Second QUIZ of MLL100

Date	: *February 12, 2022*
Day	: *Saturday*
Time	: *10:30 a.m. – 10:45 a.m.*
Marks	: *10*
Mode	: *Online (Moodle)*
Syllabus	: *Phase equilibria, Phase diagrams and Phase transformations*

MLL 100

Introduction to Materials Science and Engineering

Lecture-14 (February 08, 2022)

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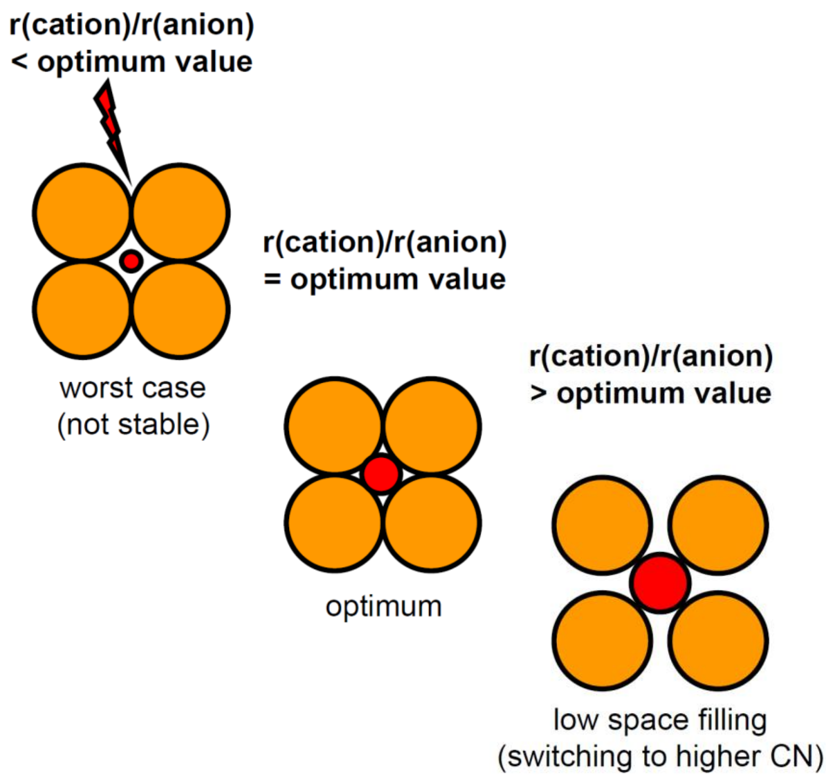
What have we learnt in Lecture-13?

- ❑ Peritectic phase diagram

  Monotectic reaction: L_1 ---------> L_2 + S

- ❑ Voids: Tetrahedral and Octahedral

- ❑ Iron-carbon phase diagram



No Rattling — *Cation should not be smaller than the void formed by the anions*

↓

Cation size larger than the void — *Cation should be larger than the void so that the anions do not touch each other*

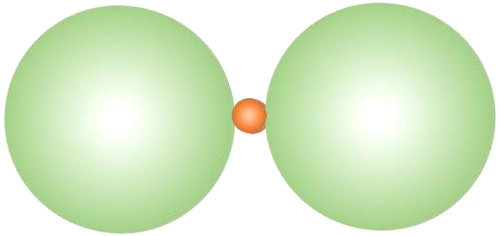
↓

Choose the largest coordination possible — *Largest coordination gives the best possible packing*

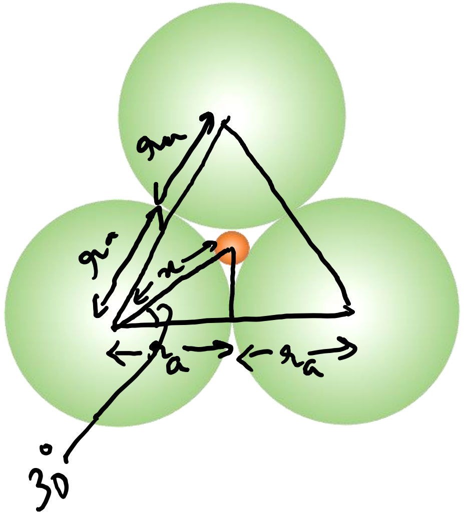
- Cations should surround themselves with as many anions as possible, and vice versa. This maximizes the attractions between neighbouring ions of opposite charge and hence maximizes the lattice energy of the crystal.

- *Radius ratio rule for ionic structures*

- A cation must be in contact with its neighbour anion -----> Lower limit on the size of a cation which may occupy a particular position.
- Neighbouring anions may or may not be in contact with each other.



$$\frac{r_c}{r_a} = 0 - 0.155$$



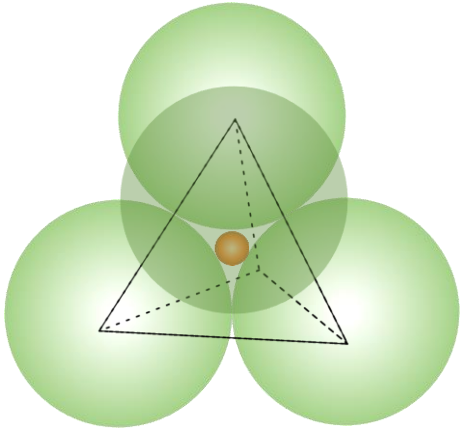
$$\frac{r_c}{r_a} = 0.155 - 0.225$$

Lower limit is governed by current coordination

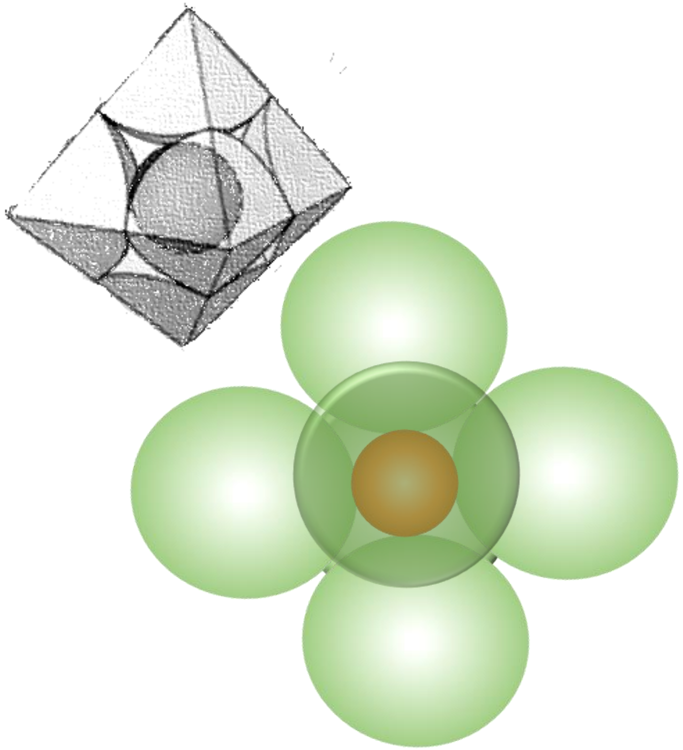
Upper limit is governed by next higher possible coordination

$$\cos 30^\circ = \frac{r_a}{(r_a + r_c)} = \frac{\sqrt{3}}{2}$$

$$\therefore \left(\frac{r_c}{r_a}\right) = 0.155$$



$$\frac{r_c}{r_a} = 0.225 - 0.414$$



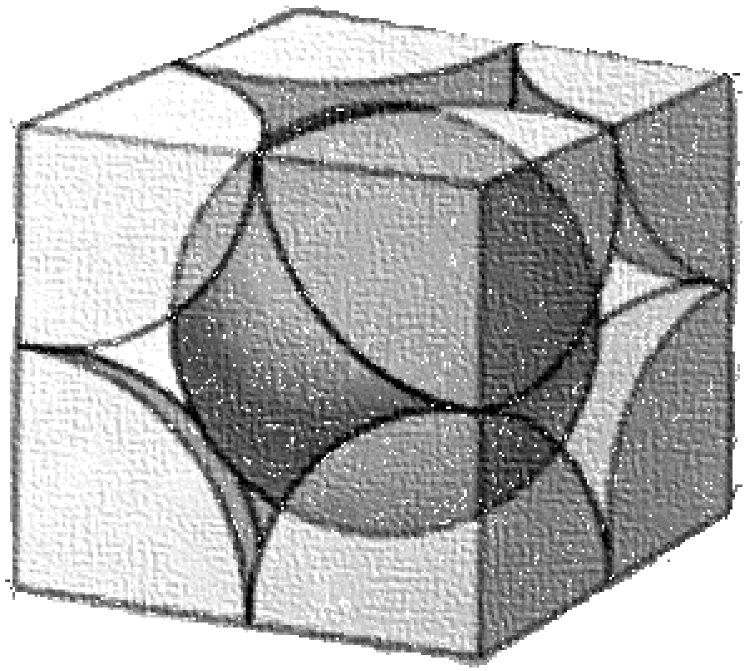
$$\frac{r_c}{r_a} = 0.414 - 0.732$$

$$(2r_a)^2 + (2r_a)^2 = \{2(r_a + r_c)\}^2$$

$$\therefore 2\sqrt{2}\, r_a = 2(r_a + r_c)$$

$$\therefore (\sqrt{2} - 1)\, r_a = r_c$$

$$\therefore \left(\frac{r_c}{r_a}\right) = 0.414$$

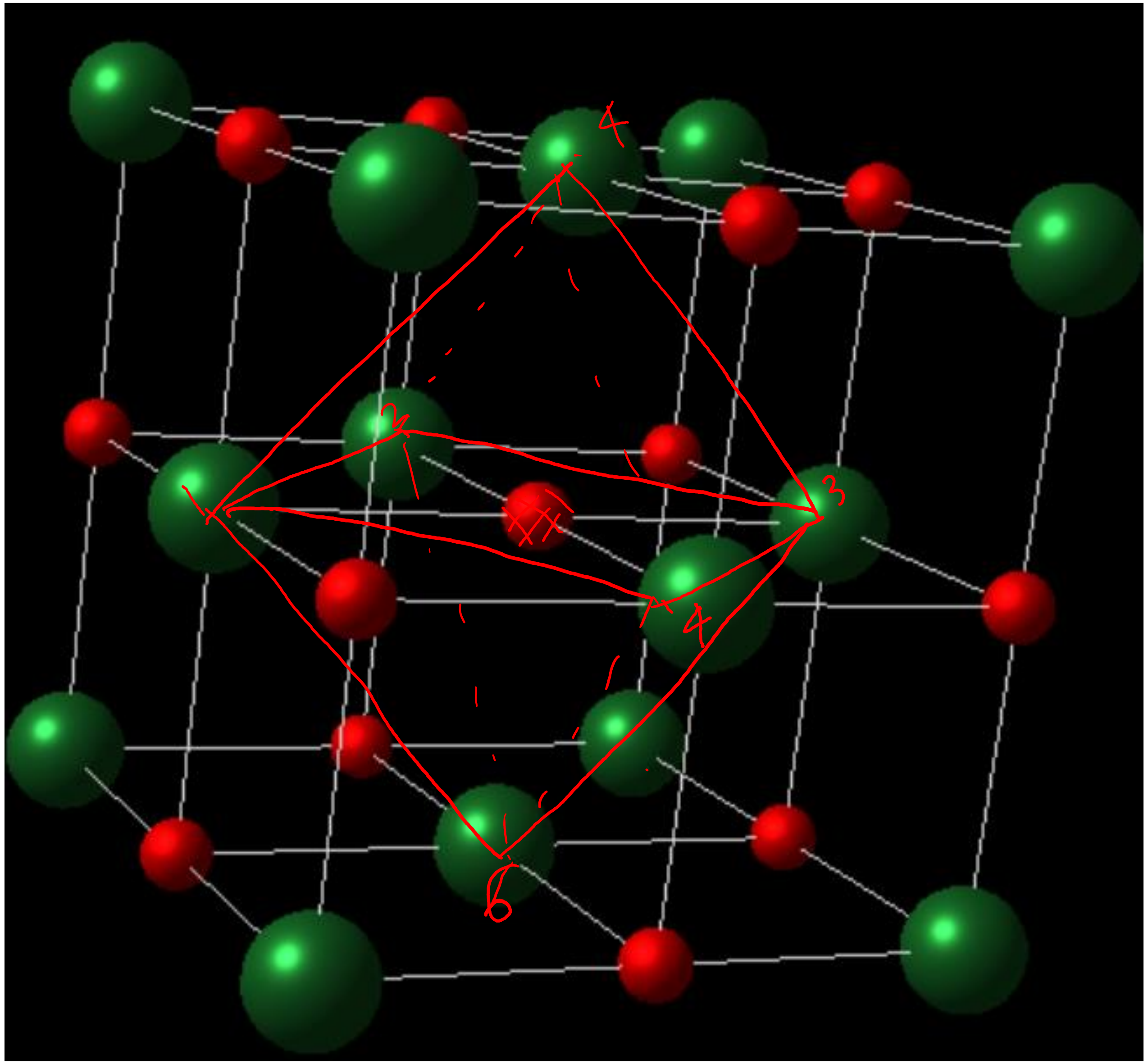


$\frac{r_c}{r_a}$ = 0.732 – 1.0

$(2r_c + 2r_a) = \text{Body diagonal}$
$= \sqrt{3}\,a = \sqrt{3}\,(2r_a)$

$\therefore \left(\frac{r_c}{r_a}\right) = 0.732$

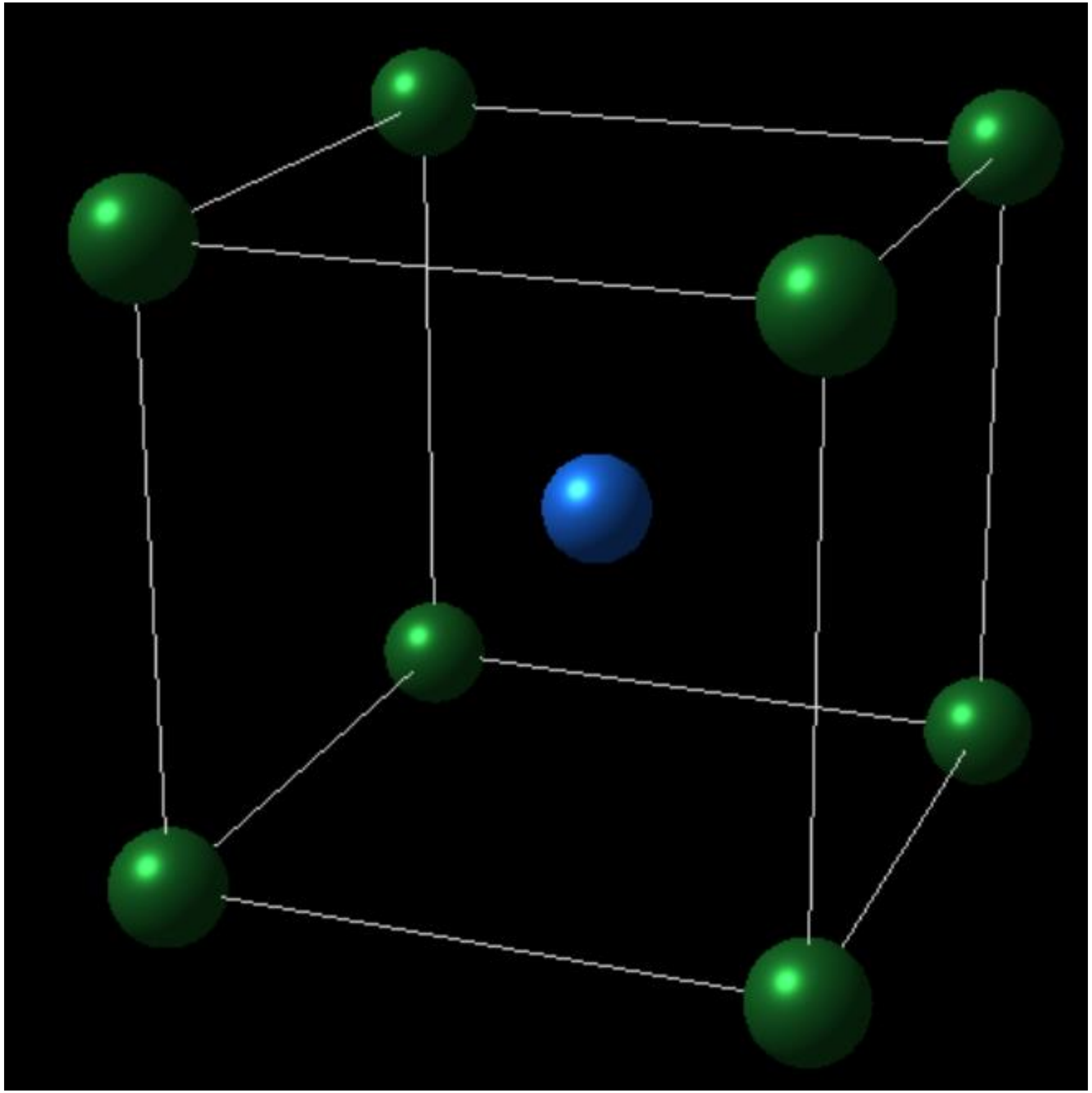
$(\frac{r_c}{r_a})$	Co-ordination number (CN)	Geometry	Crystal structures
0 – 0.155	2	Linear	
0.155 – 0.225	3	Triangular	
0.225 – 0.414	4	Tetrahedron	
0.414 – 0.732	6	Octahedron	
0.732 – 1.0	8	Cube	



$$r_{Na^+} = 0.102 \text{ nm}$$
$$r_{Cl^-} = 0.181 \text{ nm}$$

$$\frac{r_{Na^+}}{r_{Cl^-}} = 0.56$$

$(\frac{r_c}{r_a})$	Co-ordination number (CN)	Geometry	Crystal structures
0 – 0.155	2	Linear	
0.155 – 0.225	3	Triangular	
0.225 – 0.414	4	Tetrahedron	
0.414 – 0.732	6	Octahedron	
0.732 – 1.0	8	Cube	



$$r_{Cs^+} = 0.167 \text{ nm}$$

$$r_{Cl^-} = 0.181 \text{ nm}$$

$$\frac{r_{Cs^+}}{r_{Cl^-}} = 0.92$$

$(\frac{r_c}{r_a})$	Co-ordination number (CN)	Geometry	Crystal structures
0 – 0.155	2	Linear	
0.155 – 0.225	3	Triangular	
0.225 – 0.414	4	Tetrahedron	
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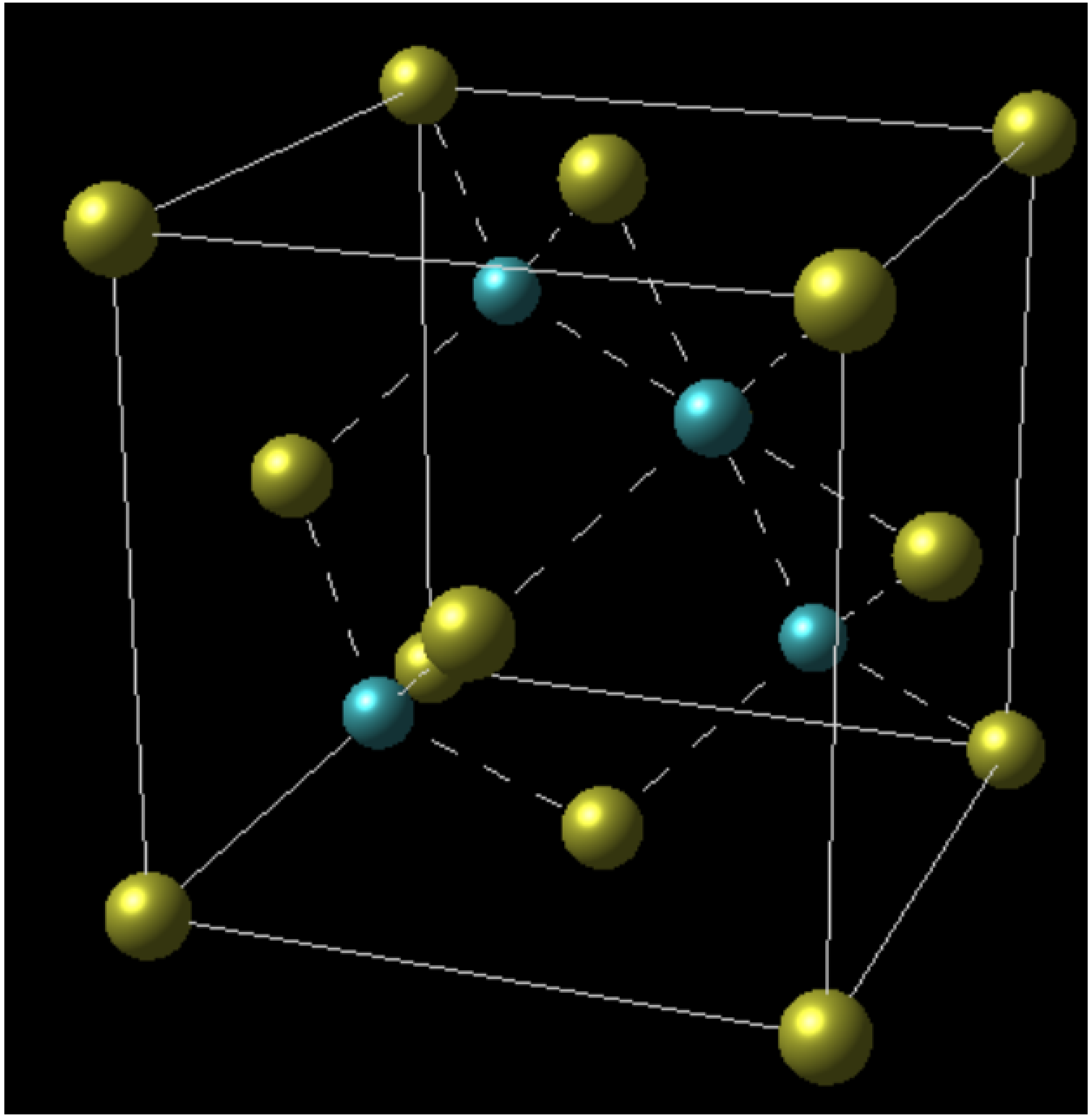
0.732 – 1.0	8	Cube	



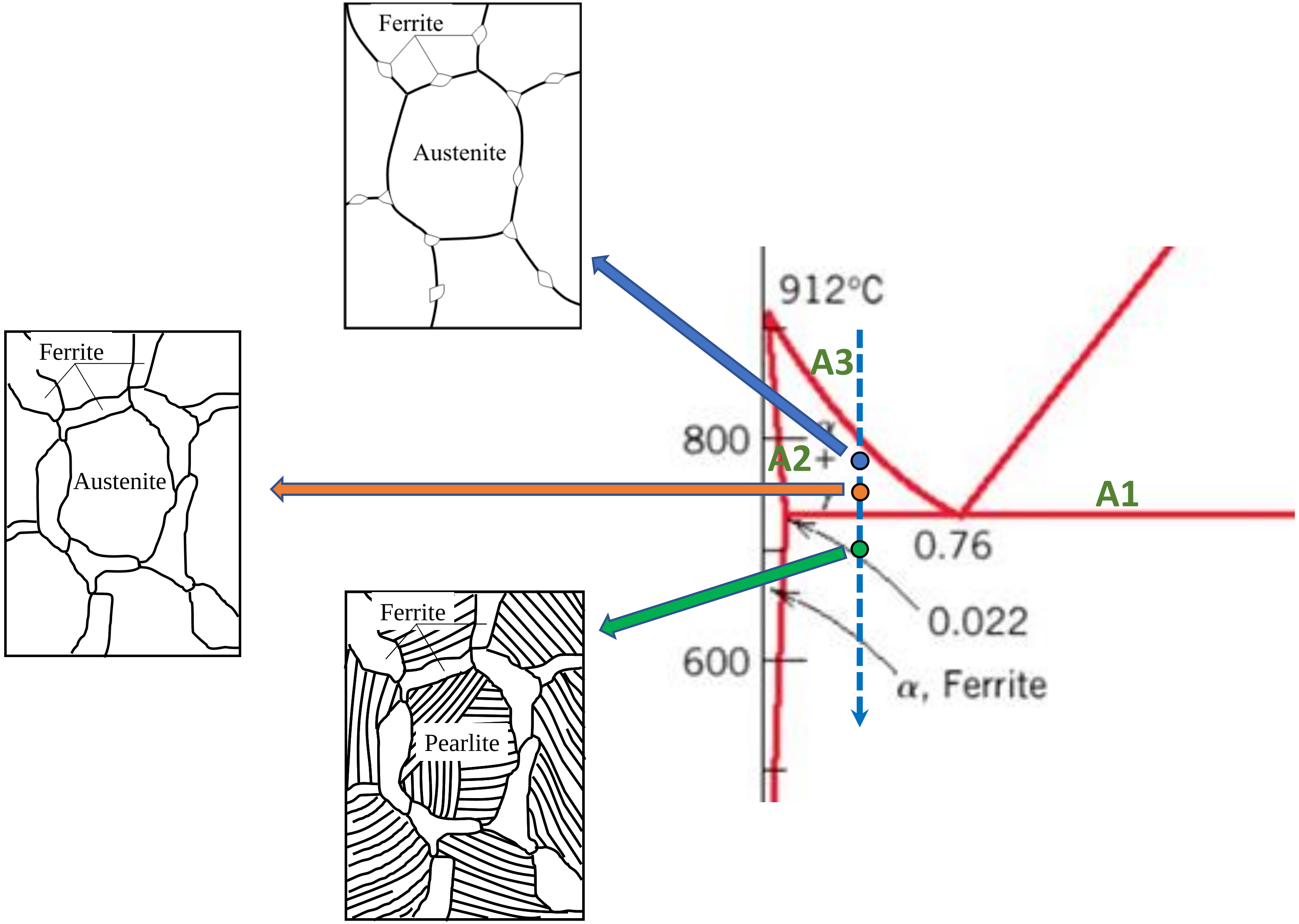
$$r_{Zn^{2+}} = 0.074 \text{ nm}$$
$$r_{S^{2-}} = 0.184 \text{ nm}$$

$$\frac{r_{Zn^{2+}}}{r_{S^{2-}}} = 0.40$$

$(\frac{r_c}{r_a})$	Co-ordination number (CN)	Geometry	Crystal structures
0 – 0.155	2	Linear	
0.155 – 0.225	3	Triangular	
0.225 – 0.414	4	Tetrahedron	
0.414 – 0.732	6	Octahedron	NaCl
0.732 – 1.0	8	Cube	CsCl

How does different phases evolve microstructurally in an Fe-C system?

Microstructural evolution of a hypoeutectic alloy

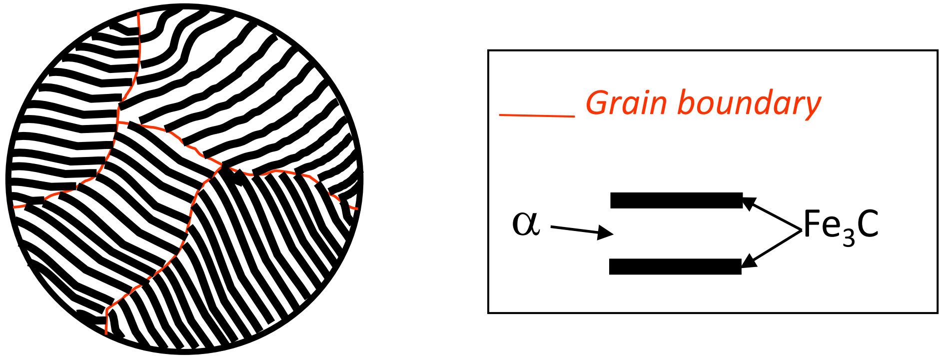


- On crossing the ‘A3’ line, the ferrite phase starts appearing on the austenite grain boundaries.
- ***Why at the grain boundaries?***

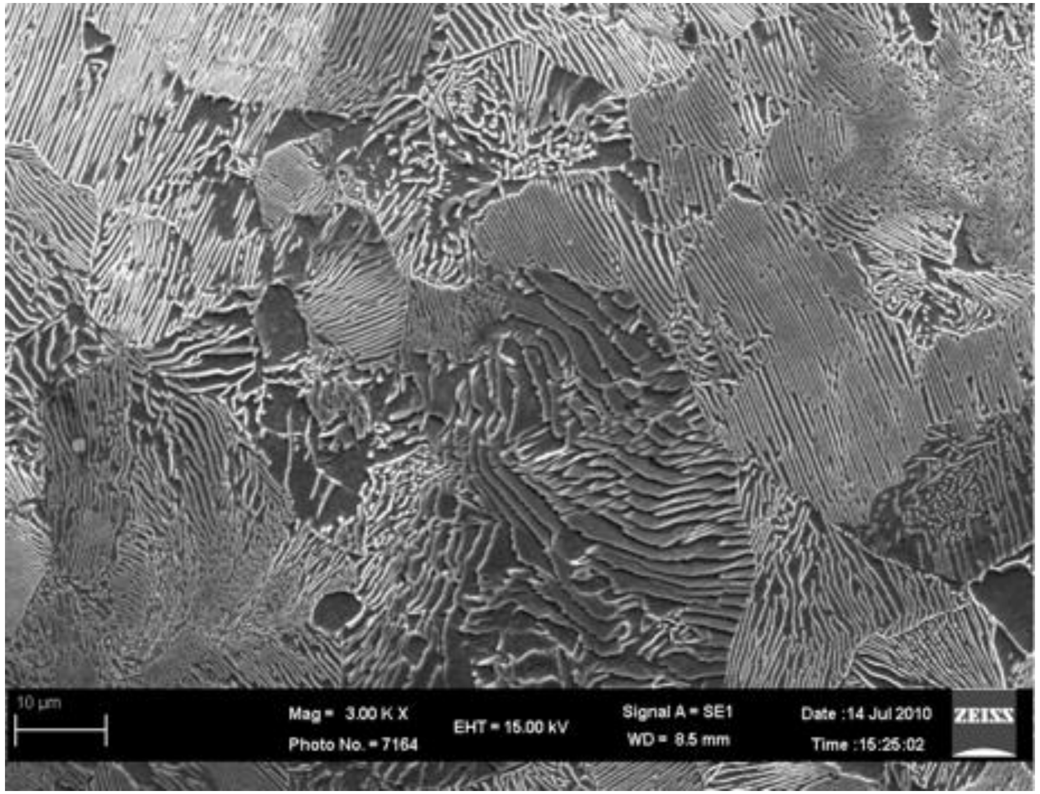
- The ferrite phase grows along the grain boundaries, and slowly protrude inside the grains of austenite.

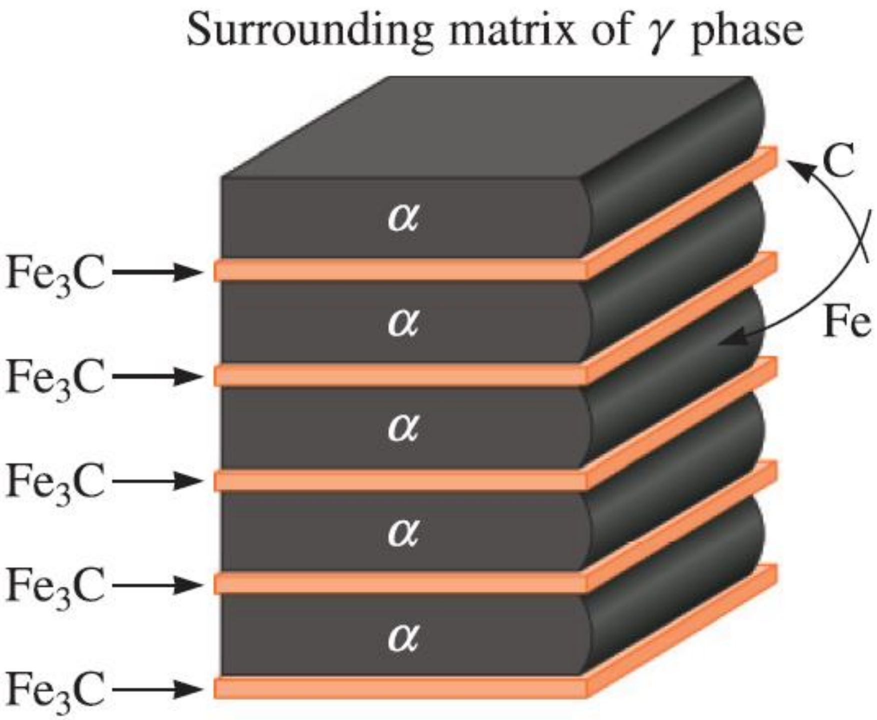
- On crossing the ‘A1’ line, the remaining austenite transforms to ‘ferrite and cementite’.
- ***Why ‘pearlite’ is mentioned in the schematic microstructure?***

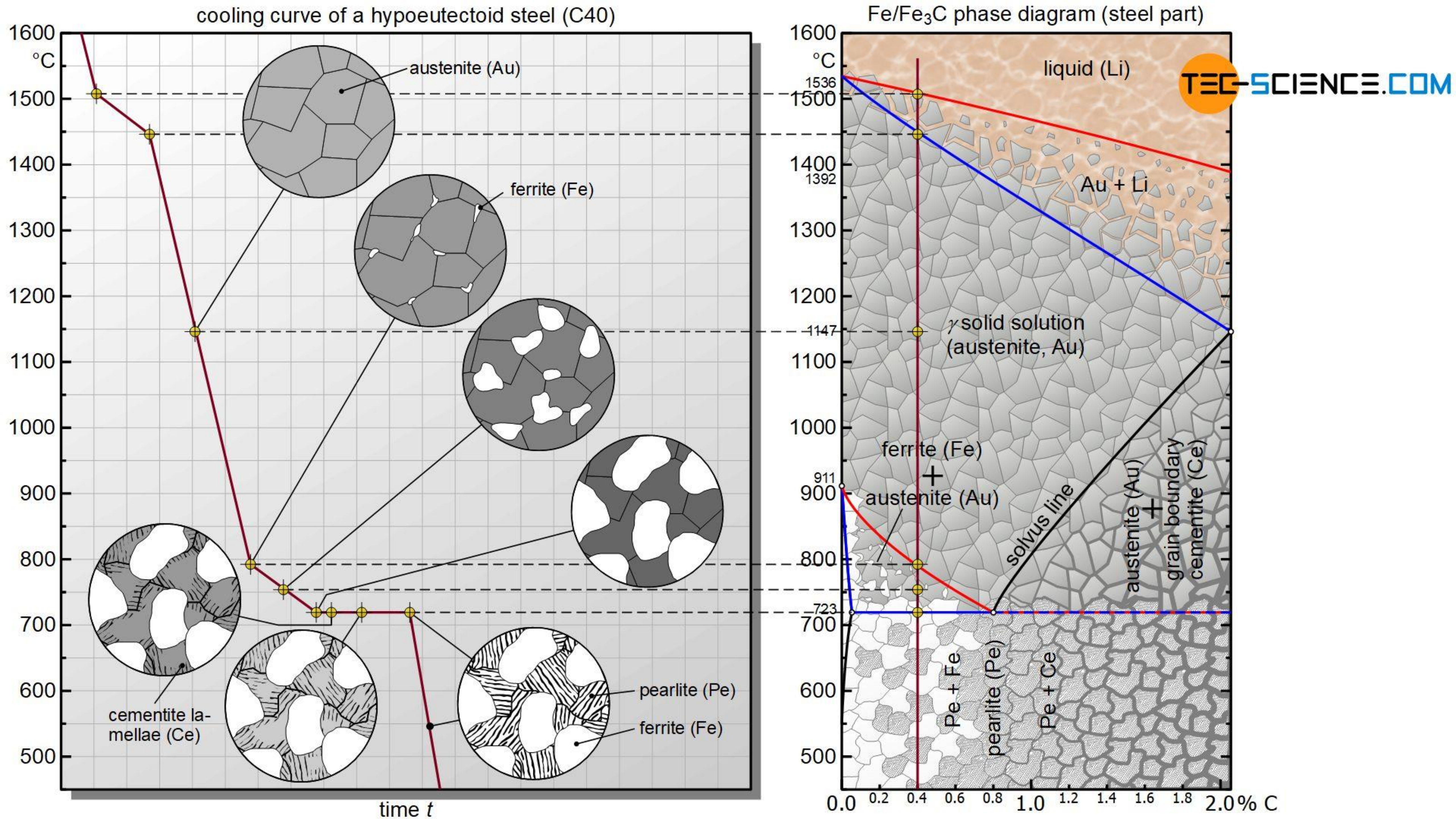
Pearlite

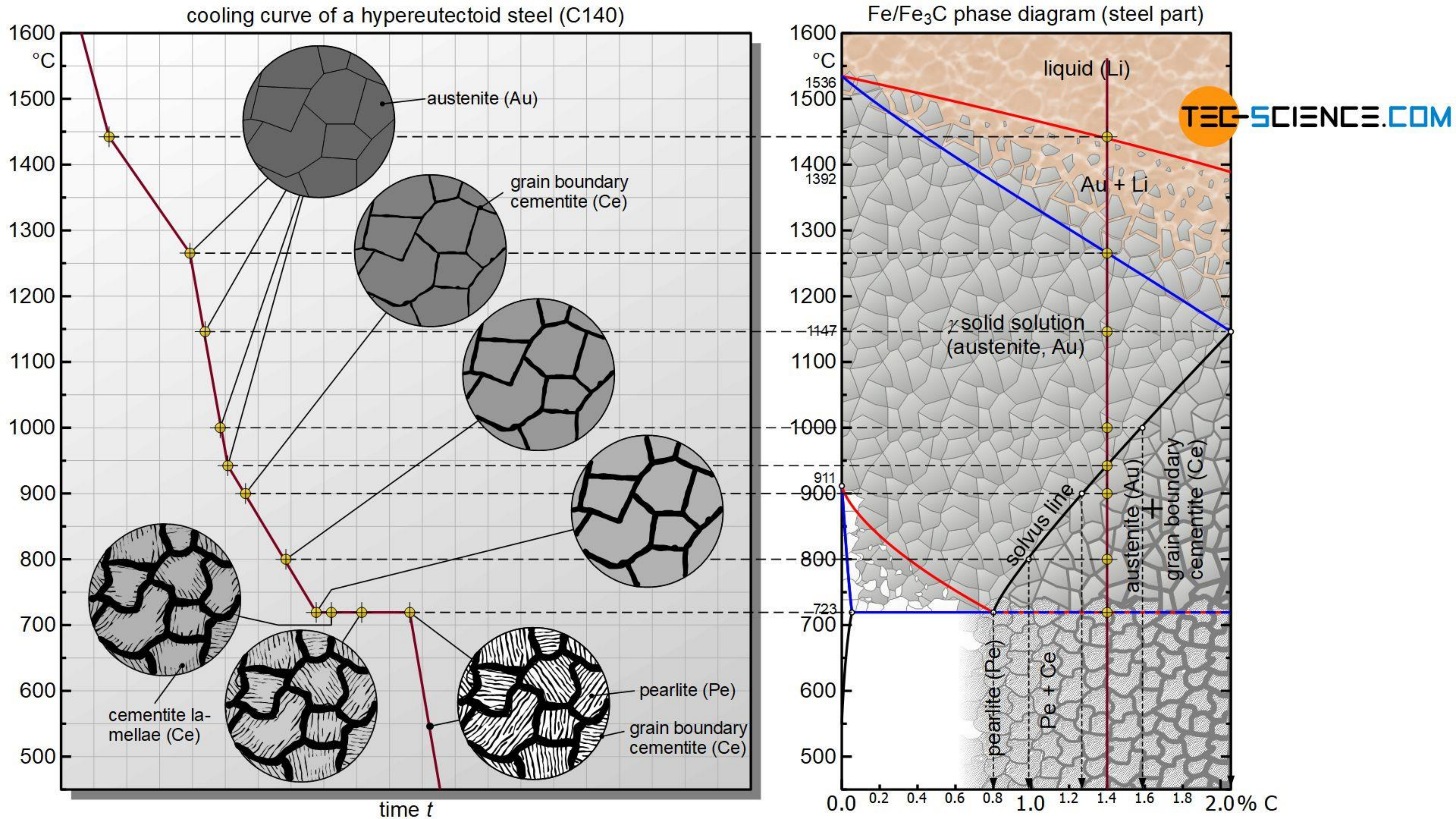


- Pearlite is a micro-constituent with alternating lamellae of cementite and ferrite.
- Pearlite is not a phase.






cooling curve of a hypoeutectoid steel (C40)
Fe/Fe3C phase diagram (steel part)
austenite (Au)
ferrite (Fe)
cementite la-
mellae (Ce)
pearlite (Pe)
ferrite (Fe)
time t
liquid (Li)
Au + Li
γ solid solution
(austenite, Au)
ferrite (Fe)
+
austenite (Au)
solvus line
austenite (Au)
+
grain boundary
cementite (Ce)
Pe + Fe
pearlite (Pe)
Pe + Ce
1536
1392
1147
911
723
°C
% C
TEC-SCIENCE.COM



cooling curve of a hypereutectoid steel (C140)
1600
°C
1500
1400
1300
1200
1100
1000
900
800
700
600
500
austenite (Au)
grain boundary
cementite (Ce)
cementite la-
mellae (Ce)
pearlite (Pe)
grain boundary
cementite (Ce)
time t
Fe/Fe3C phase diagram (steel part)
1536
1392
1147
911
723
liquid (Li)
Au + Li
γ solid solution
(austenite, Au)
solvus line
austenite (Au)
+
grain boundary
cementite (Ce)
pearlite (Pe)
Pe + Ce
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0 % C
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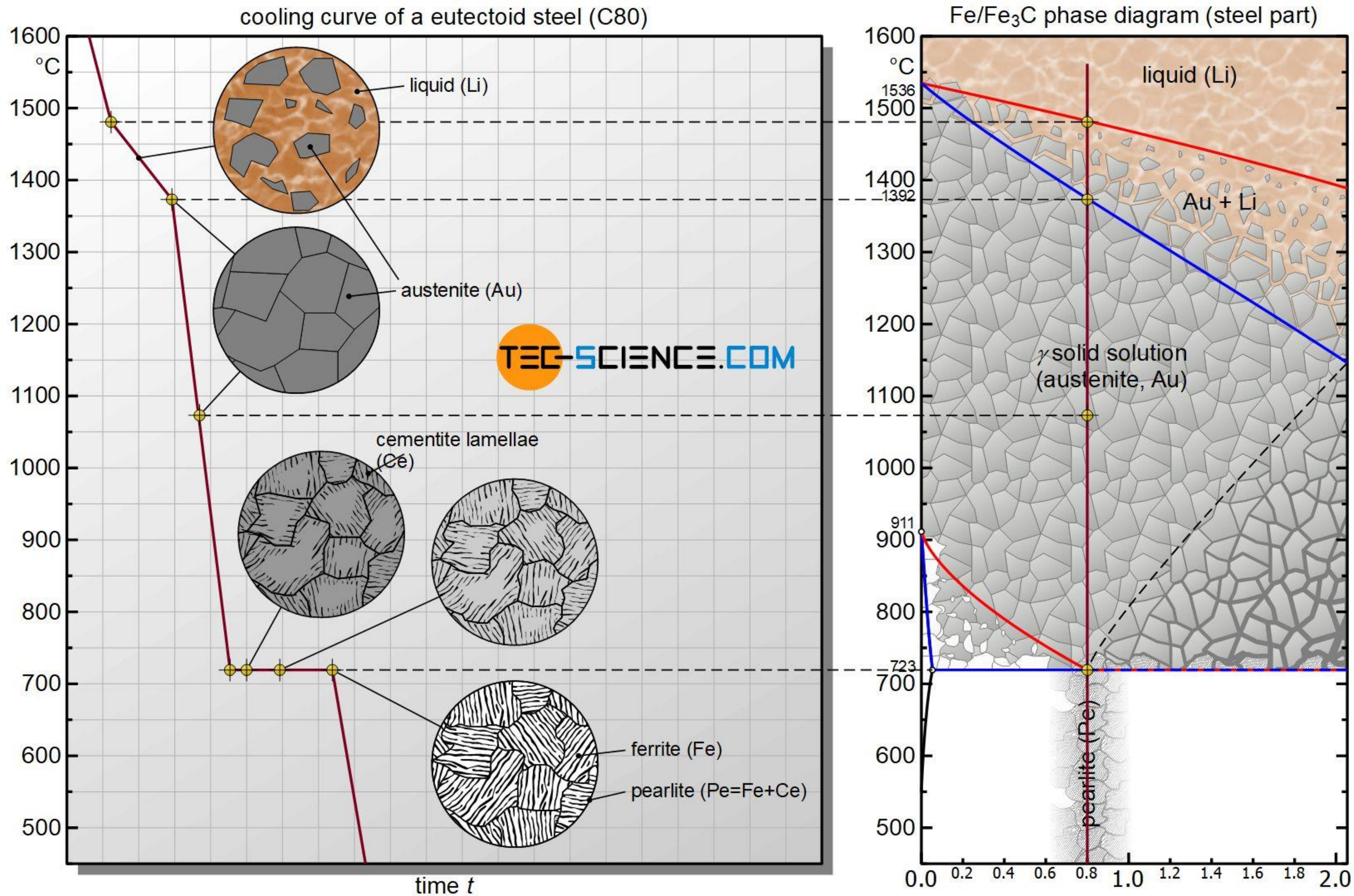


Pearlite

⇓

Two-phase mixture

$(\alpha + Fe_3C)$

Ferrite

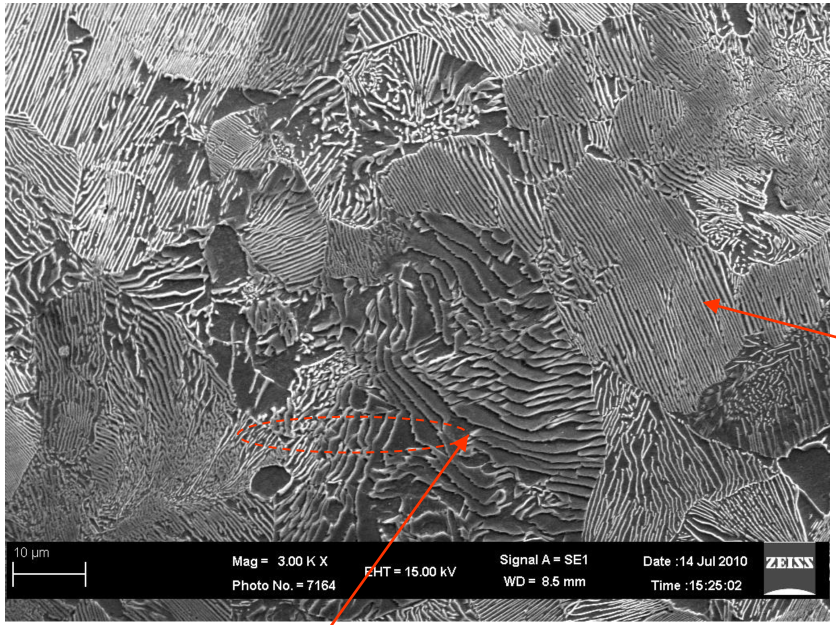
Bcc-Fe with C-solubility

Cementite

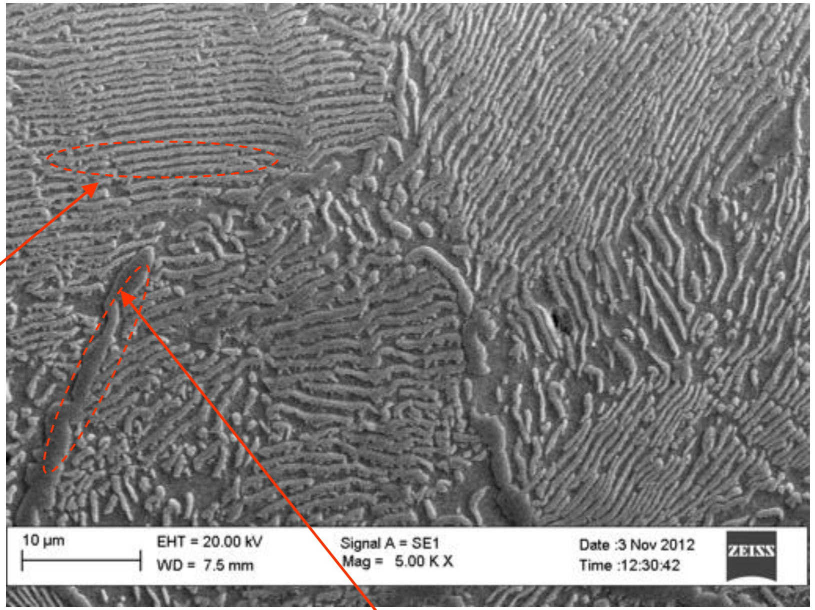
(Fe_3C)

SEM micrograph of pearlite in eutectoid composition (0.8% C) of steel

SEM micrograph of pearlite in hypo-eutectoid composition (1% C) of steel



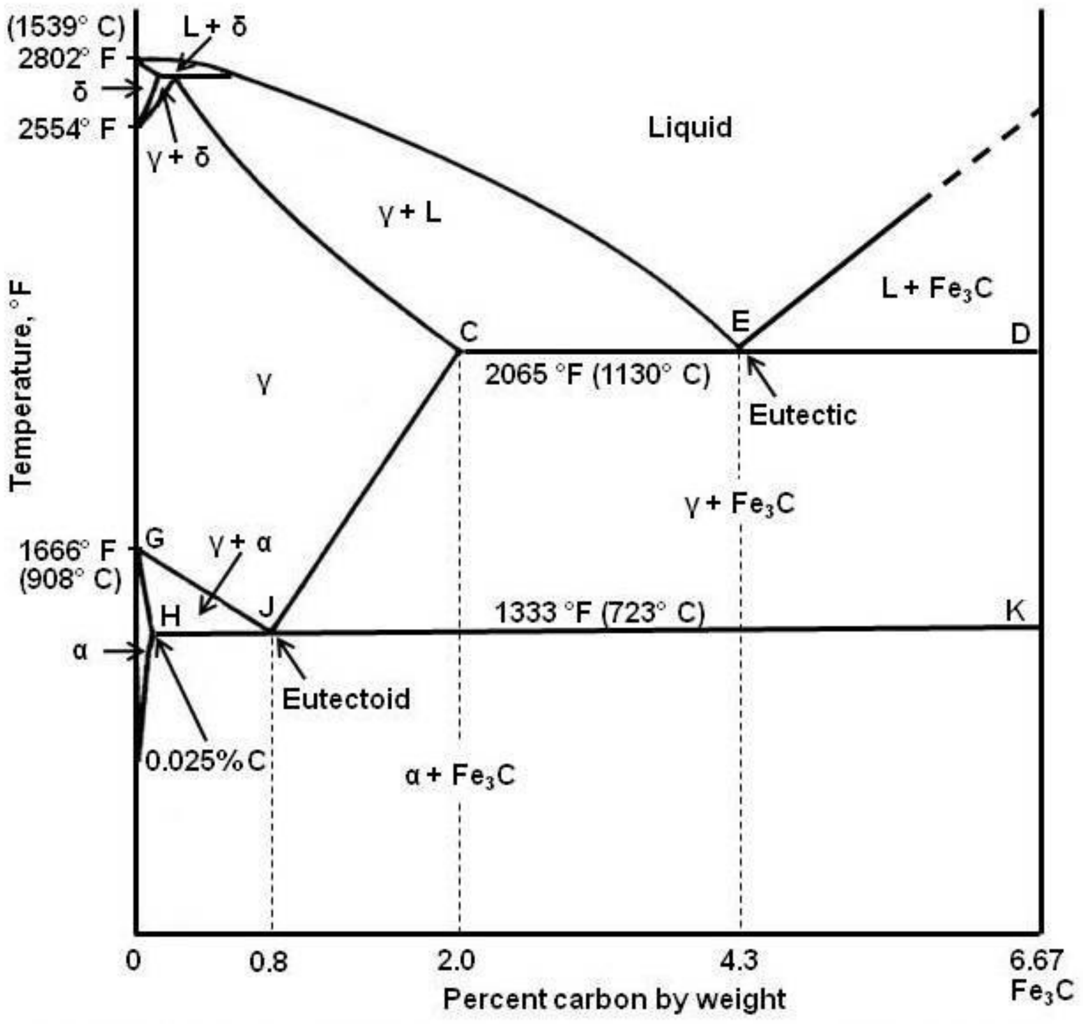
Pearlite



lamellar spacing in the micrograph: different orientation of the lamellae

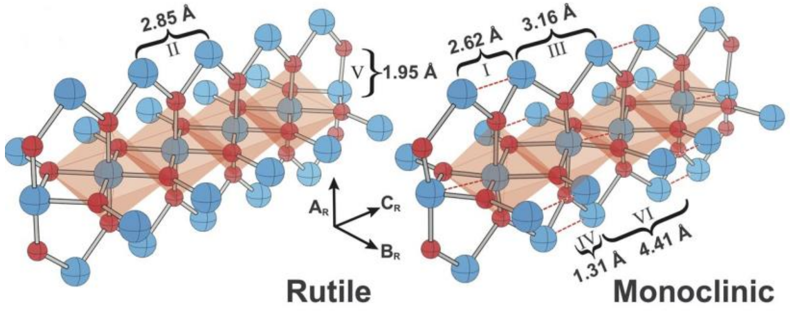
Pro-eutectoid Cementite along prior austenite grain boundaries

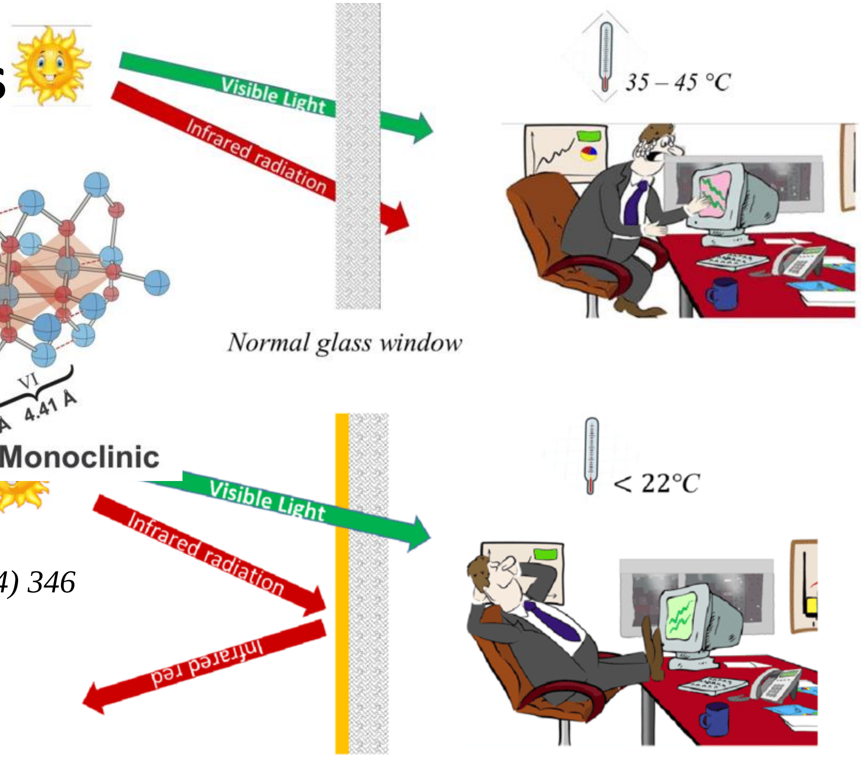
A steel contains 20% pearlite and 80% pro-eutectoid (primary) ferrite at room temperature. Is the steel hypoeutectoid or hypereutectoid?



Phase Transformation

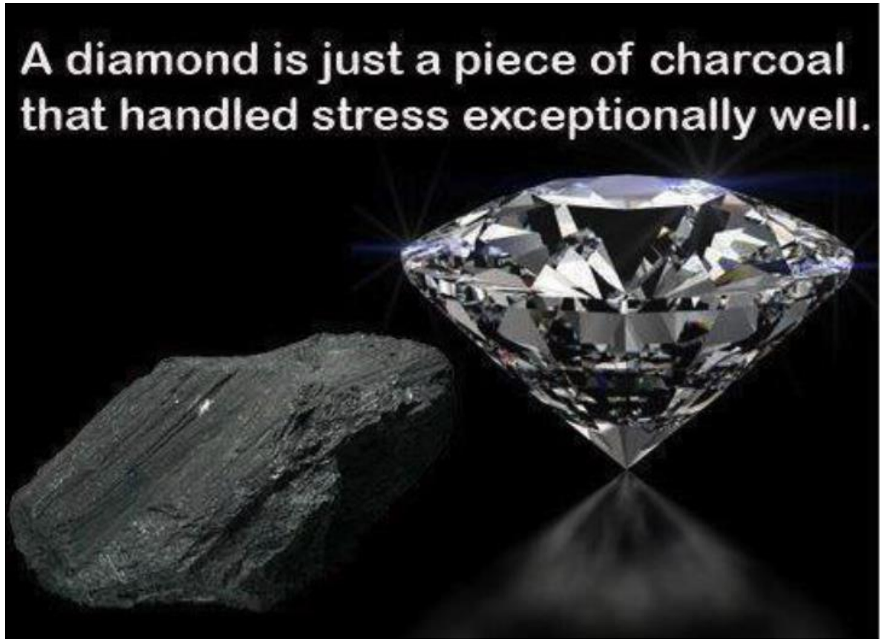
Smart windows

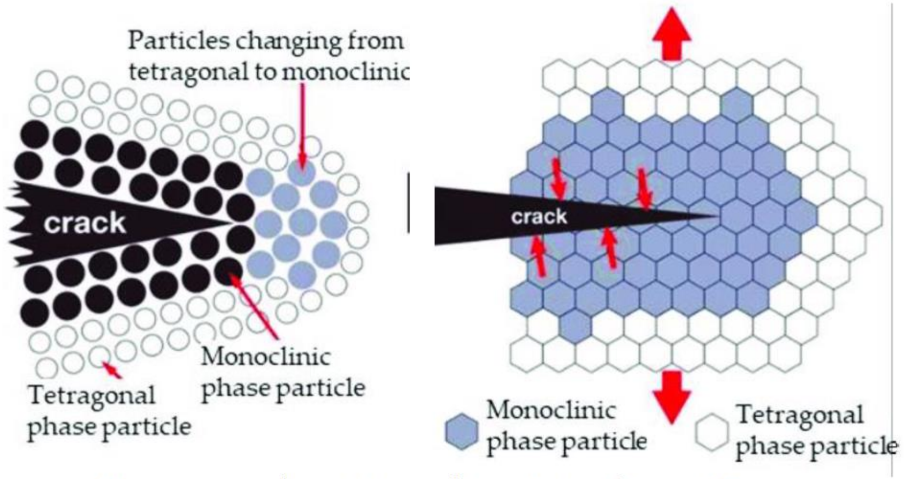




Morrison et al., Science (2014) 346

VO_2 based smart window





Stress can also cause phase transformation

Why should one learn phase transformation?

- ❑ What causes phase transformation? -----> Temperature and Pressure
- ❑ Knowledge about phase transformation will aid at designing the material.

Engineering of Microstructure and phase → Enhancement of desired properties in applications