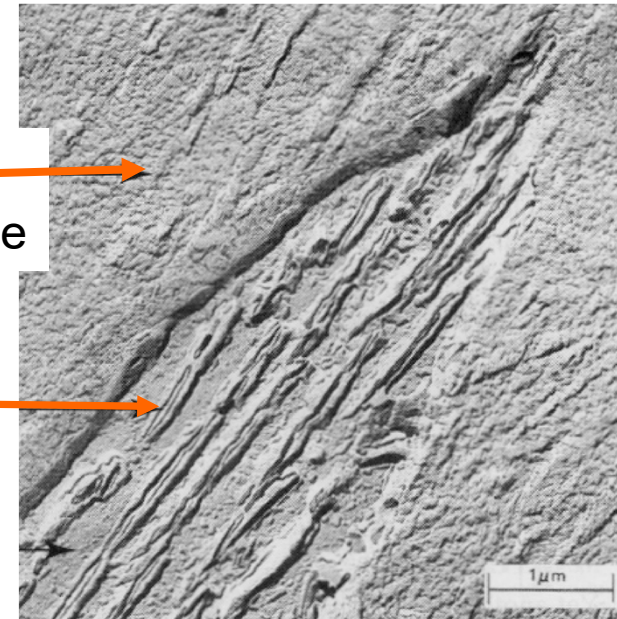
Microstructure control by phase transformation

d. Control of Phases by Heat Treatment



Martensite ;
Non-equilibrium phase
(Very hard)

Pearlite
(Fe₃C+ferrite)



Heat Treatment

Process control

Phase & Microstructure

Properties of Material

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



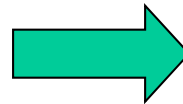
Martensite

Tip of needle shape grain

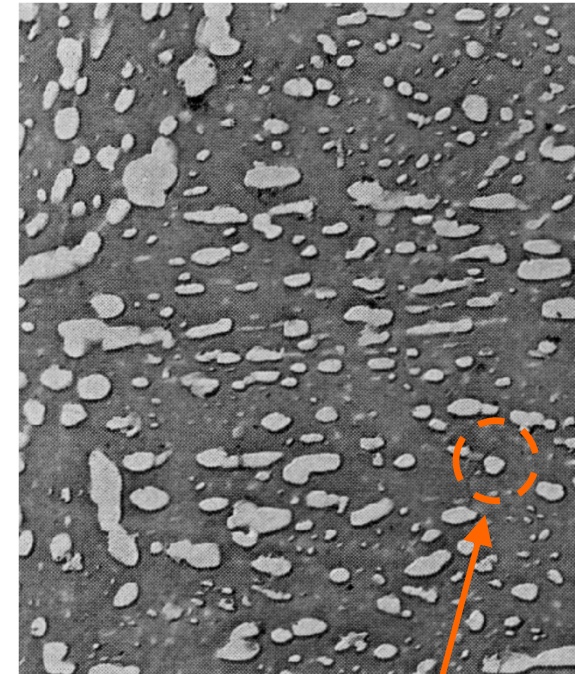
Nucleation site of fracture

Brittle

Process control



Proper heat treatment
(tempering)



Tempered martensite

Very small & spherical shape grain

Good strength, ductility, toughness

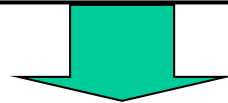
② Diffusionless Transformation

Individual atomic movements are less than one interatomic spacing.

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

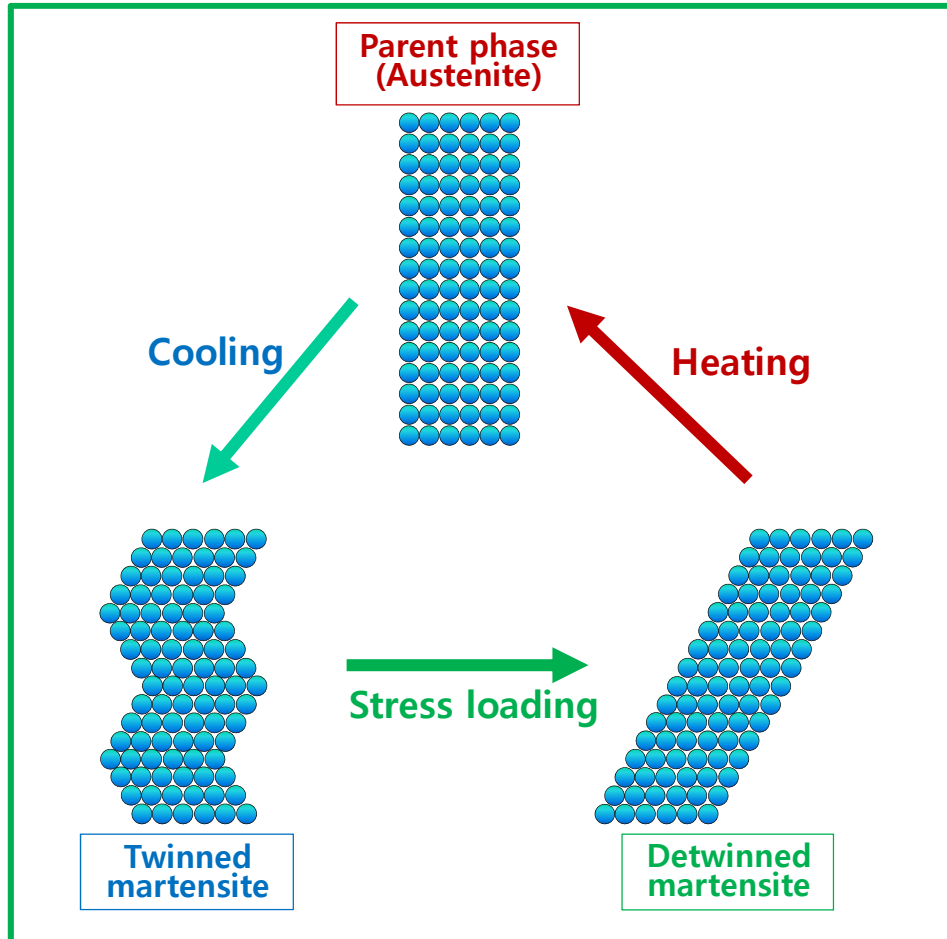
e.g. b Martensitic transformation in Ni-Ti alloy ;

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

Alloy design &
Processing

Performance

“Phase Transformation”

Microstructure
down to atomic scale

Properties

“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