



EVROPSKÁ UNIE  
Evropské strukturální a investiční fondy  
Operační program Výzkum, vývoj a vzdělávání



Audio test:



# Materials and its structure

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## Brno, PS

Tento učební materiál vznikl v rámci projektu Rozvoj doktorského studia chemie  
č. CZ.02.2.69/0.0/0.0/16\_018/0002593

# Material

## [Material - Wikipedia](#)

**Material** is a [substance](#) or [mixture](#) of substances that constitutes an [object](#). Materials can be pure or impure, living or non-living matter. Materials can be classified on the basis of their [physical](#) and [chemical properties](#), or on their [geological](#) origin or [biological](#) function. [Materials science](#) is the study of materials, their properties and their applications.

Materials can be broadly categorized in terms of their use, for example:

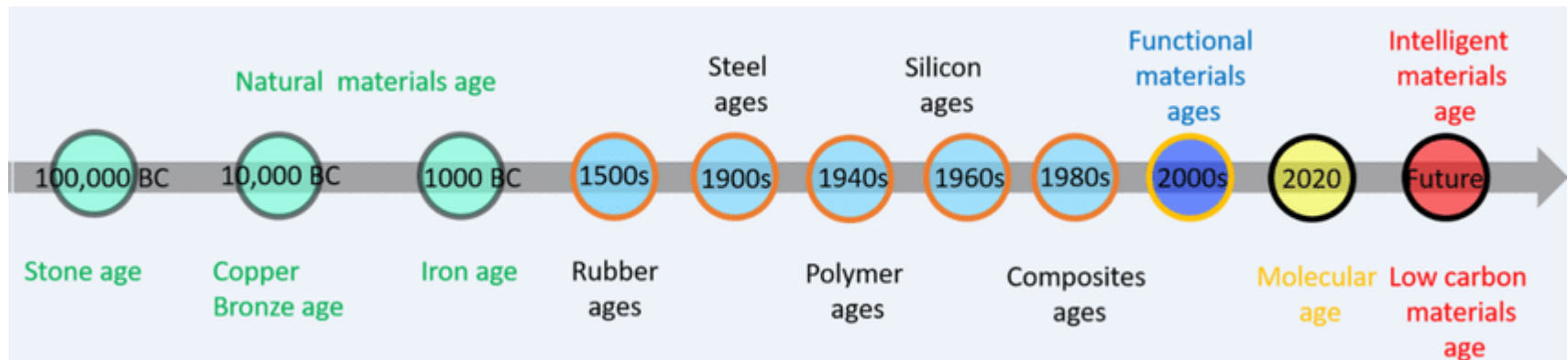
- [Building materials](#) are used for construction
- [Building insulation materials](#) are used to retain heat within buildings
- [Refractory materials](#) are used for high-temperature applications
- [Nuclear materials](#) are used for nuclear power and weapons
- [Aerospace materials](#) are used in aircraft and other aerospace applications
- [Biomaterials](#) are used for applications interacting with living systems

[Material selection](#) is a process to determine which material should be used for a given application.

# History and technologies

Materials chart the history of humanity. The system of the three prehistoric ages ([Stone Age](#), [Bronze Age](#), [Iron Age](#)) were succeeded by historical ages: steel age in the 19th century, polymer age in the middle of the following century (plastic age) and silicon age in the second half of the 20th century.<sup>[2]</sup>

[The timeline for major materials \(reproduced with permission from Liu... | Download Scientific Diagram \(researchgate.net\)\)](#)



# Linear economy vs. Circular economy

LINEAR ECONOMY



RECYCLING ECONOMY

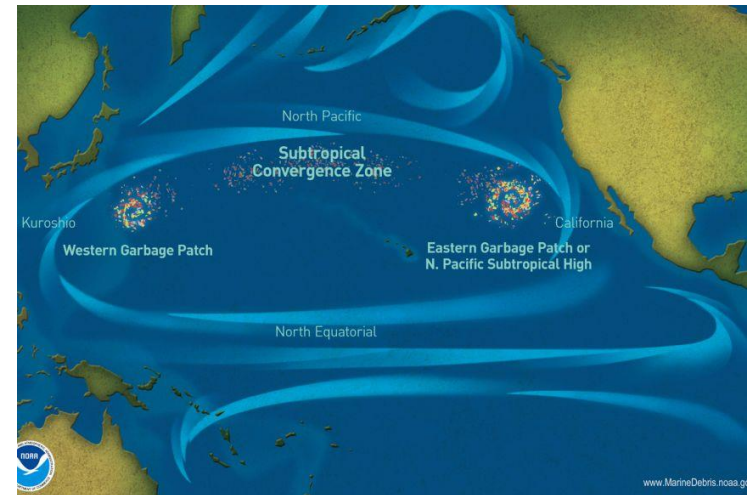


CIRCULAR ECONOMY



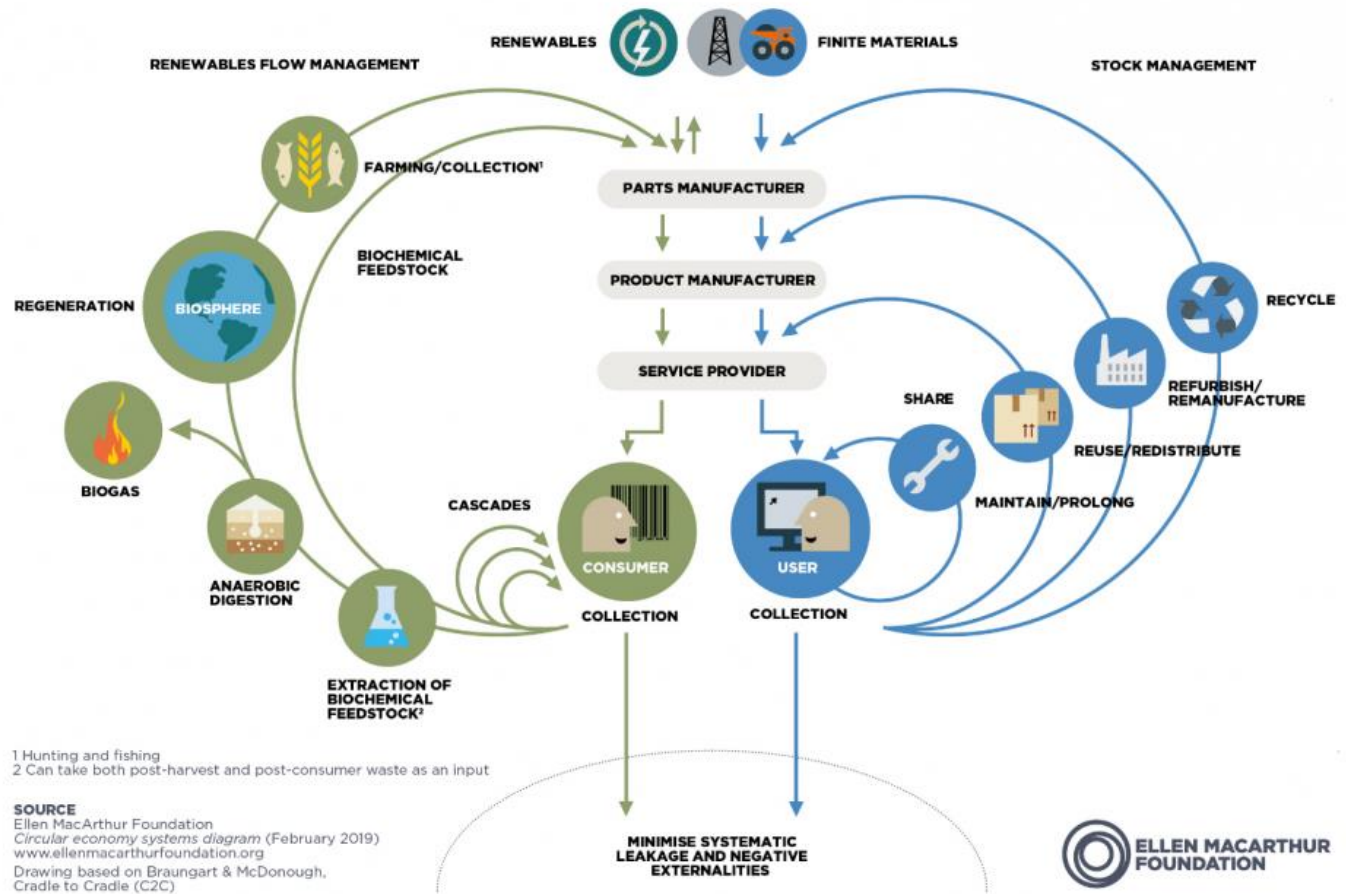
[Circular Economy](#)  
[Resource Box \(KS3/4\) -](#)  
[Zone \(recycledevon.org\)](#)

[Great Pacific Garbage Patch](#)  
[\(nationalgeographic.org\)](#)



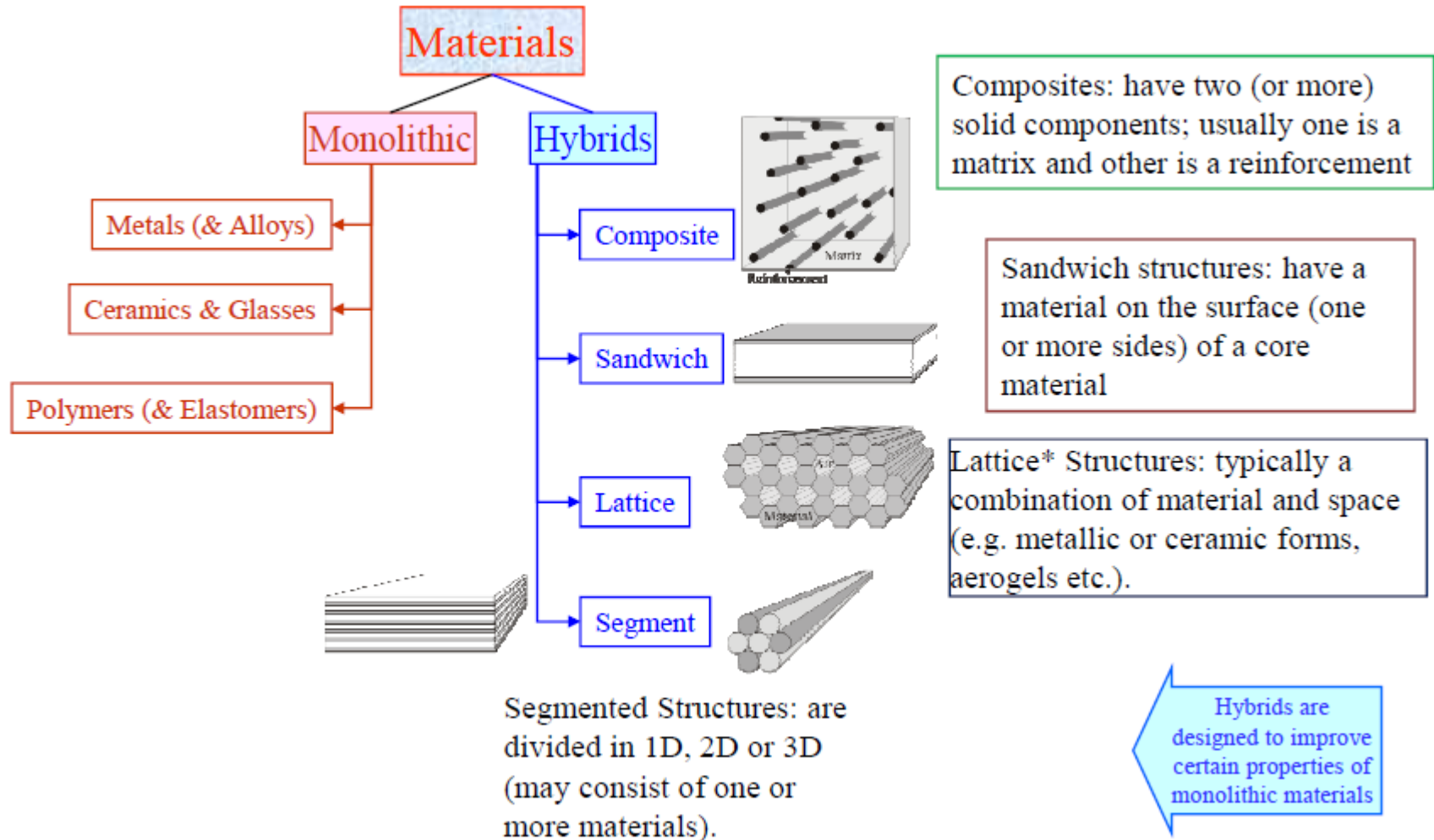
# Circular Economy

A circular economy keeps materials, products, and services in circulation for as long as possible.



# Material classification

According Kumar

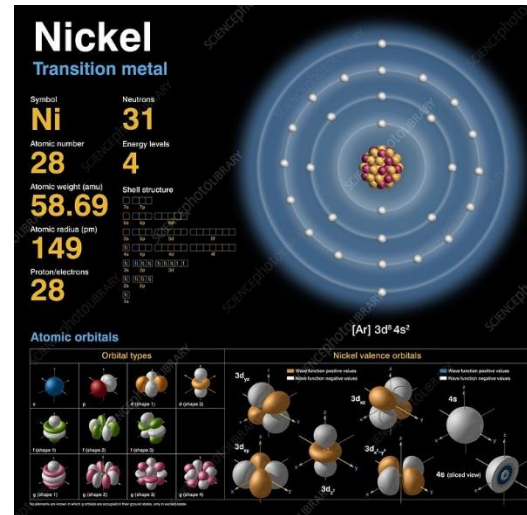




# From atom to component



[Do we actually know what atoms look like? - Quora](#)



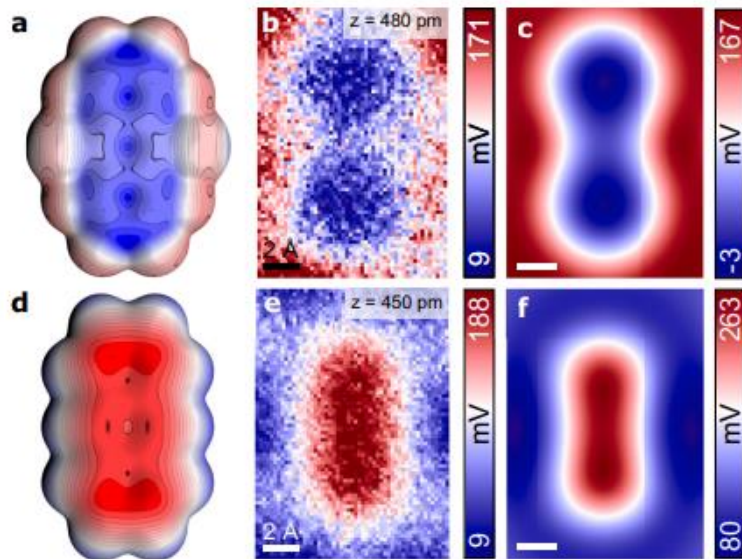
[Nickel, atomic structure - Stock Image - C018/3709 - Science Photo Library](#)



[Turbo TDO6-17A Turbocharger 49179-00110 ME037701 for Mitsubishi Engine 6D31T 6D14T 6D14CT 6D14-2CT \(fridayparts.com\)](#)

# Experimental measurement of Submolecular charge distribution

Mallada, B., Ondráček, M., Lamanec, M. *et al.* Visualization of  $\pi$ -hole in molecules by means of Kelvin probe force microscopy. *Nat Commun* **14**, 4954 (2023). <https://doi.org/10.1038/s41467-023-40593-3>

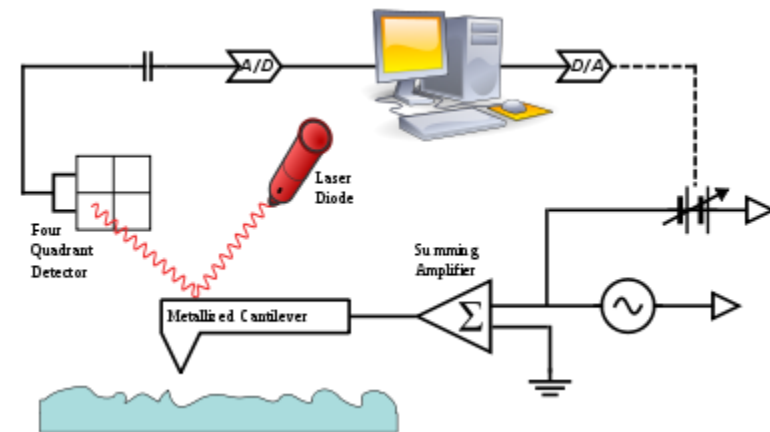


**Fig. 3 | Simulated and experimental charge distributions of FCI-An and An.**  
**a, d** Electrostatic potential maps of free-standing FCI-An and An molecules.  
**b, e** Experimental LCPD maps of FCI-An and An acquired with the same CO-tip in constant height mode. **c, f** Probe particle simulated LCPD maps of FCI-An and An. Source data are provided as a Source Data file.

[Visualization of  \$\pi\$ -hole in molecules by means of Kelvin probe force microscopy | Nature Communications](#)

experimentally visualize the  $\pi$ -hole in 9,10-Dichlorooctafluoroanthracene  $C_{14}F_8Cl_2$  (FCI-An) molecule and, at the same time, its absence in anthracene  $C_{14}H_{10}$  (An).

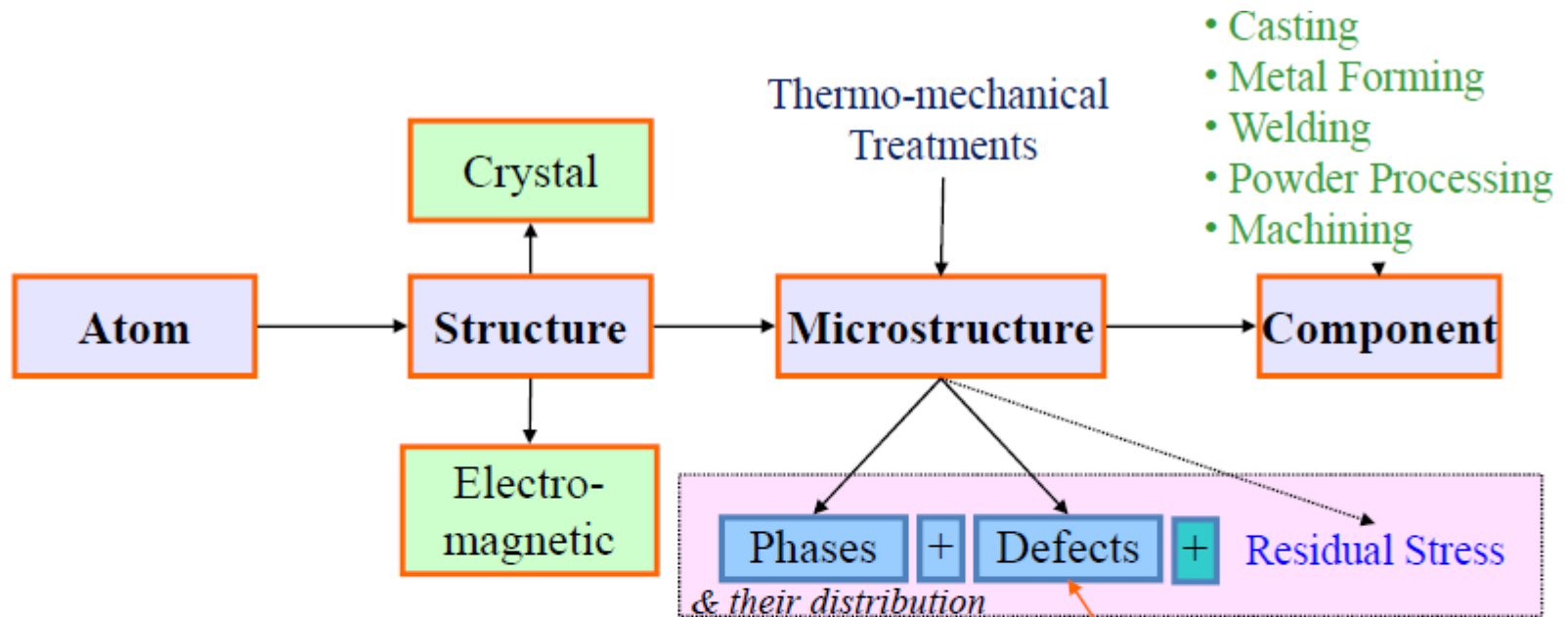
the ordered self-assembly structure of An and FCI-An molecules on Au(111).



[Kelvin probe force microscope - Wikipedia](#)



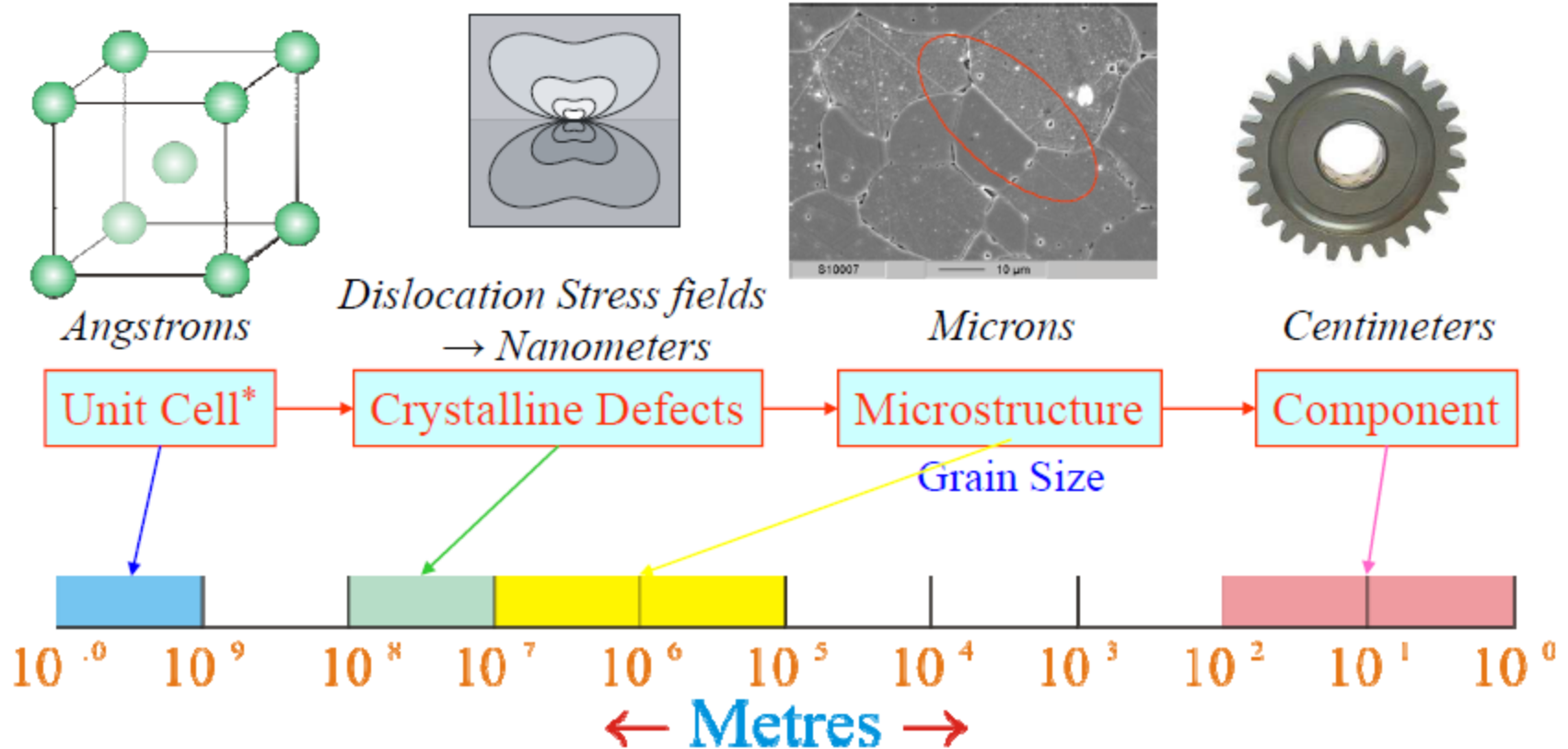
# Length scales in metallurgy



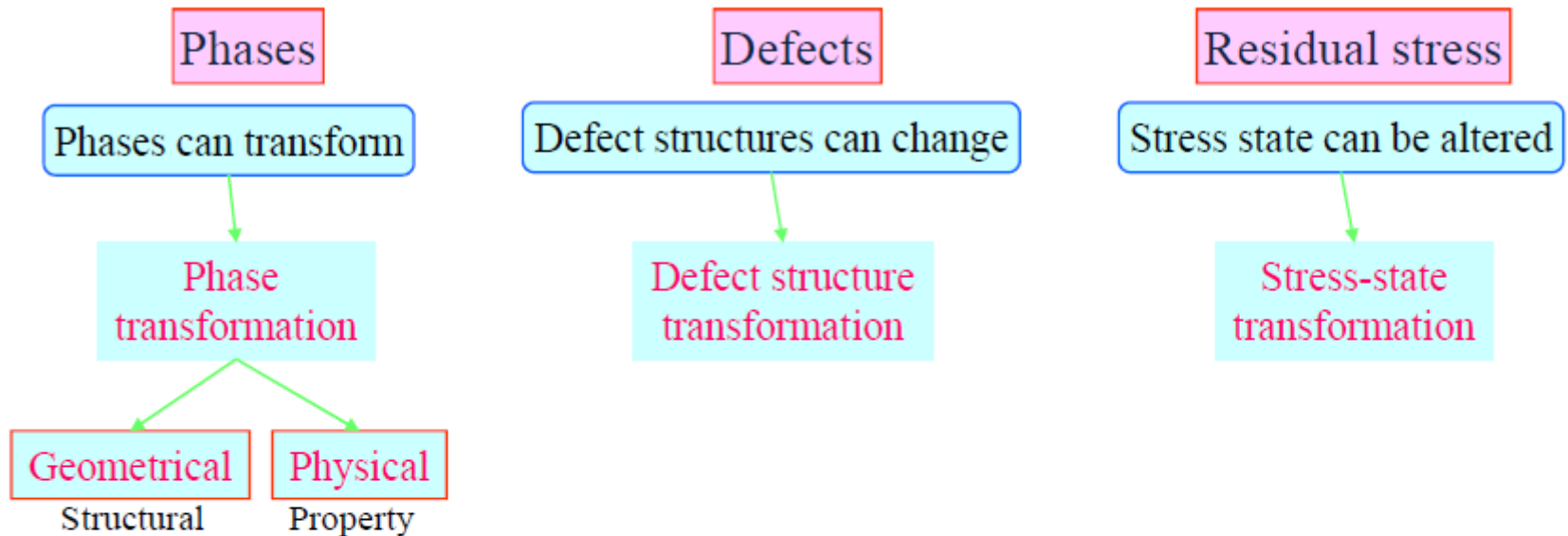
- ❑ Structure could imply two types of structure:
  - Crystal structure
  - Electromagnetic structure
  - *Fundamentally these aspects are two sides of the same coin*
- ❑ Microstructure can be defined as:  
(Phases + Defect Structure + Residual Stress) and their distributions
- ❑ Microstructure can be 'tailored' by thermo-mechanical treatments

- Vacancies
- Dislocations
- Twins
- Stacking Faults
- Grain Boundaries
- Voids
- Cracks

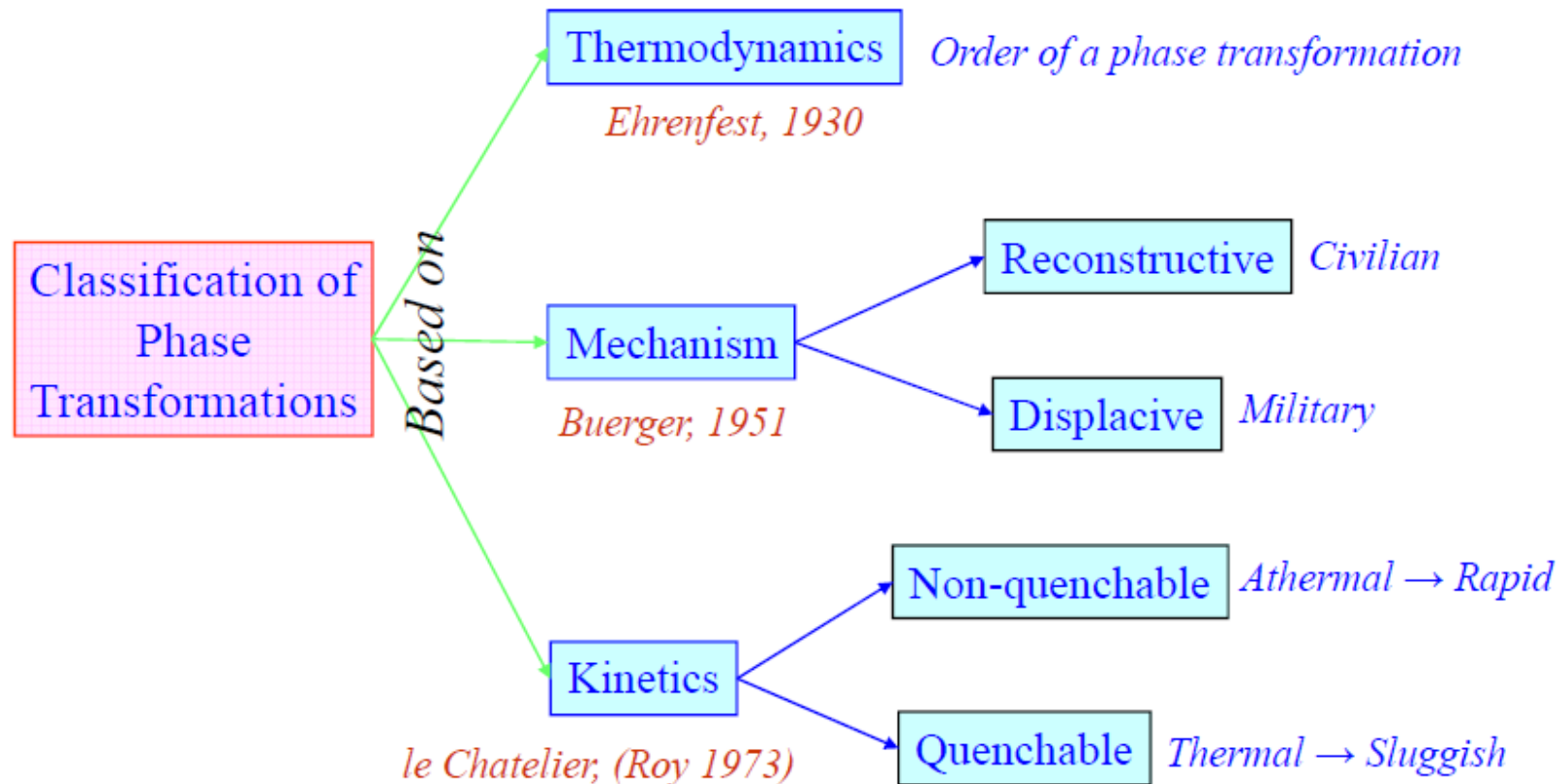
# Length scales



# Transformations and changes in materials



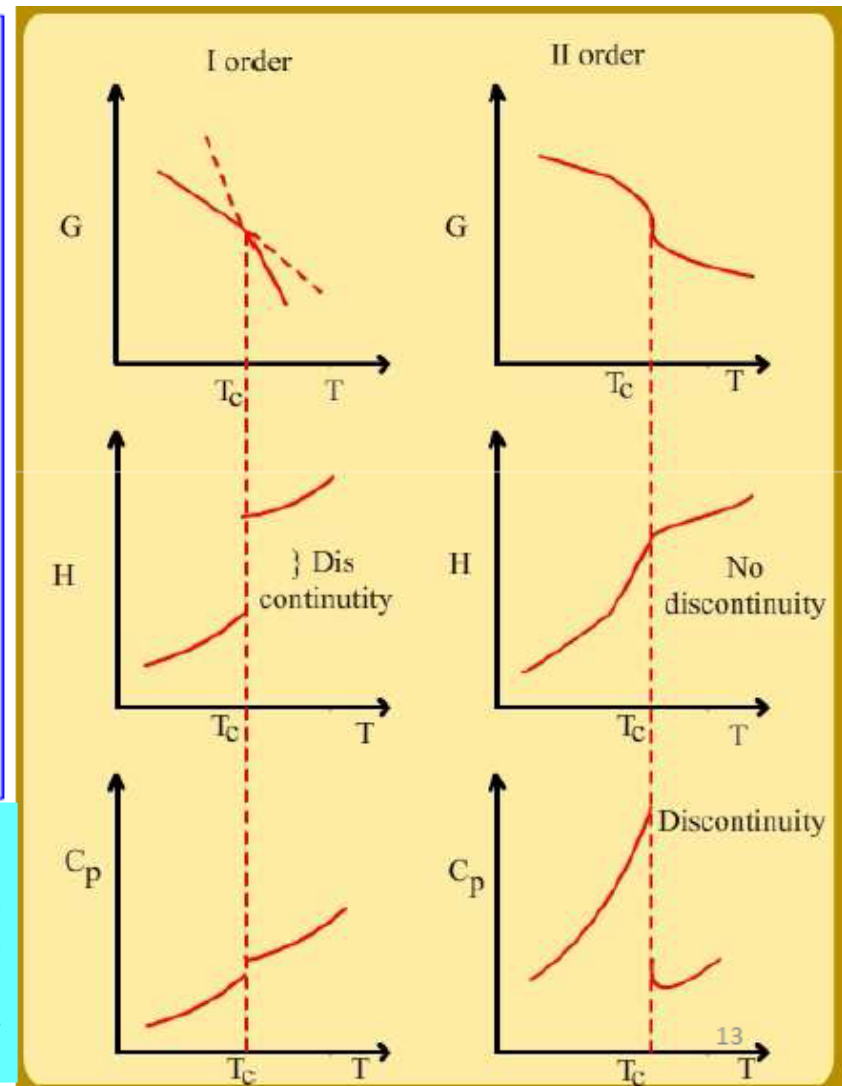
# Classification of Transformations



# Classification of PT according to thermodynamics

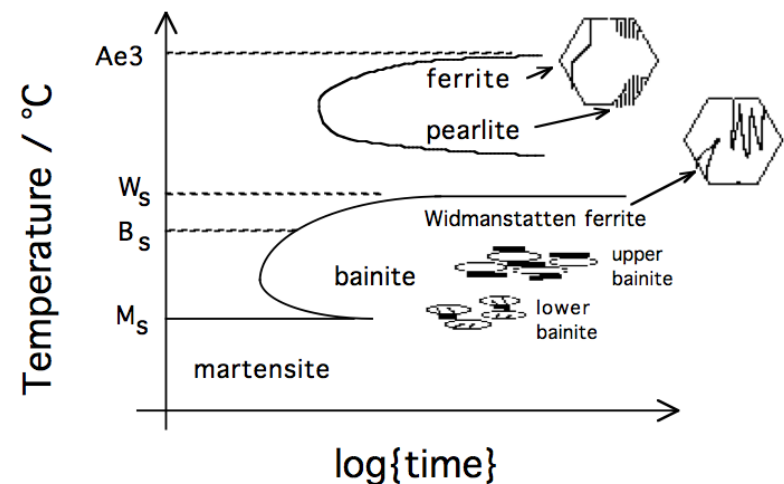
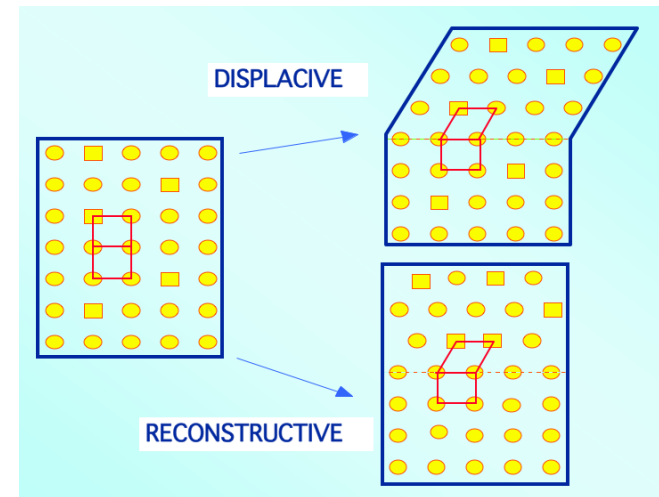
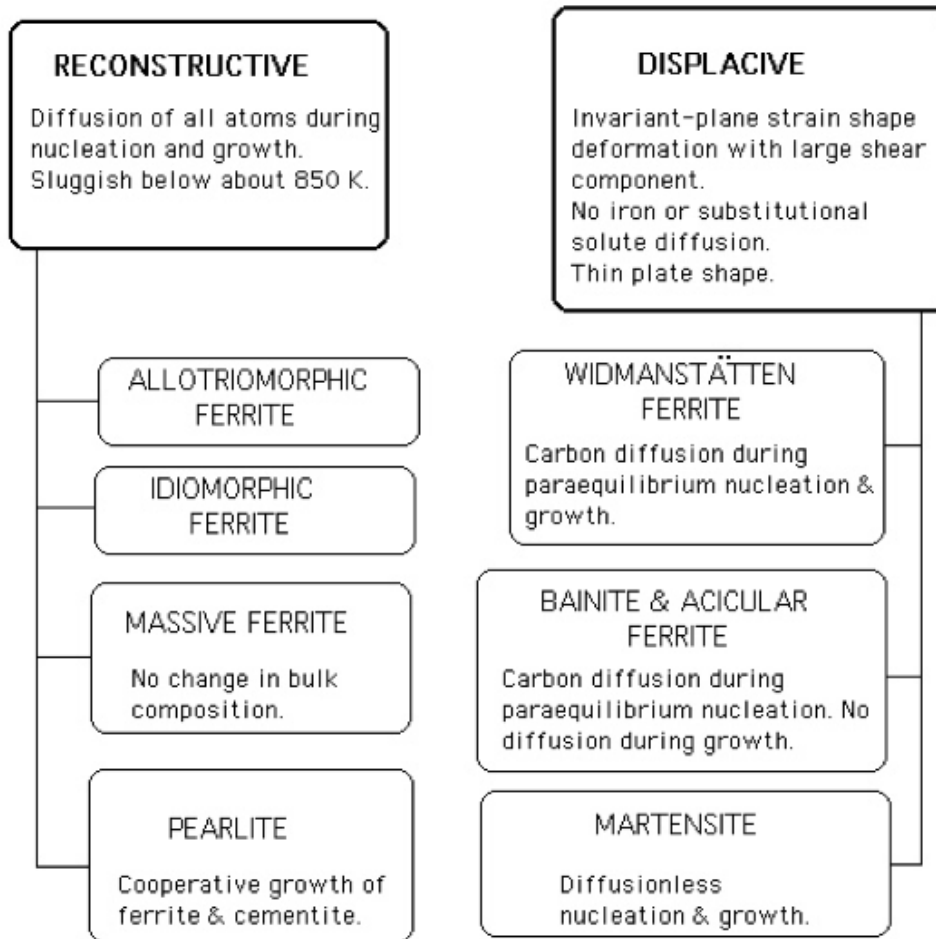
- ❑ The thermodynamic characteristics associated with the phase transformations can be used to classify transformations; in this classification methodology, if the  $n^{\text{th}}$  derivative of free energy ( $G$ ) with respect to temperature ( $T$ ) and pressure ( $P$ ) is discontinuous, it is defined as the  $n^{\text{th}}$  order transformation.
- ❑ As shown in Fig., in transformations such as melting, the first derivative has the discontinuity; hence, melting is a first order transformation; on the other hand, in some of the order/disorder transformations, it is the second derivative which is discontinuous, making it the second order transformation.

Figure: The thermodynamic classification of transformations: the first derivative of the free energy ' $G$ ' with respect to temperature ' $T$ ', that is the enthalpy ' $H$ ' is discontinuous at the transformation temperature  $T_c$  as shown in the first column; the second derivative of the free energy with respect to temperature  $C_p$  is discontinuous while ' $H$ ' is not in the second column, making the order of transformation second.



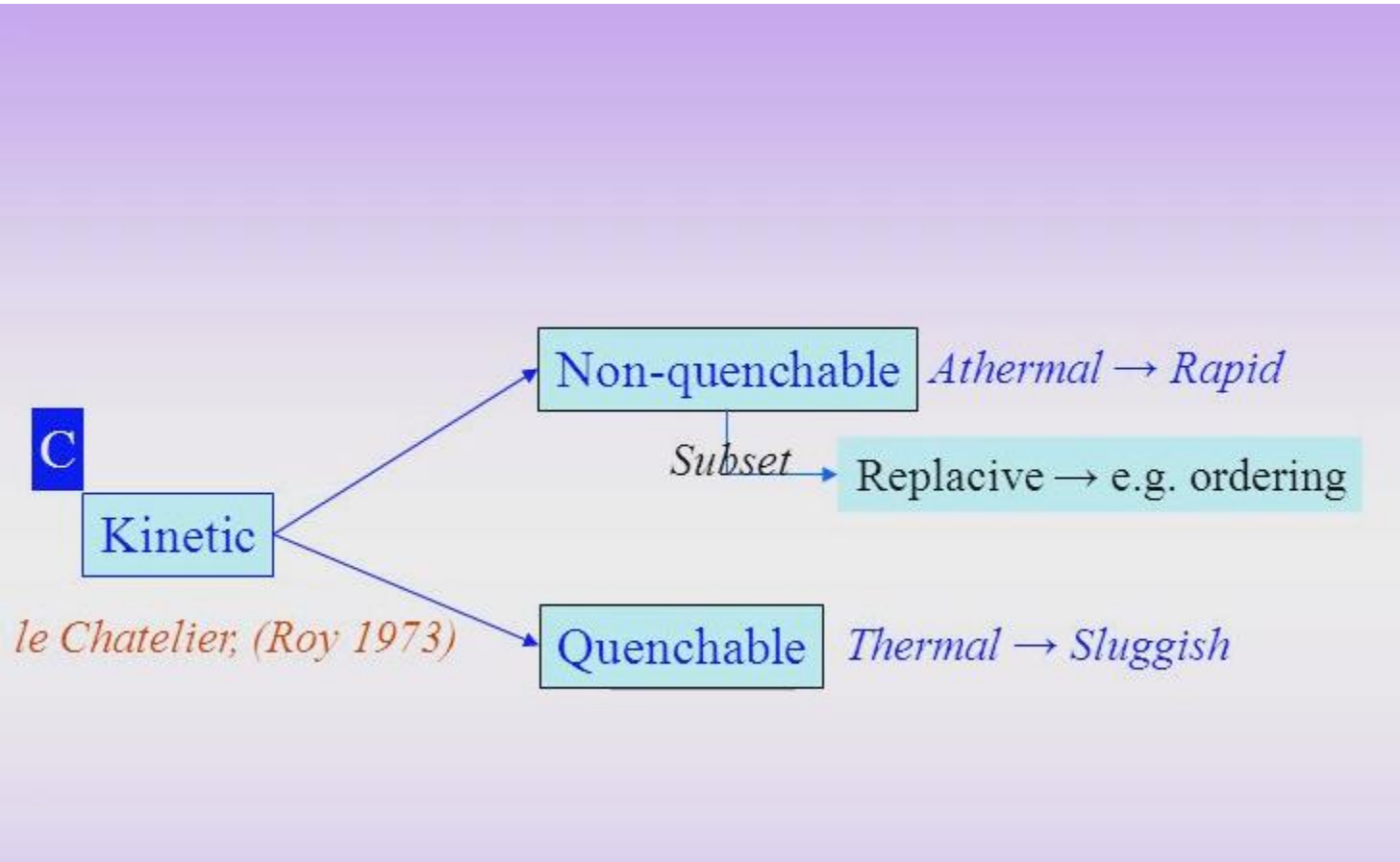
# Classification of PT according to mechanism

[Metallography of Steels \(cam.ac.uk\)](http://cam.ac.uk)

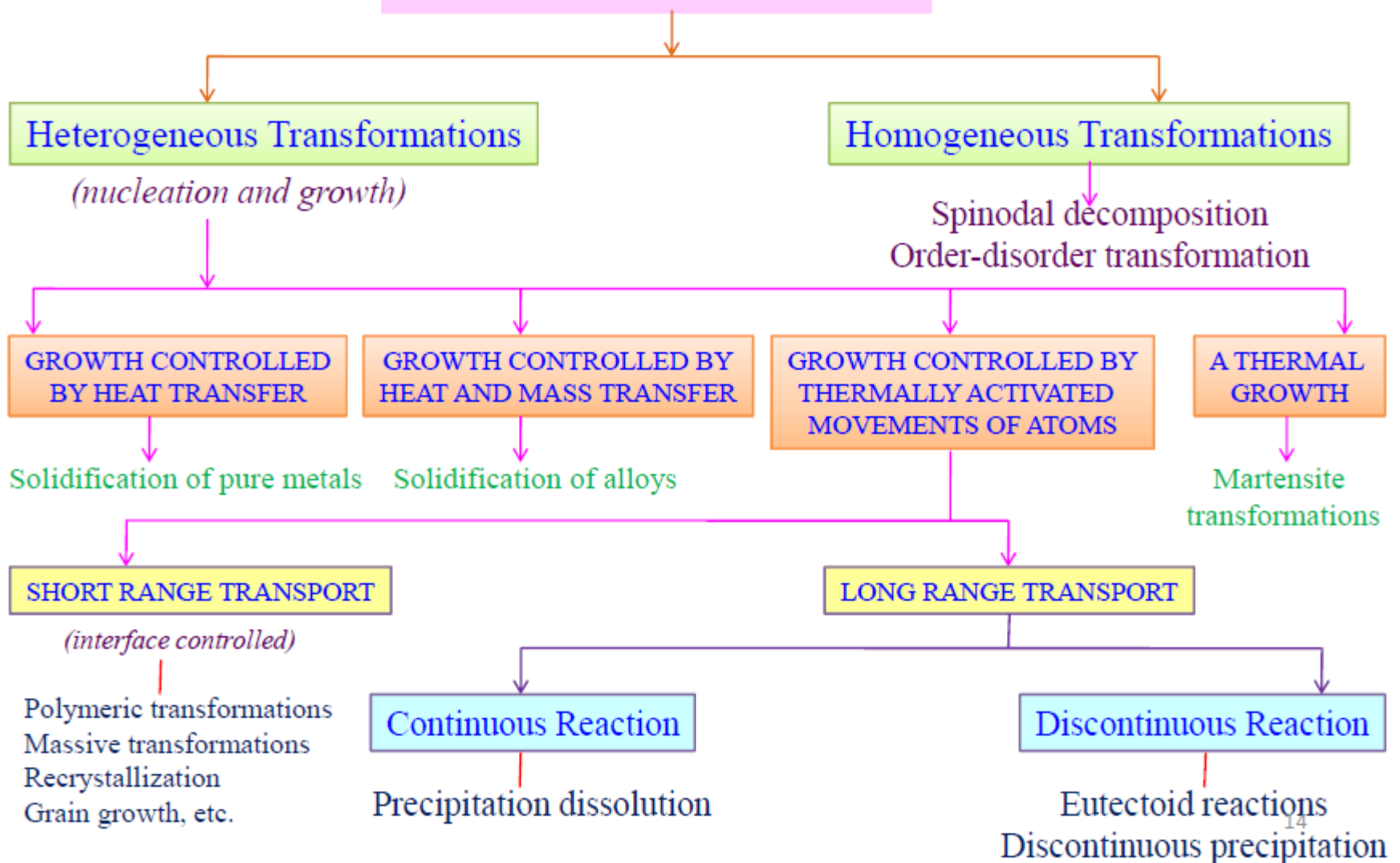




# Classification of PT according to kinetics



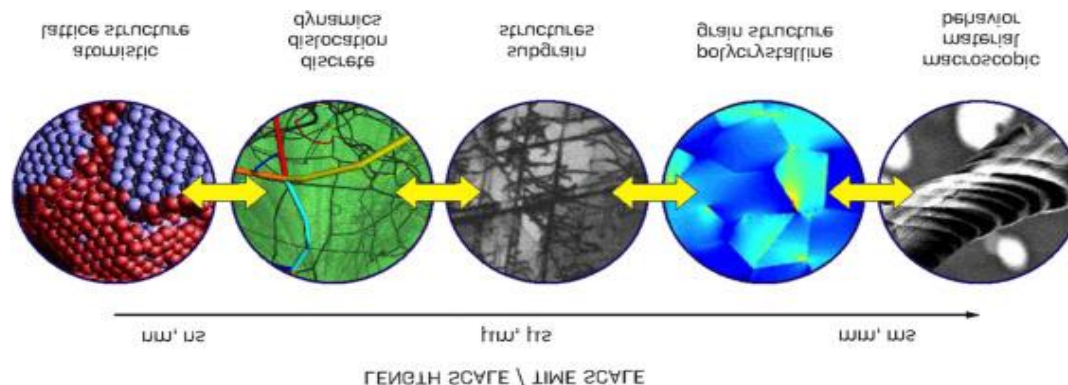
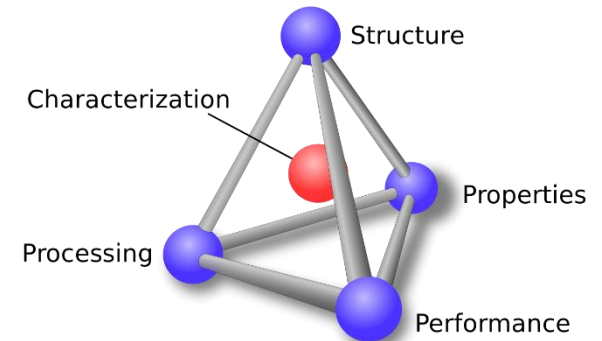
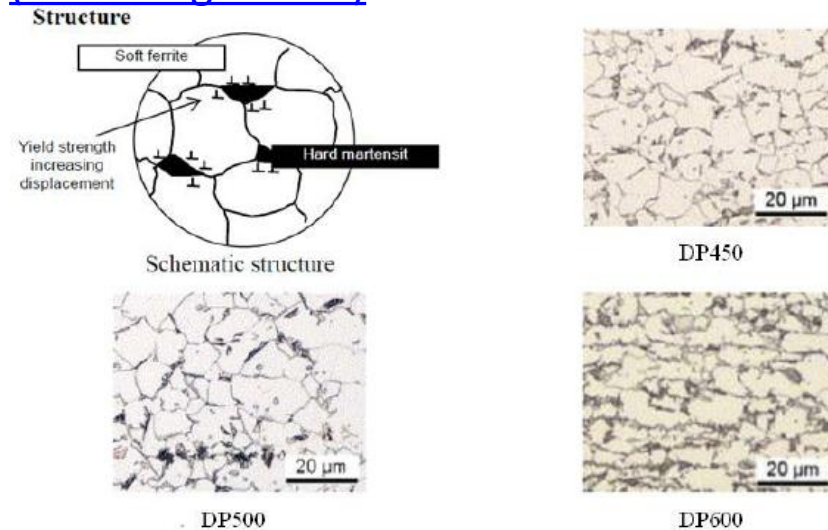
# Classification of Transformations



# Structure of materials

[1: The schematic structure and microstructures of DP steel \(Material... | Download Scientific Diagram \(researchgate.net\)\)](#)

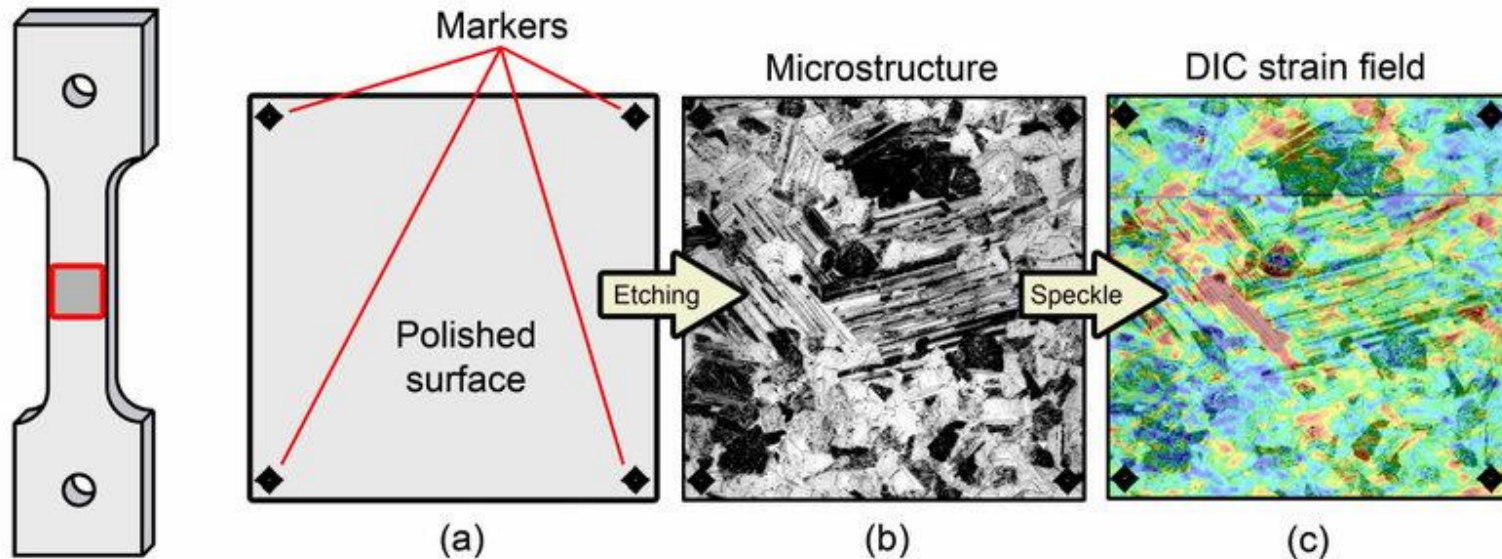
[Materials Science and Engineering | MATSE 81: Materials In Today's World \(psu.edu\)](#)



[The new frontiers in computational modeling of material structures - ScienceDirect](#)

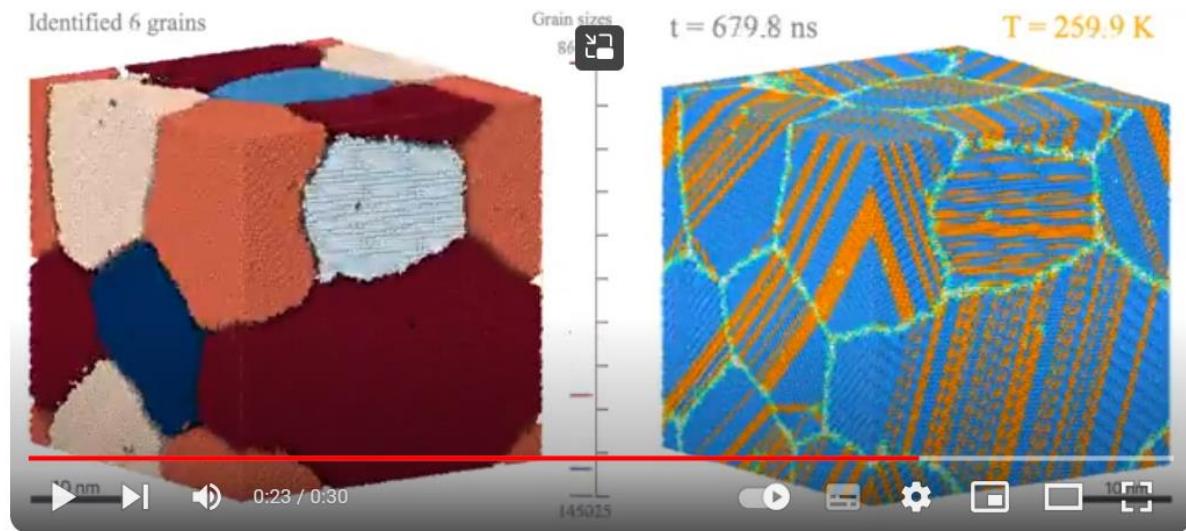
# Microstructure

[Specimen preparation, positioning of fiducial markers \(a\),... | Download Scientific Diagram \(researchgate.net\)](#)



# Capturing 3D microstructures in real time

[Capturing 3D microstructures in real time | Argonne Leadership Computing Facility \(anl.gov\)](#)



Capturing 3D microstructures in real time

**Video:** [Capturing 3D microstructures in real time - YouTube](#)



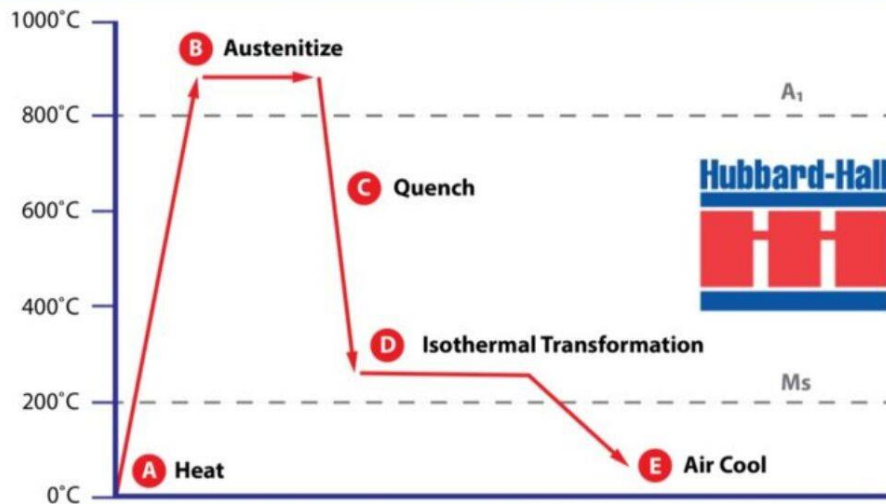
# How to prepare „(Micro) structure“?

## „Anthropogenic“ ways

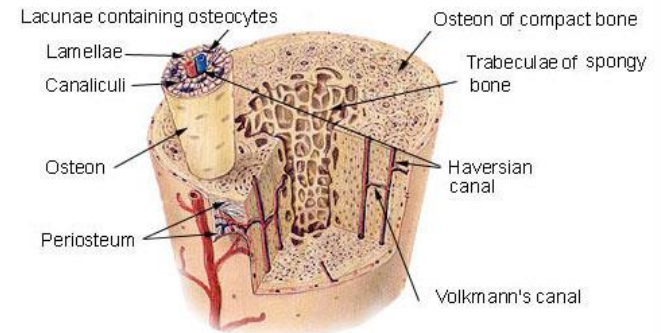
- Heat treatment
- Nano printing
- Multilayer
- templates

## „Nature“ ways

- Cell tailoring (much more possibilities) .....



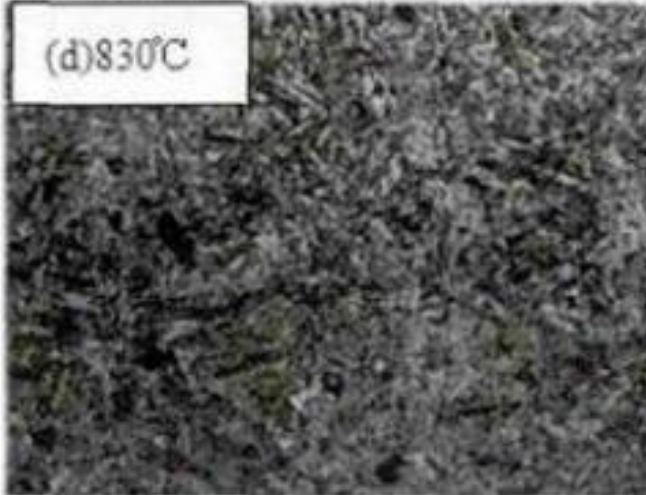
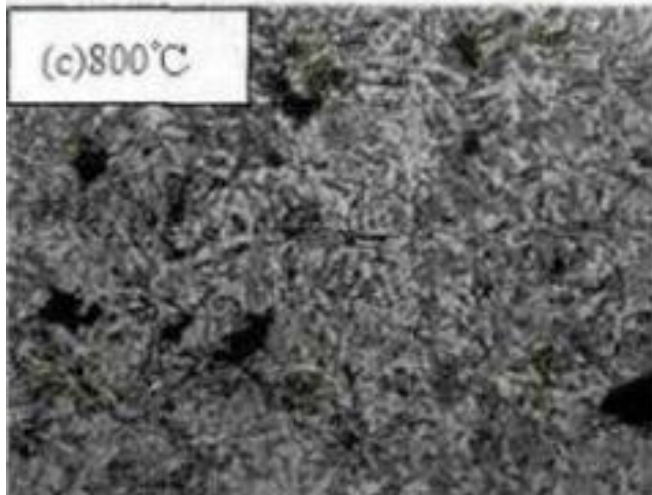
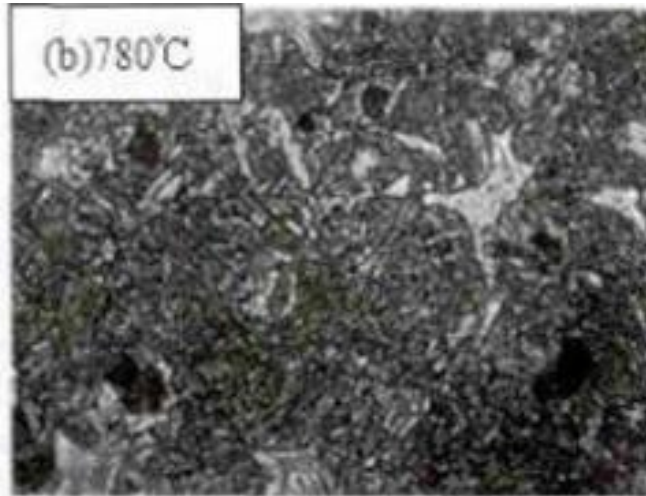
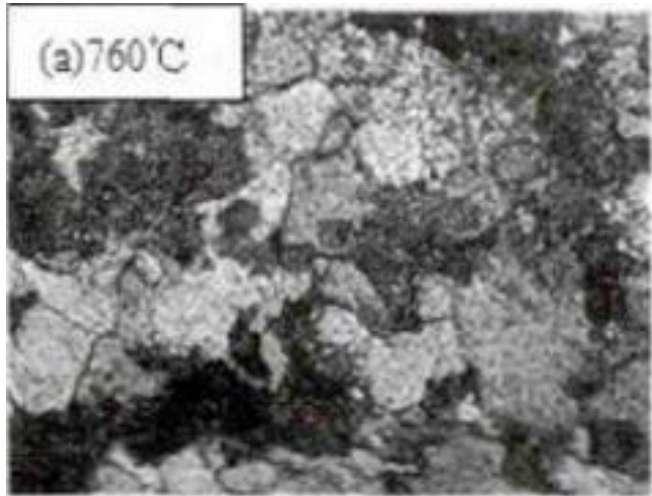
### Compact Bone & Spongy (Cancellous Bone)



[Structure of Bone Tissue | SEER Training \(cancer.gov\)](https://seer.cancer.gov/structure-of-bone-tissue/)



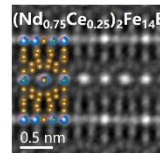
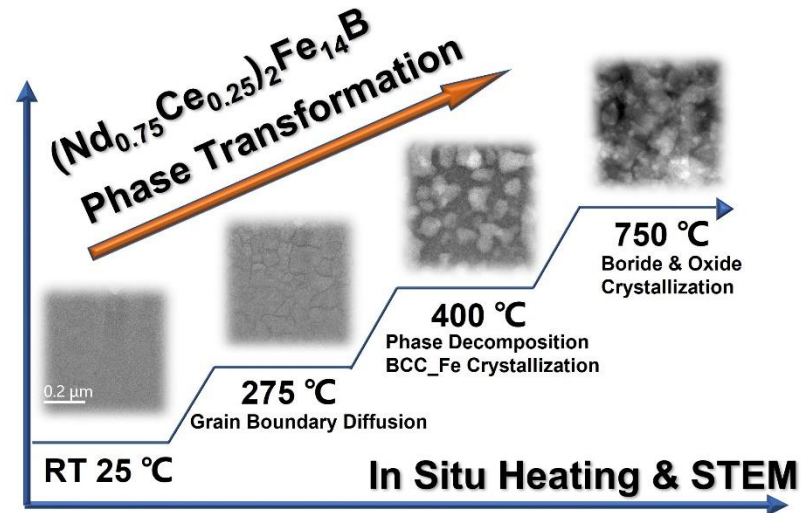
# Heat treatment of steels



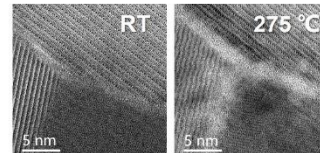
[Study on the effect of different heat treatment processes on the microstructure and properties of 45 # steel - China piping solution supplier - China piping solution supplier \(epowermetals.com\)](#)

# Most used path to structural anthropogenic material - Phase transformation

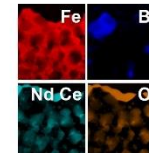
[In-situ STEM study on thermally induced phase & microstructure evolution of lanthanide magnetic - American Chemical Society \(digitellinc.com\)](#)



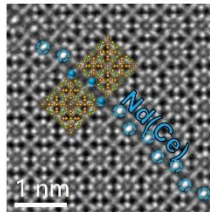
Atomic Resolved  
STEM Imaging



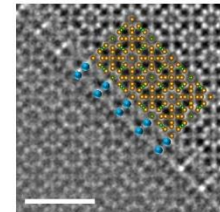
Grain Boundary  
Diffusion Analysis



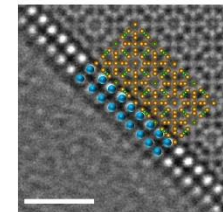
EELS & EDS  
Elemental Analysis



Single La Atom  
Grain Boundary



Partial Substituting  
La Interface



Pure La atom  
Interface

# Discussion