Generalisation

www.msm.cam.ac.uk/phase-trans

S. Khare, K. Y. Lee, H. K. D. H. Bhadeshia, *Metallurgical and Materials Transactions* **41A** (2009) 922-928

J. H. Jang, I. G. Kim, H. K. D. H. Bhadeshia, *Computational Materials Science* **44** (2009) 1319-1326

J. H. Jang, I. G. Kim, H. K. D. H. Bhadeshia, *Scripta Materialia* **63** (2010) 121-123

G. Gomez, T. Perez and H. K. D. H. Bhadeshia, *Materials Science and Technology* **25** (2009) 1502-1517

G. Cola and S. S. Babu, *Materials Science and Technology, in press*

S. Khare, K. Y. Lee, H. K. D. H. Bhadeshia, *International Journal of Materials Research* **100** (2009) 1513-1529

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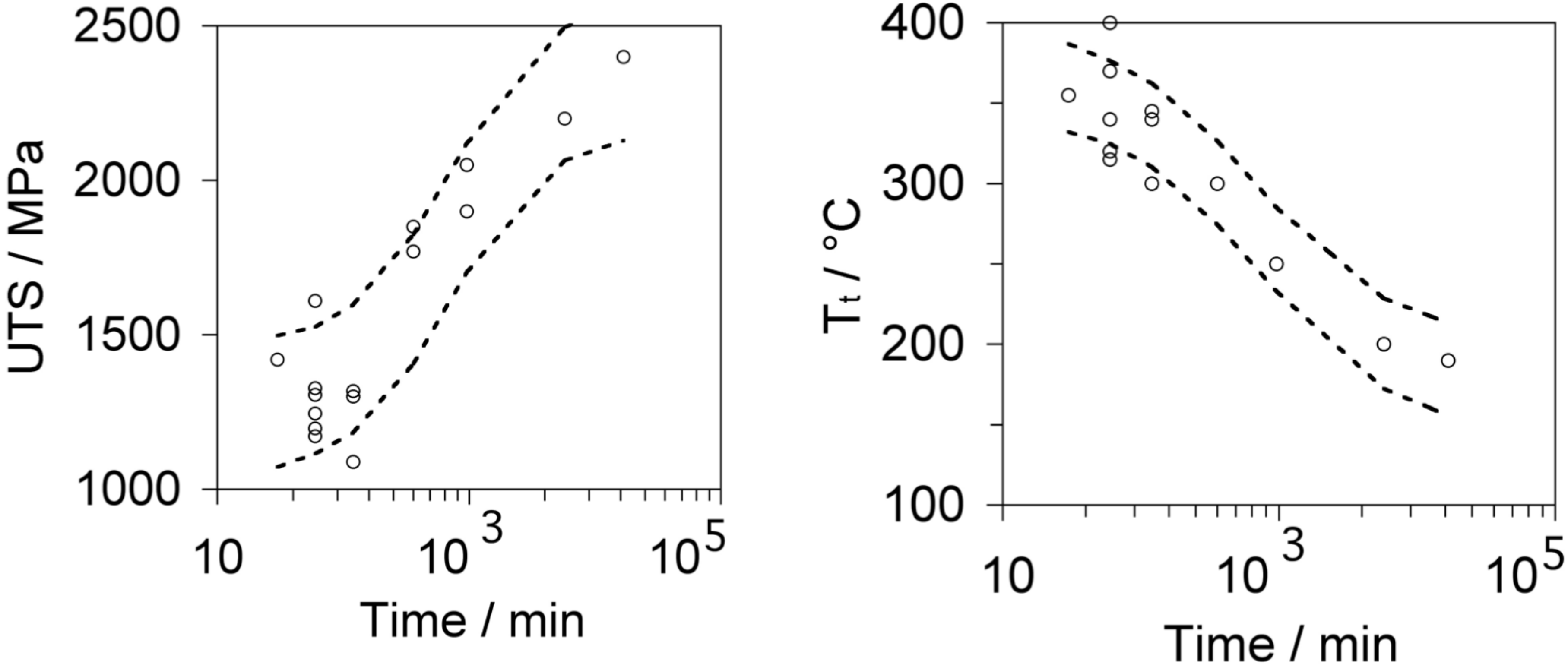
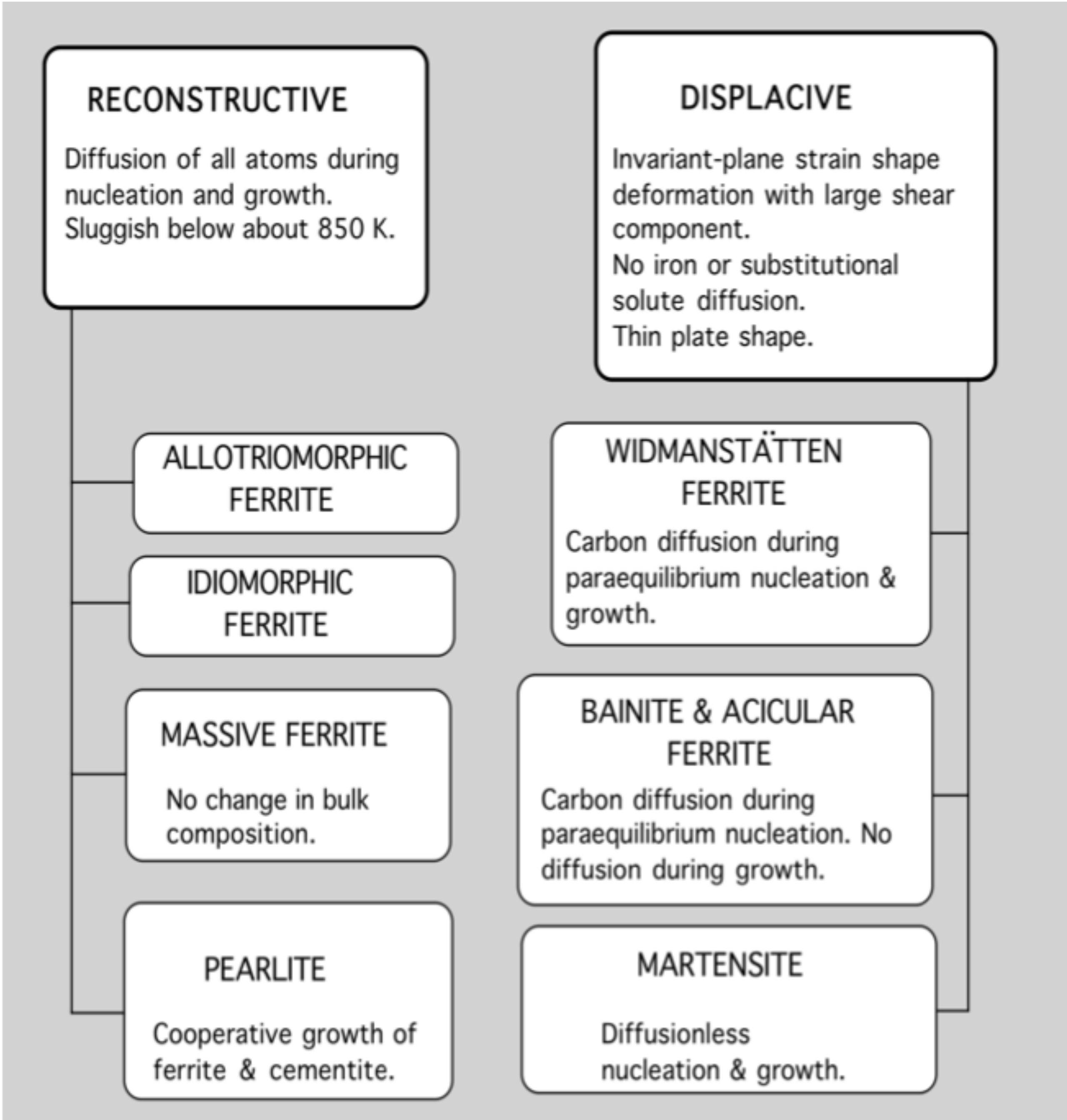
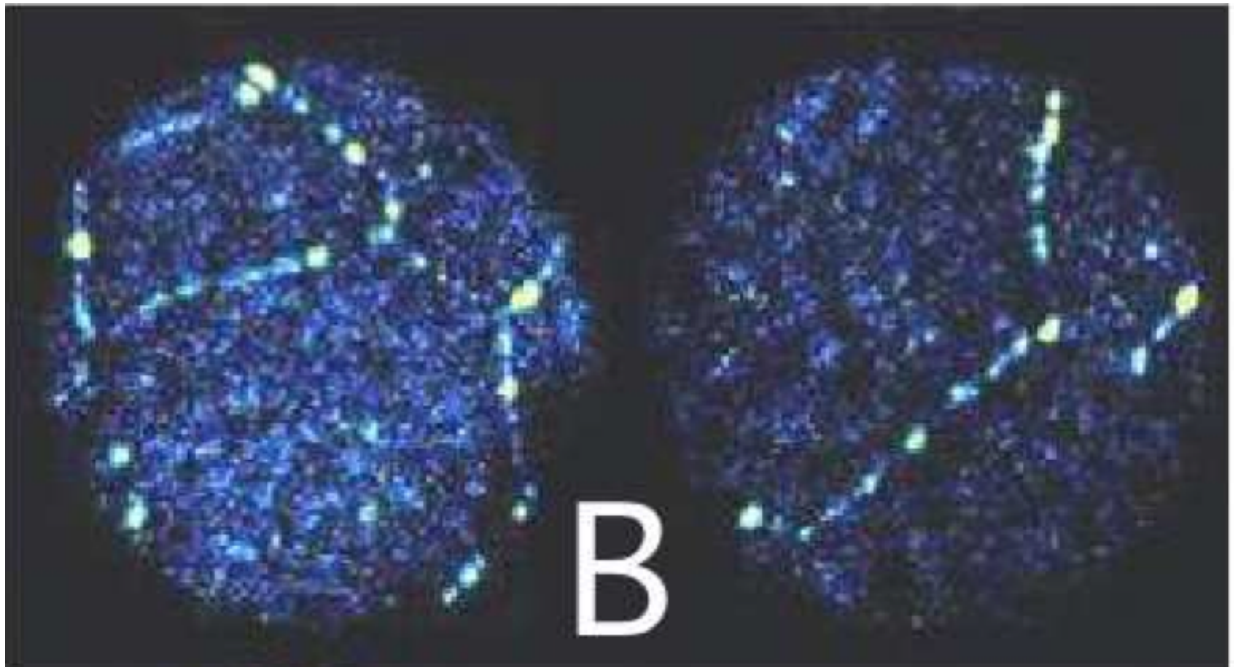

2500
2000
1500
1000
UTS / MPa
10
10^3
10^5
Time / min
400
300
200
100
T_t / °C
10
10^3
10^5
Time / min

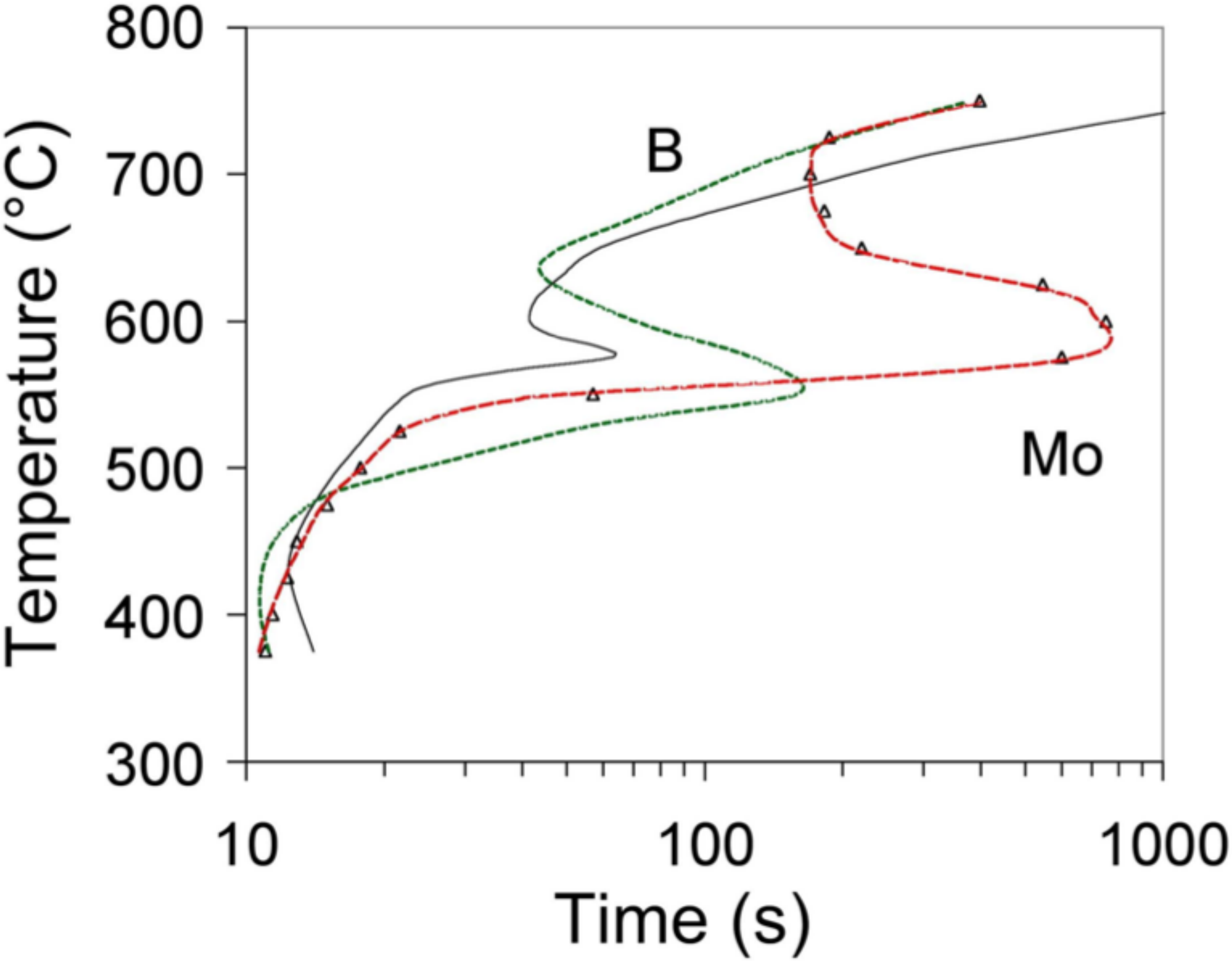

RECONSTRUCTIVE
Diffusion of all atoms during nucleation and growth. Sluggish below about 850 K.
DISPLACIVE
Invariant-plane strain shape deformation with large shear component.
No iron or substitutional solute diffusion.
Thin plate shape.
ALLOTRIOMORPHIC FERRITE
IDIOMORPHIC FERRITE
MASSIVE FERRITE
No change in bulk composition.
PEARLITE
Cooperative growth of ferrite & cementite.
WIDMANSTÄTTEN FERRITE
Carbon diffusion during paraequilibrium nucleation & growth.
BAINITE & ACICULAR FERRITE
Carbon diffusion during paraequilibrium nucleation. No diffusion during growth.
MARTENSITE
Diffusionless nucleation & growth.

Kinetics of tranformation:

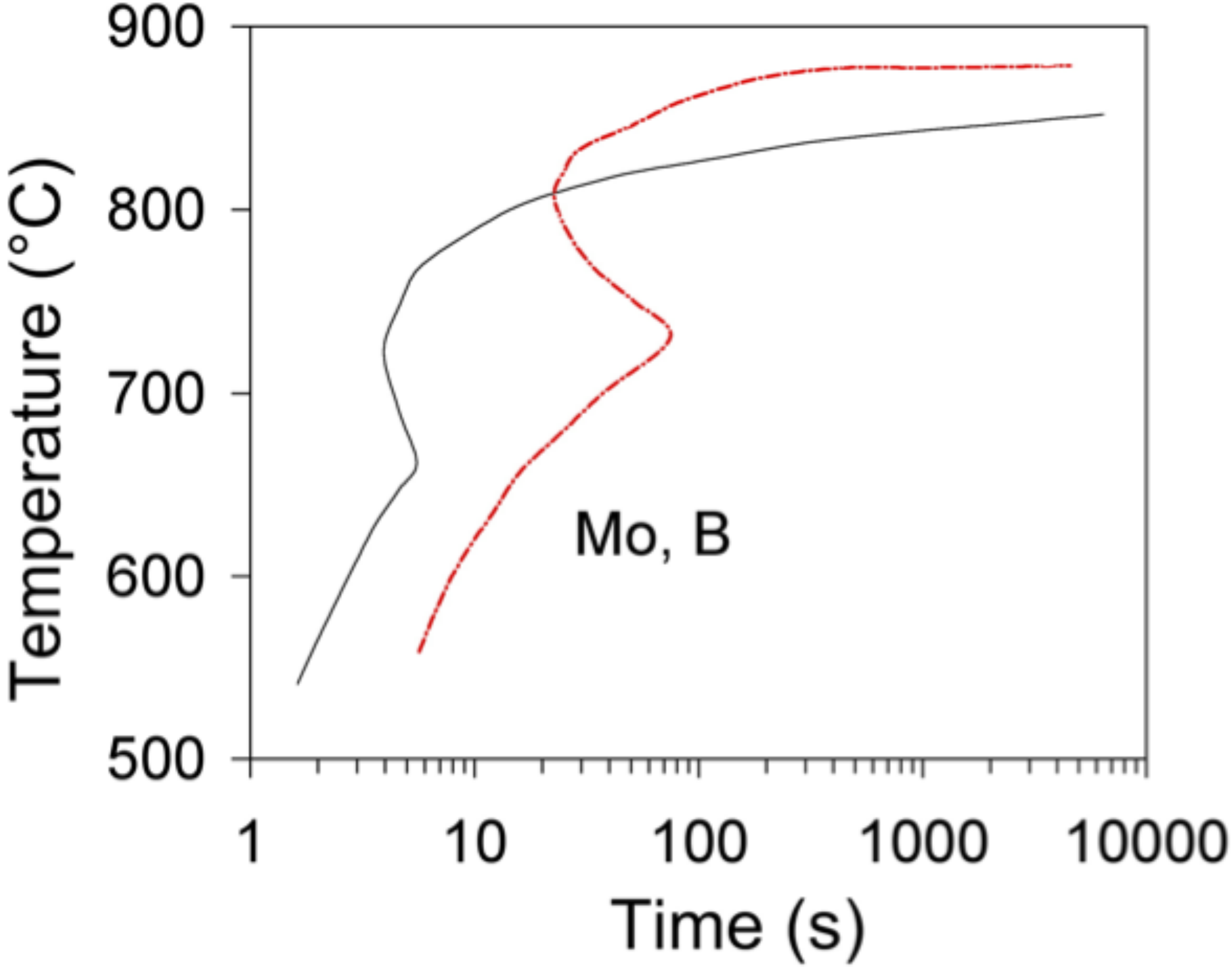
Molybdenum and Boron

	C	Si	Mn	Al	Co	Mo	N	B	Ti
Alloy 1	0.32	1.47	1.98	1.06	1.08	0	0.0034	0	0
Alloy 2–B	0.33	1.47	1.96	1.06	1.08	0	0.0030	**0.0028**	0.01
Alloy 3–Mo	0.32	1.47	1.98	1.07	1.08	**0.25**	0.0030	0	0

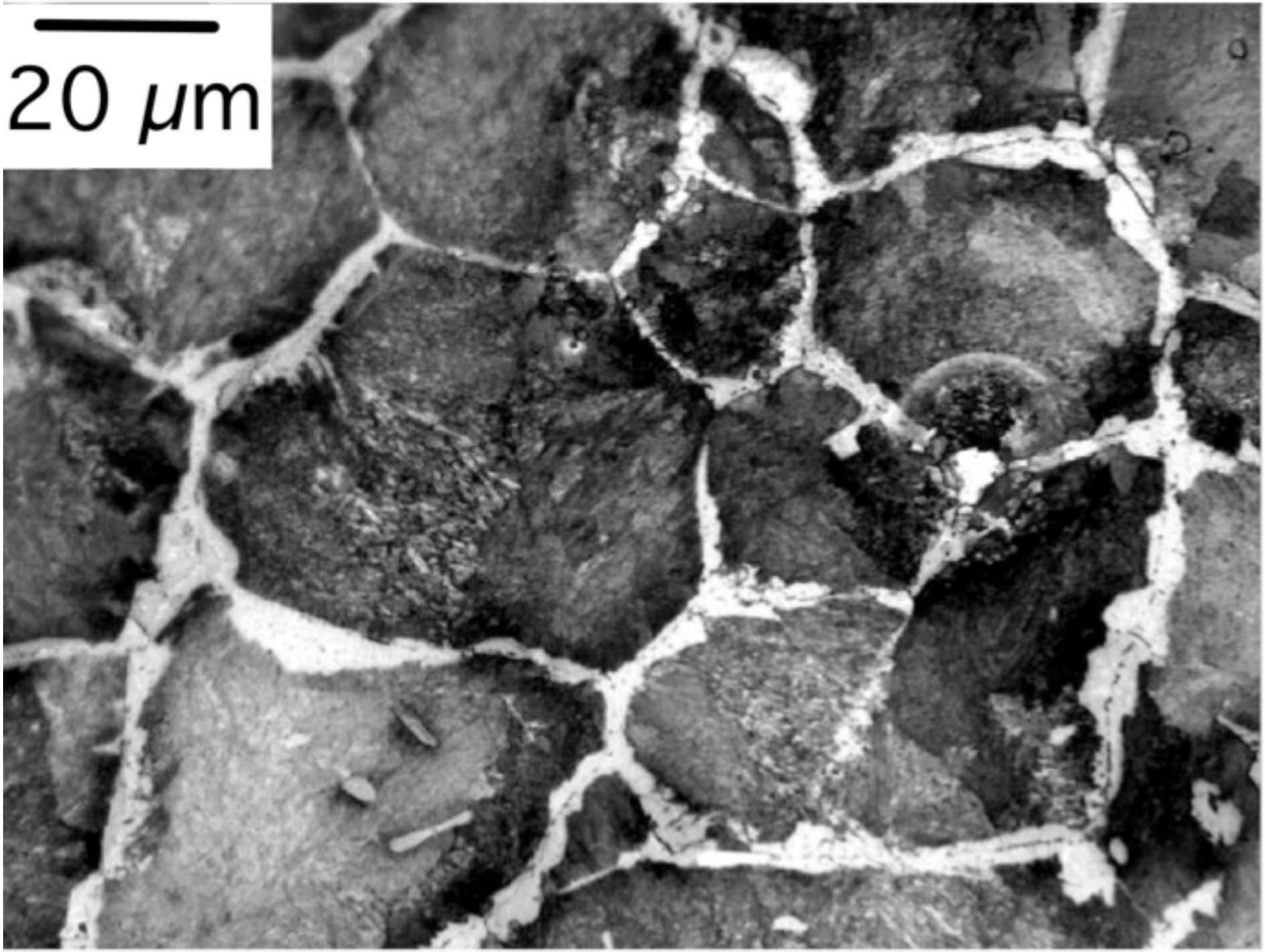


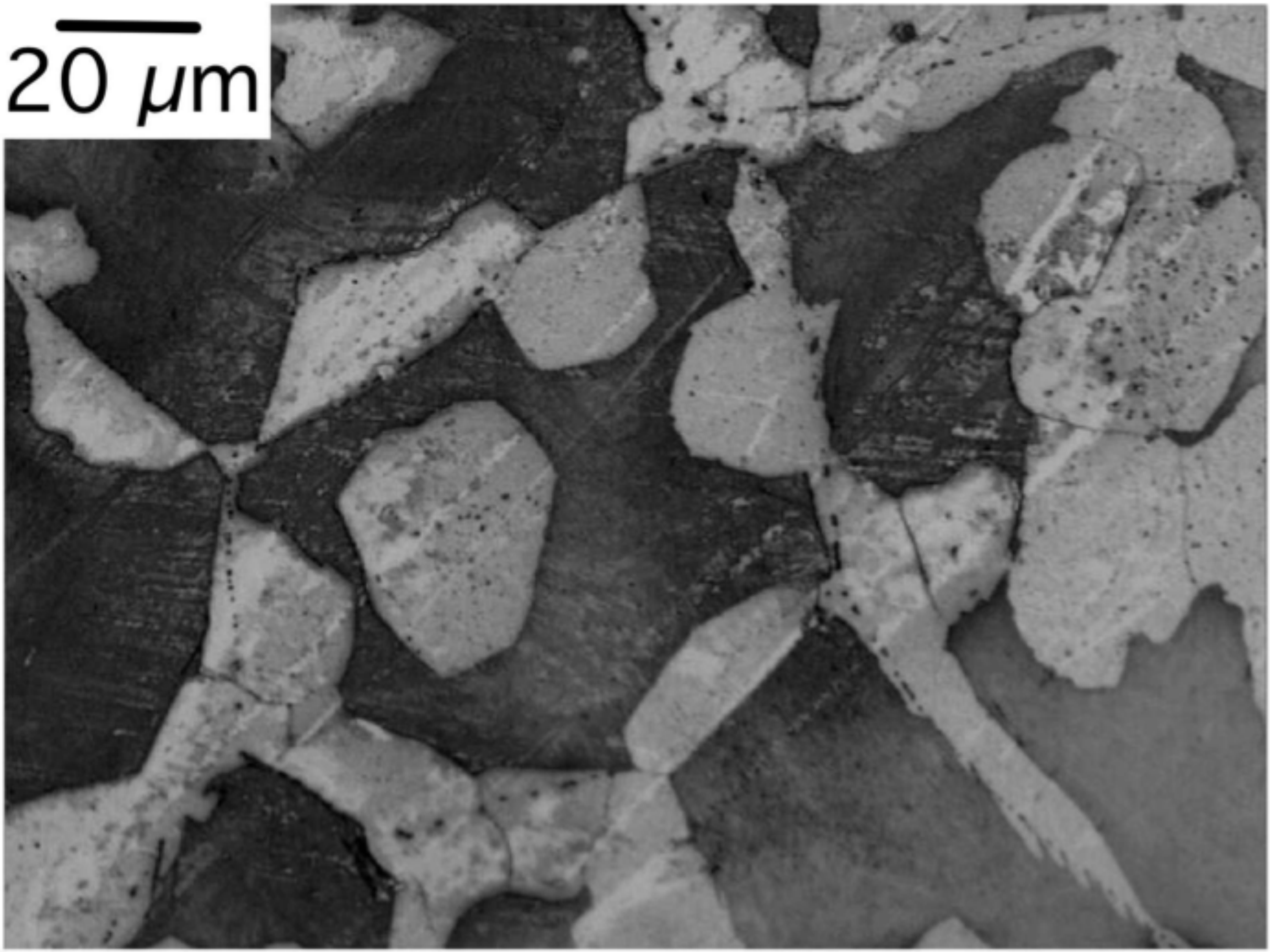


800
700
600
500
400
300
Temperature (°C)
B
Mo
10
100
1000
Time (s)

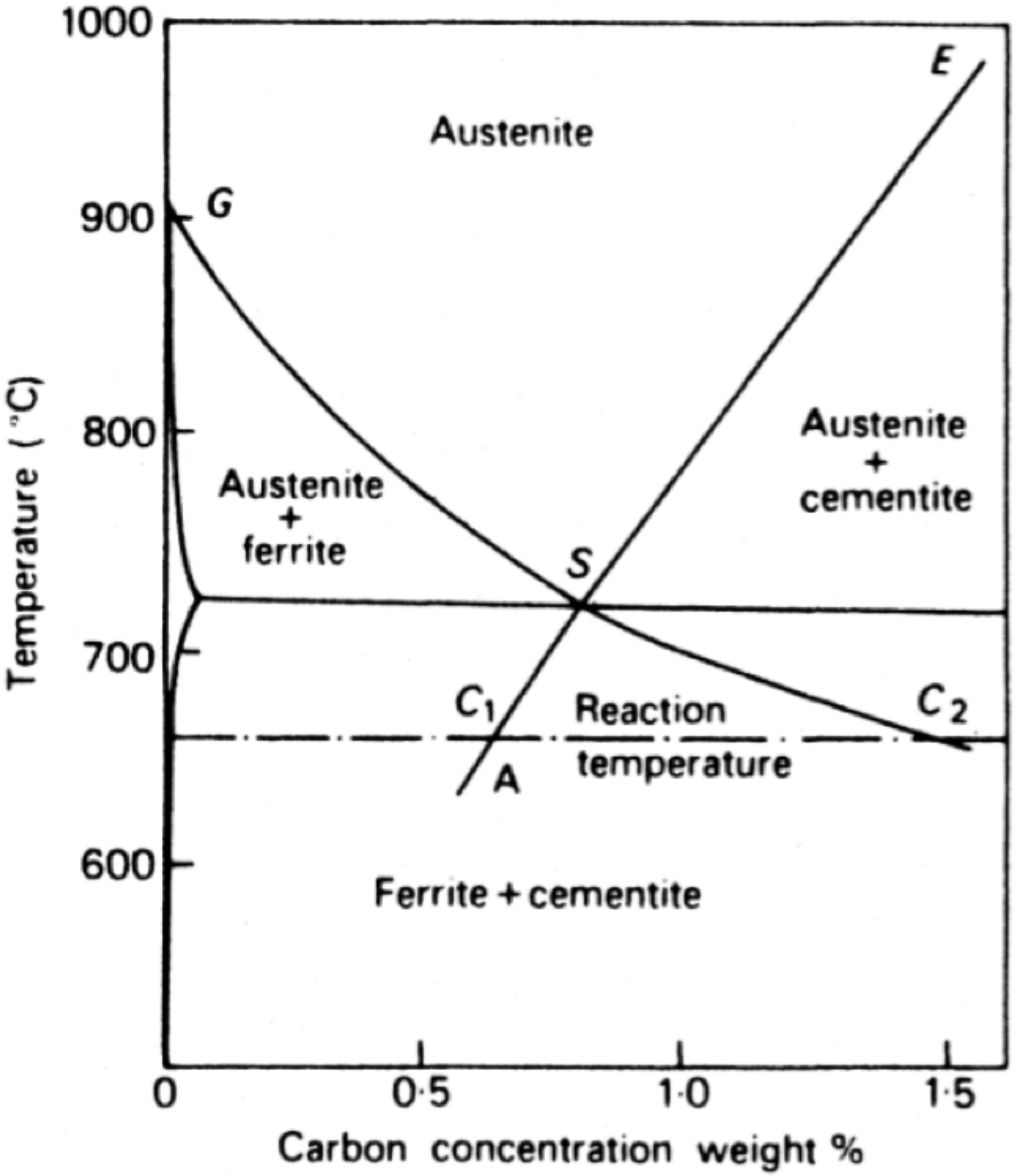


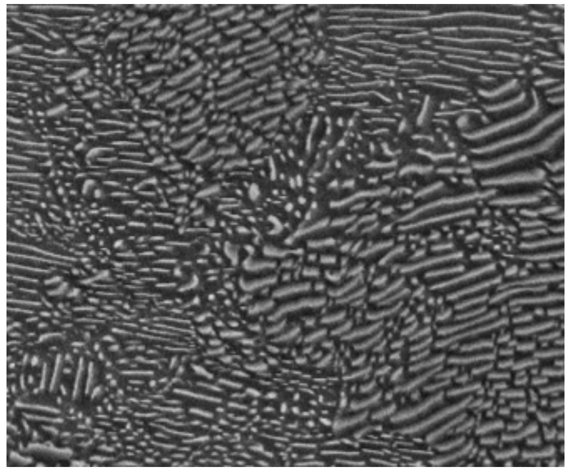
K. J. Irvine, F. B. Pickering and W. C. Haselwood
Journal of the Iron and Steel Institute, **186** (1957) 54-67


20 μm


20 μm

Hultgren extrapolation





First-Principles Calculation

Quantum Mechanics

↓

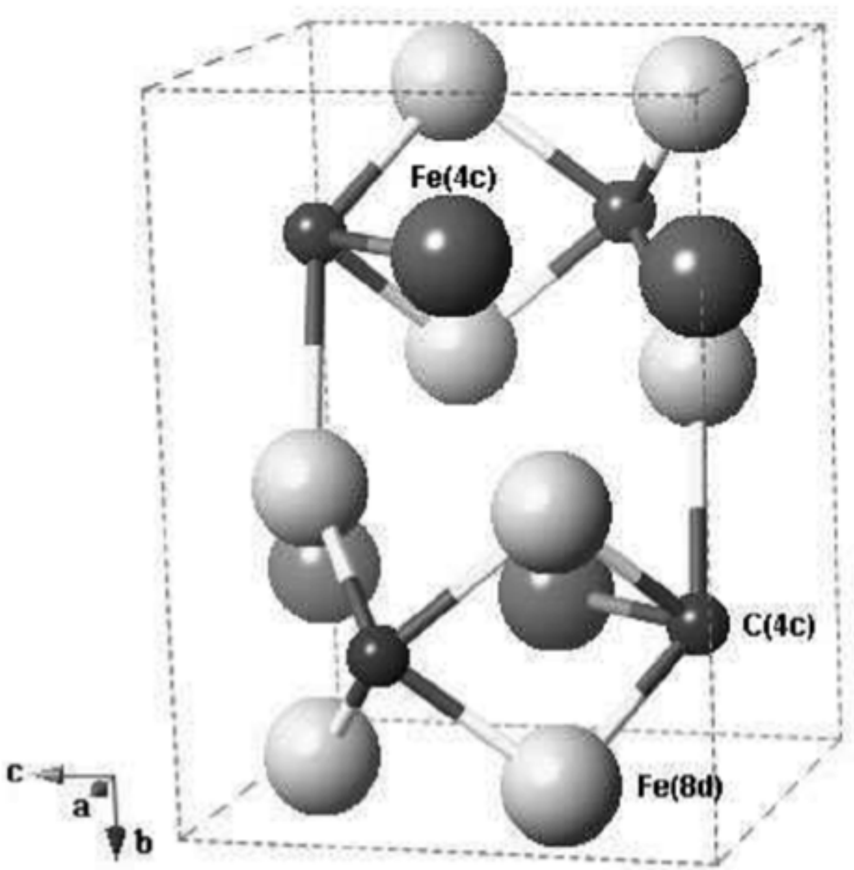
Atomic Position → Schrödinger Equation → Electron Density

↓

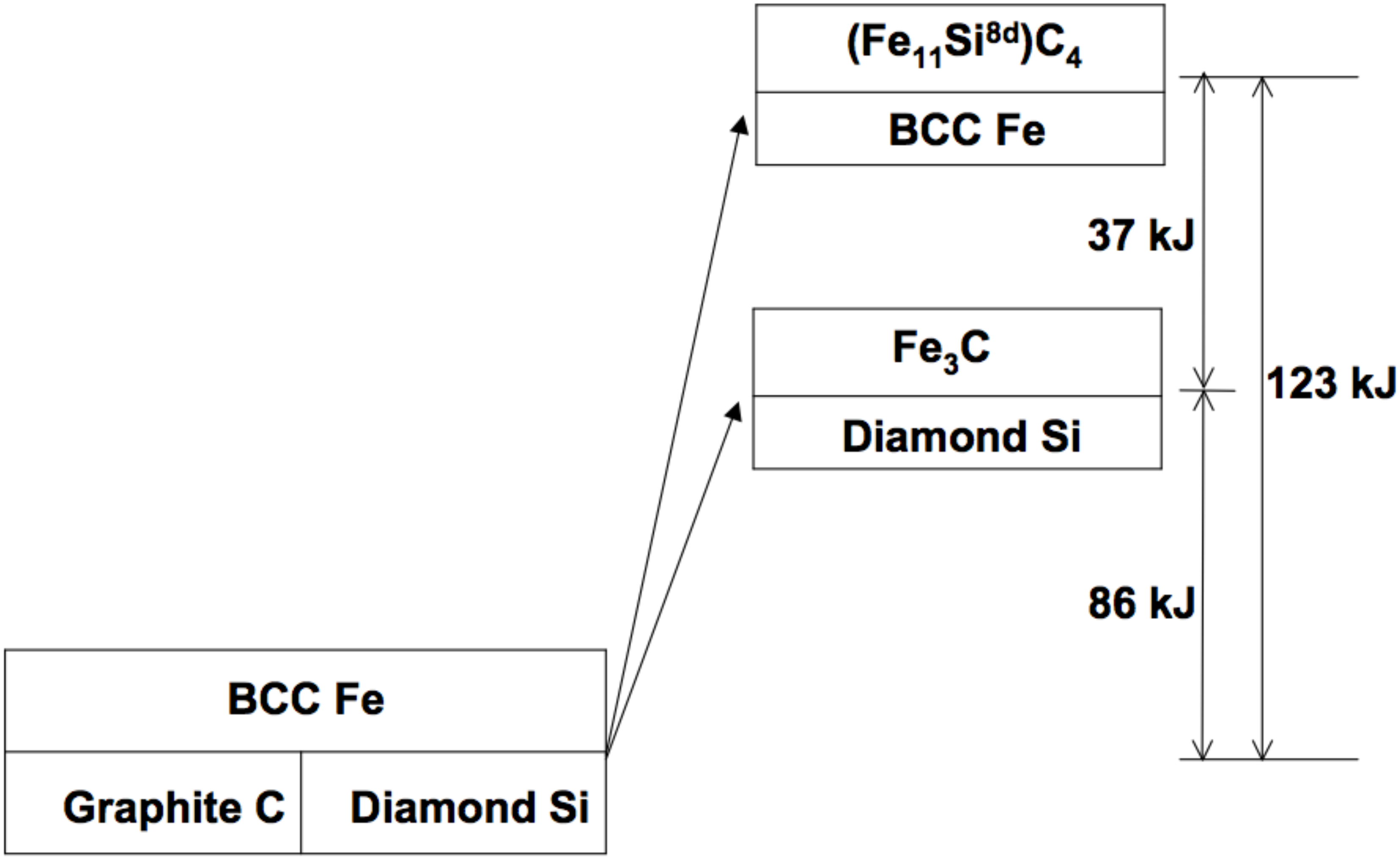
Physical Principles

↓

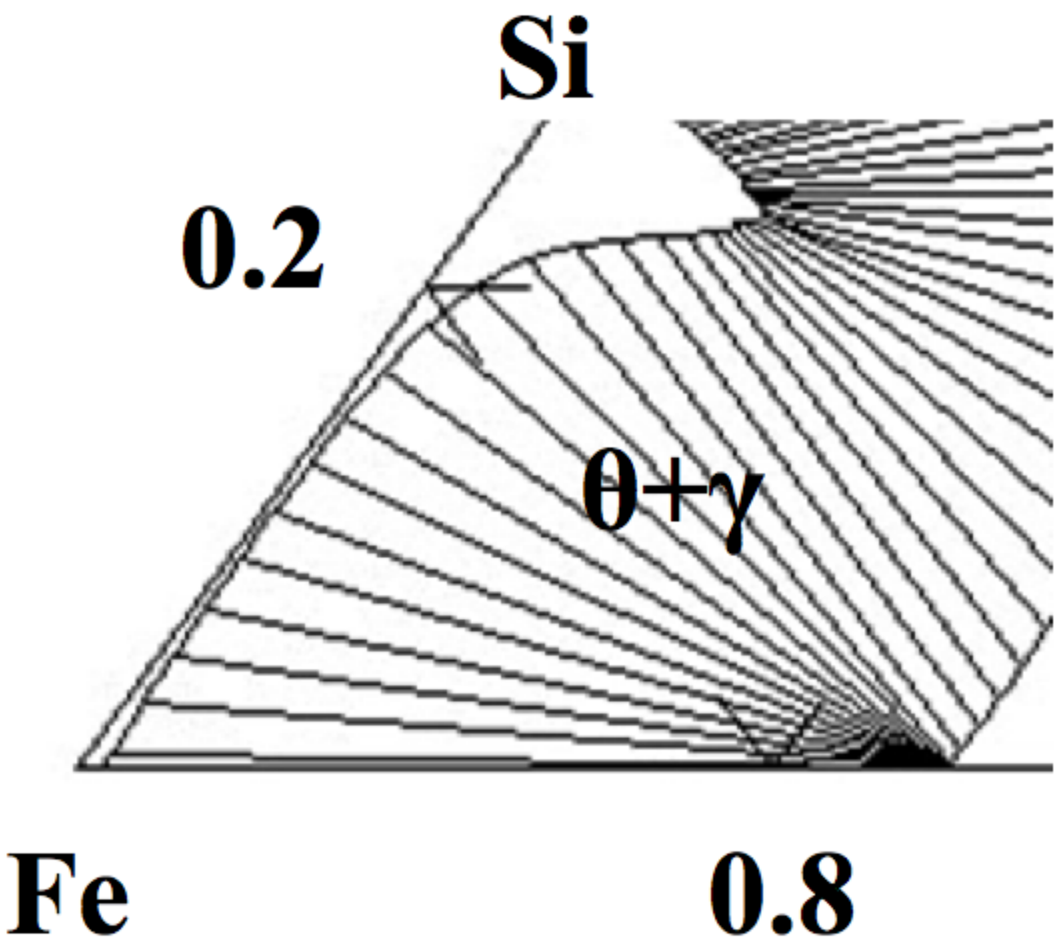
Structure	**Thermodynamic**	**Mechanical**	**Electrical**
Molecular	Internal Energy	Compressibility	Electron
Crystal	Entropy	Elastic Constants	Ionization
Density	Free Energy	Bulk Modulus	Energy Band
Defect	Formation Energy	Vibrations	Band Gaps
Surface	Phase Transform		Magnetic
Interface	Phase Diagrams		



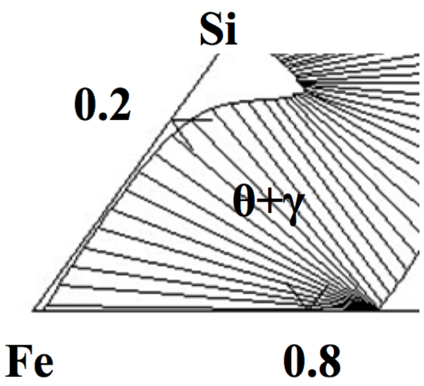
Phase	Cementite
Structure	Orthorhombic
Space Group	*Pmna*
a	5.0896 Å (5.1281 Å)
b	6.7443 Å (6.6512 Å)
c	4.5248 Å (4.4623 Å)


(Fe11Si8d)C4
BCC Fe
Fe3C
Diamond Si
37 kJ
123 kJ
86 kJ
BCC Fe
Graphite C
Diamond Si

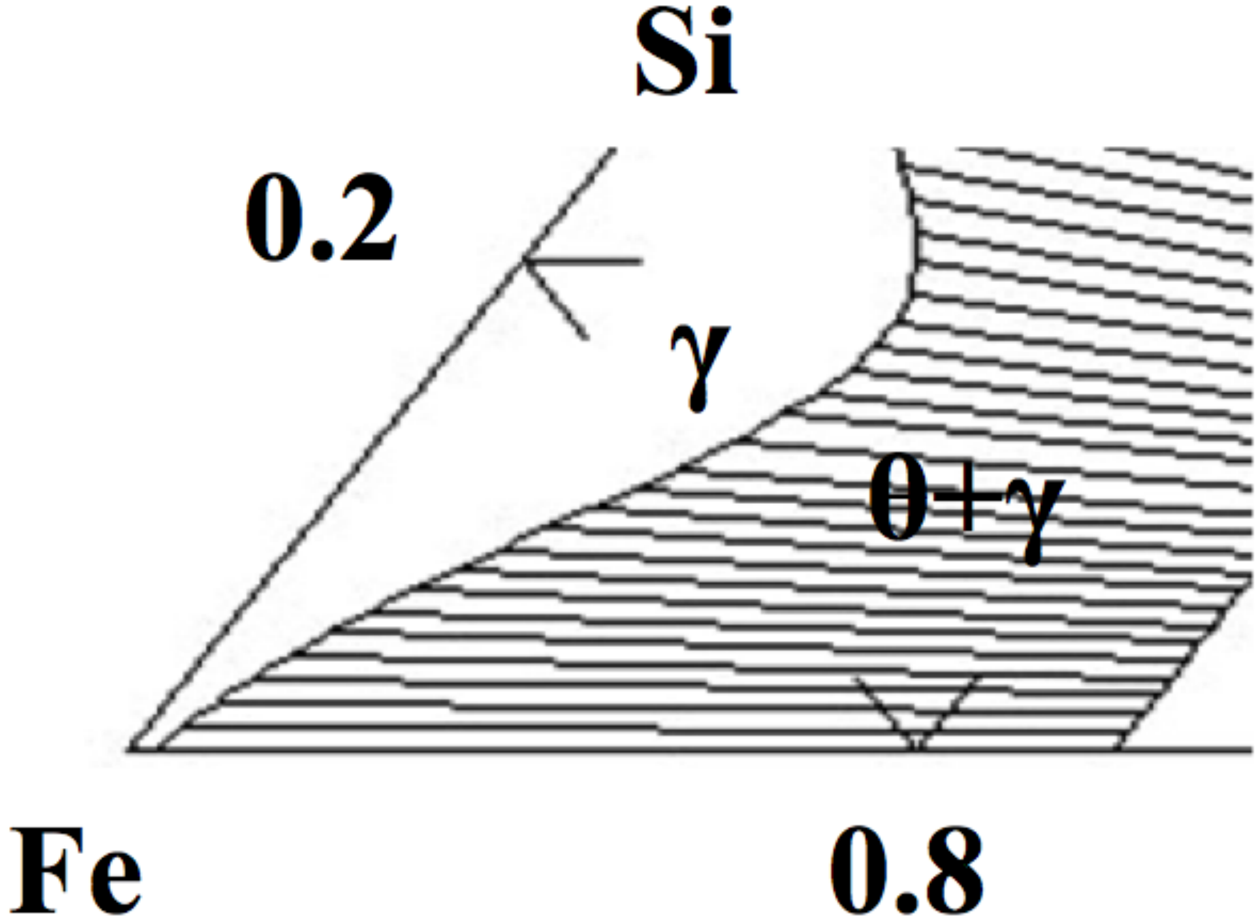
Equilibrium

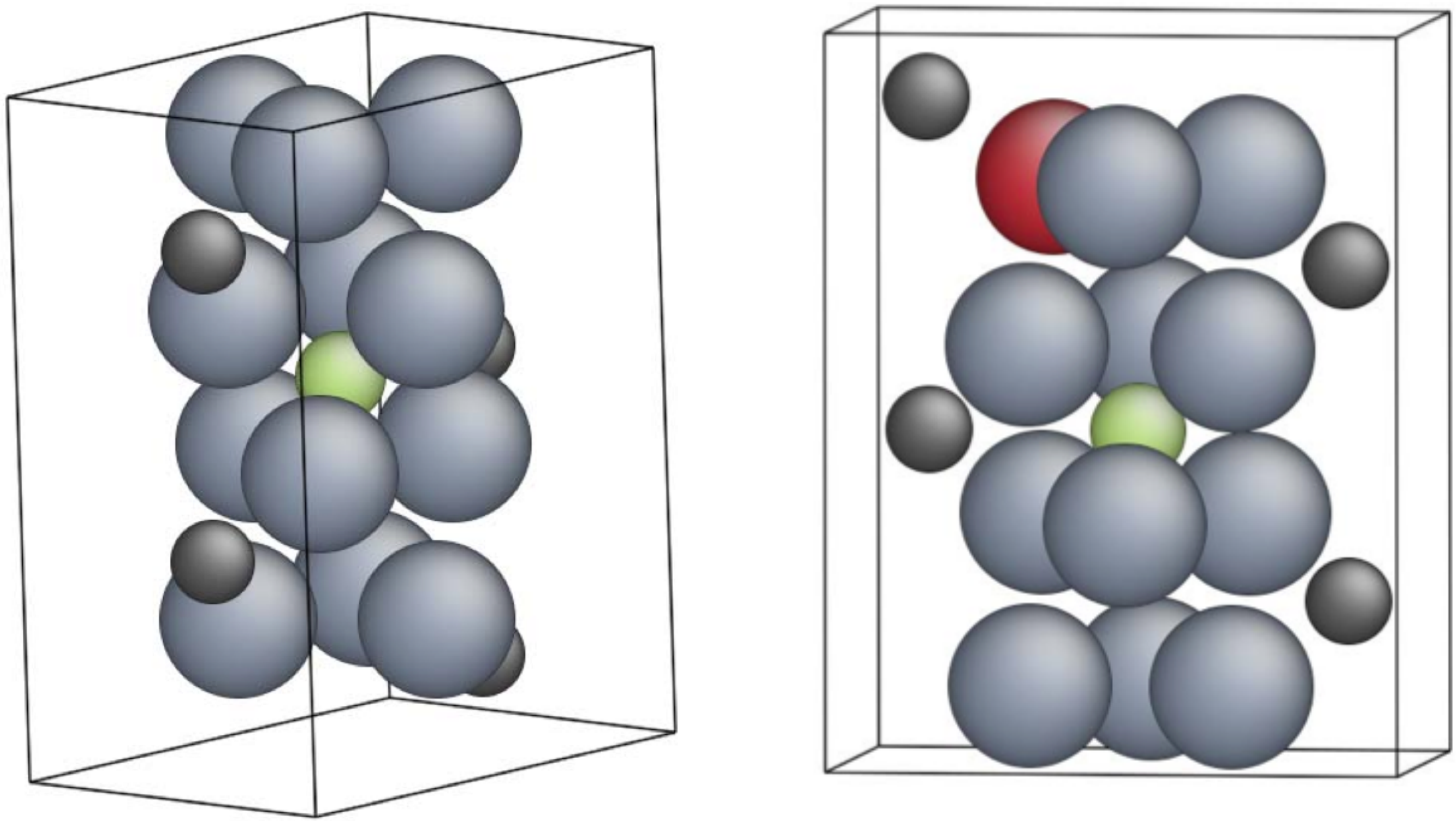


Equilibrium

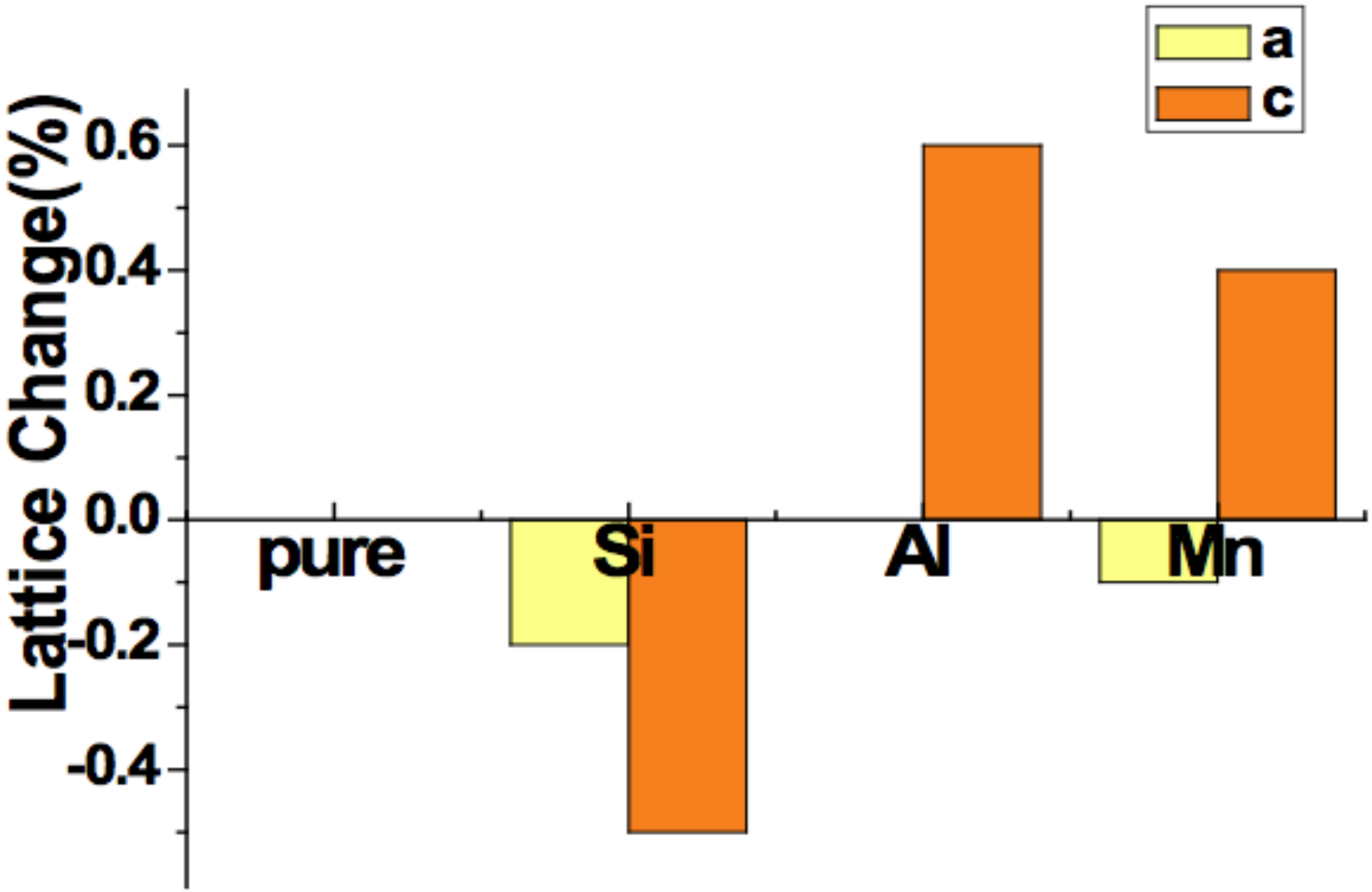


Para-equilibrium



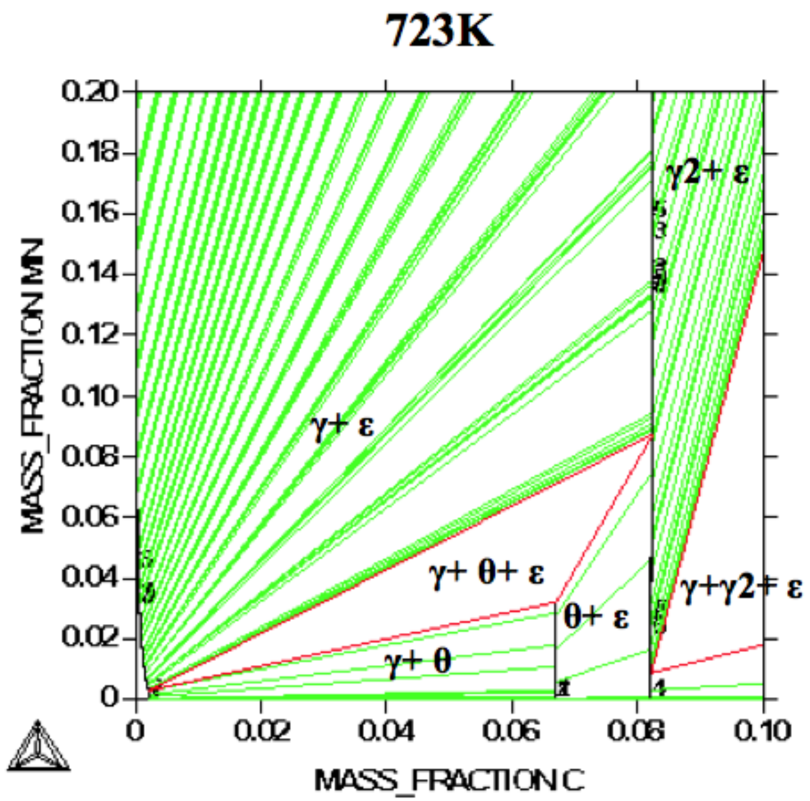


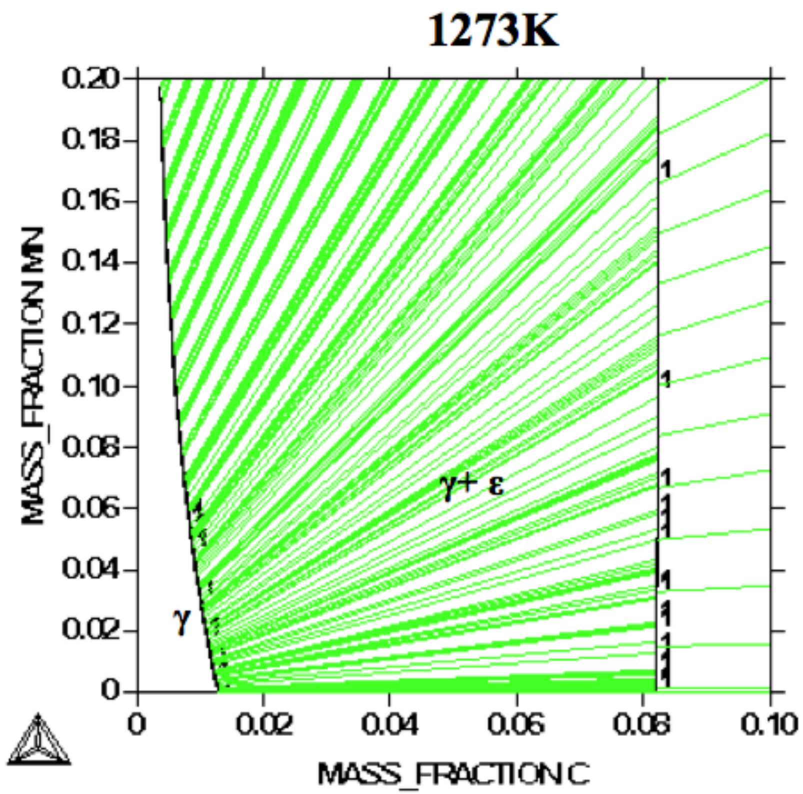
ΔH (kJ/mol)	ε-carbide	cementite
pure-carbide	106.0	86.1
Si substituted	154.4(+48.4)	123.2(+37.1)
Al substituted	84.7(−21.3)	72.5(−13.6)
Mn substituted	74.8(−31.2)	81.1(−5.0)

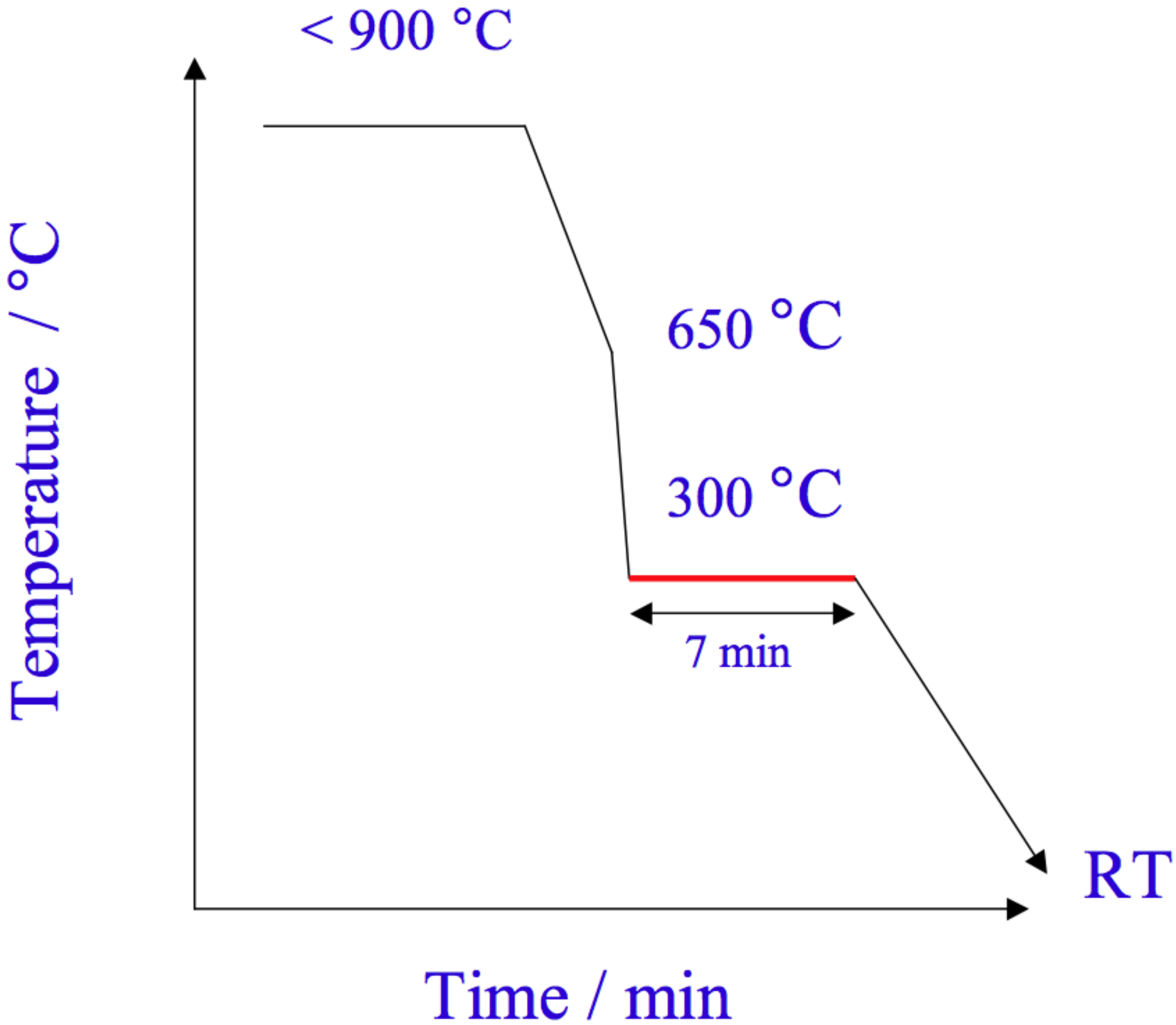


a
c
Lattice Change(%)
0.6
0.4
0.2
0.0
-0.2
-0.4
pure
Si
Al
Mn

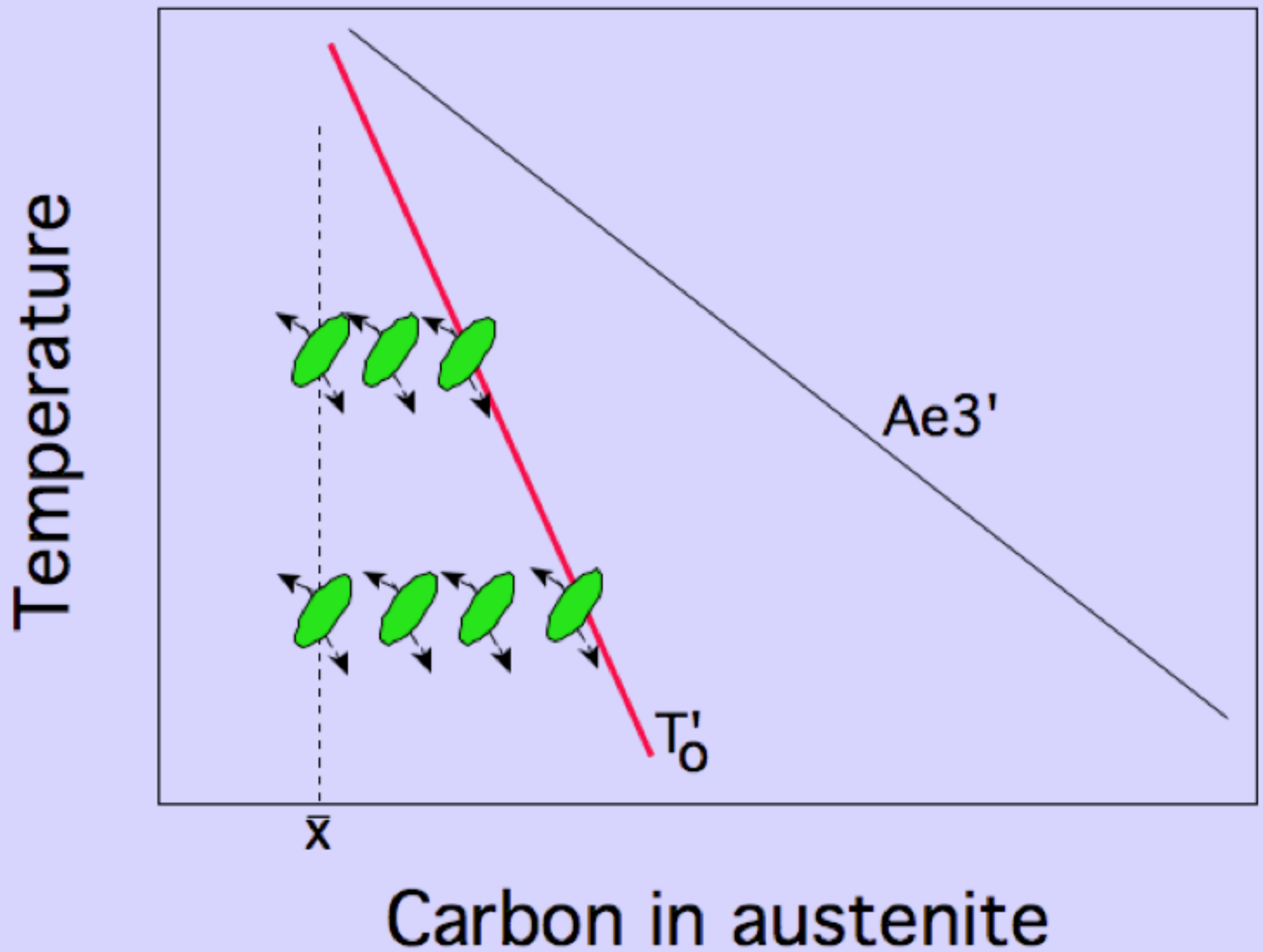
- **Phase Boundary Calculation (PE/LPE/NPLE)**
- **Alloy Design (Stable Epsilon Carbide)**



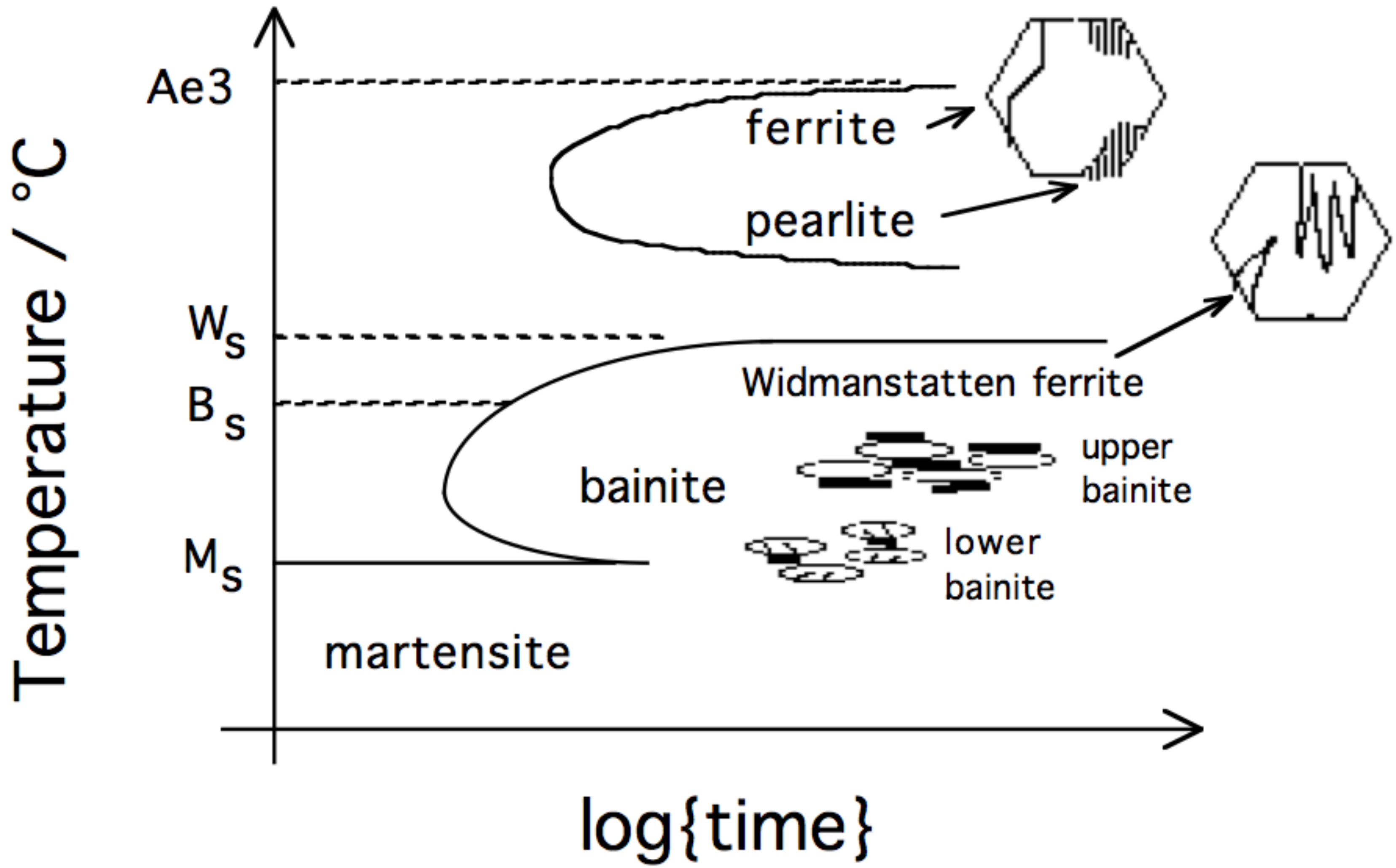



< 900 °C
650 °C
300 °C
7 min
RT
Temperature / °C
Time / min

Methods: phase diagrams, thermodynamics

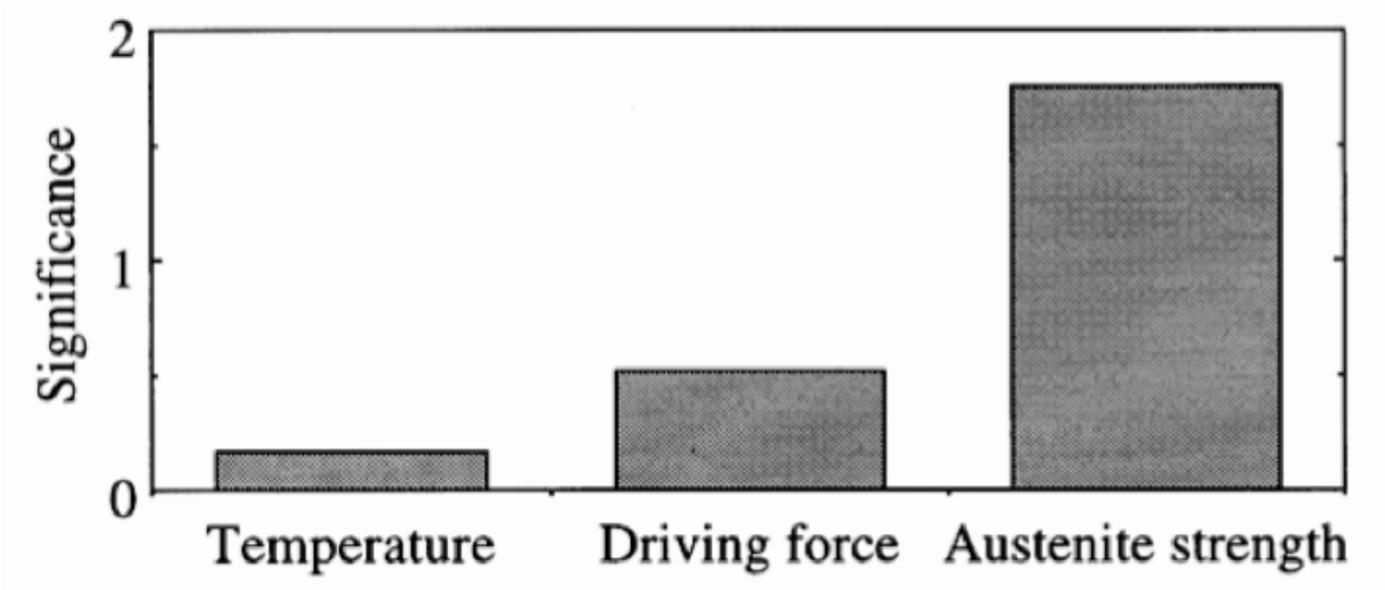


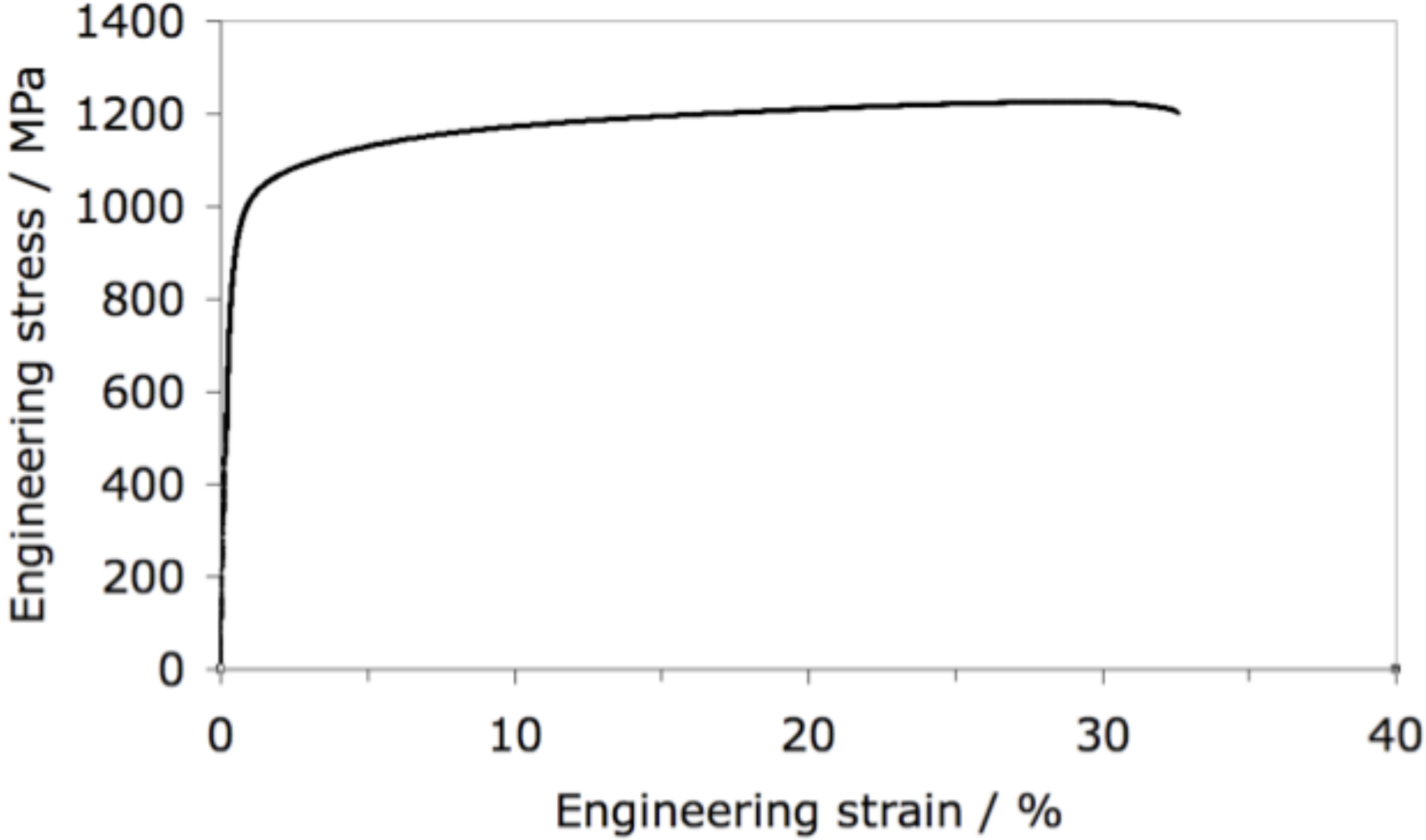
Methods: TTT diagrams, transformation temperatures



Methods: thickness of bainite plates

- Chemical free energy available for nucleation
- Strength of austenite at transformation temperature
- Transformation temperature

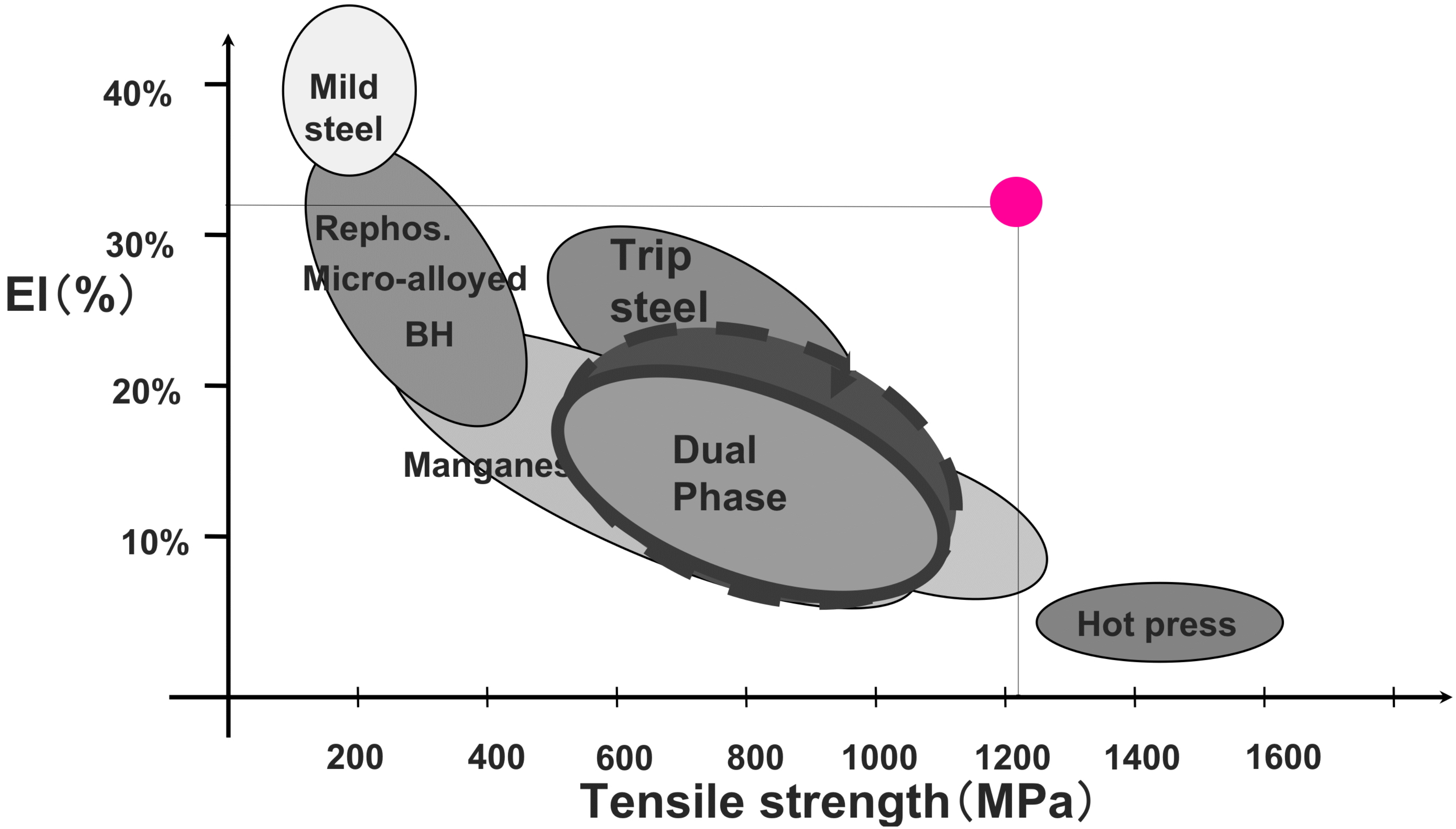




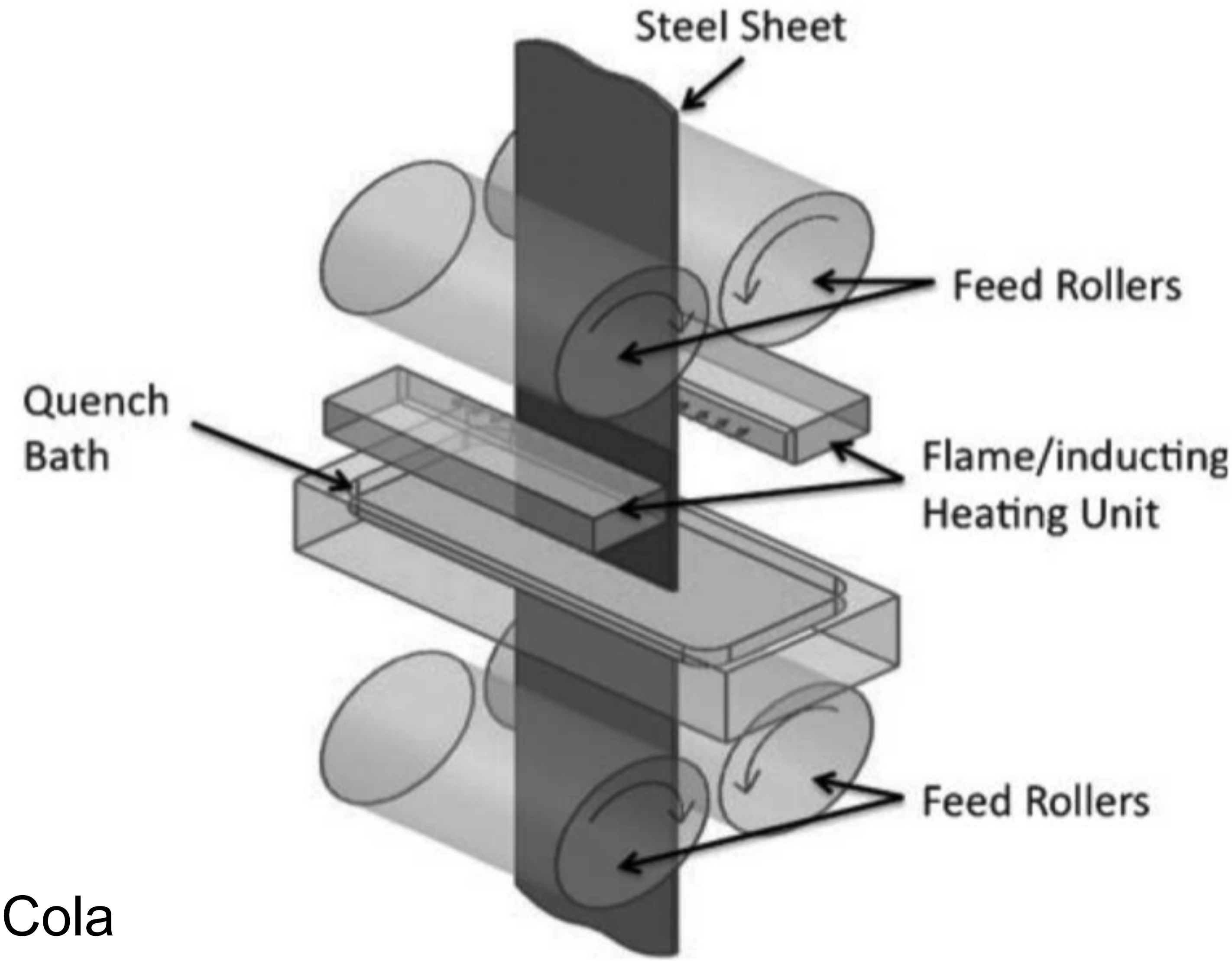
Engineering stress / MPa
1400
1200
1000
800
600
400
200
0
0
10
20
30
40
Engineering strain / %

Novel steel designed by Computational Metallurgy Laboratory, GIFT for production on continuous annealing line.

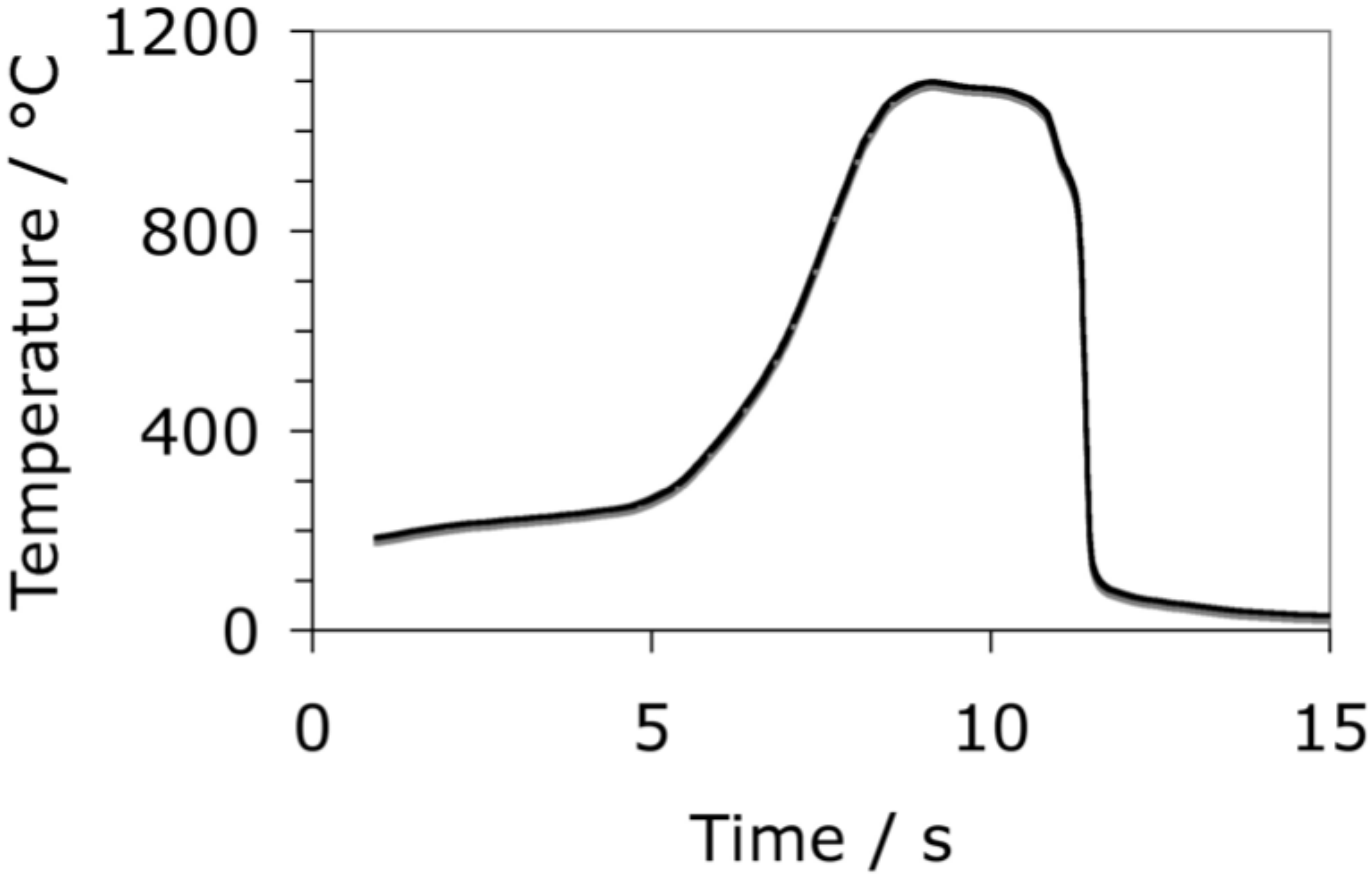
Product of UTS and elongation = 39500 MPa %



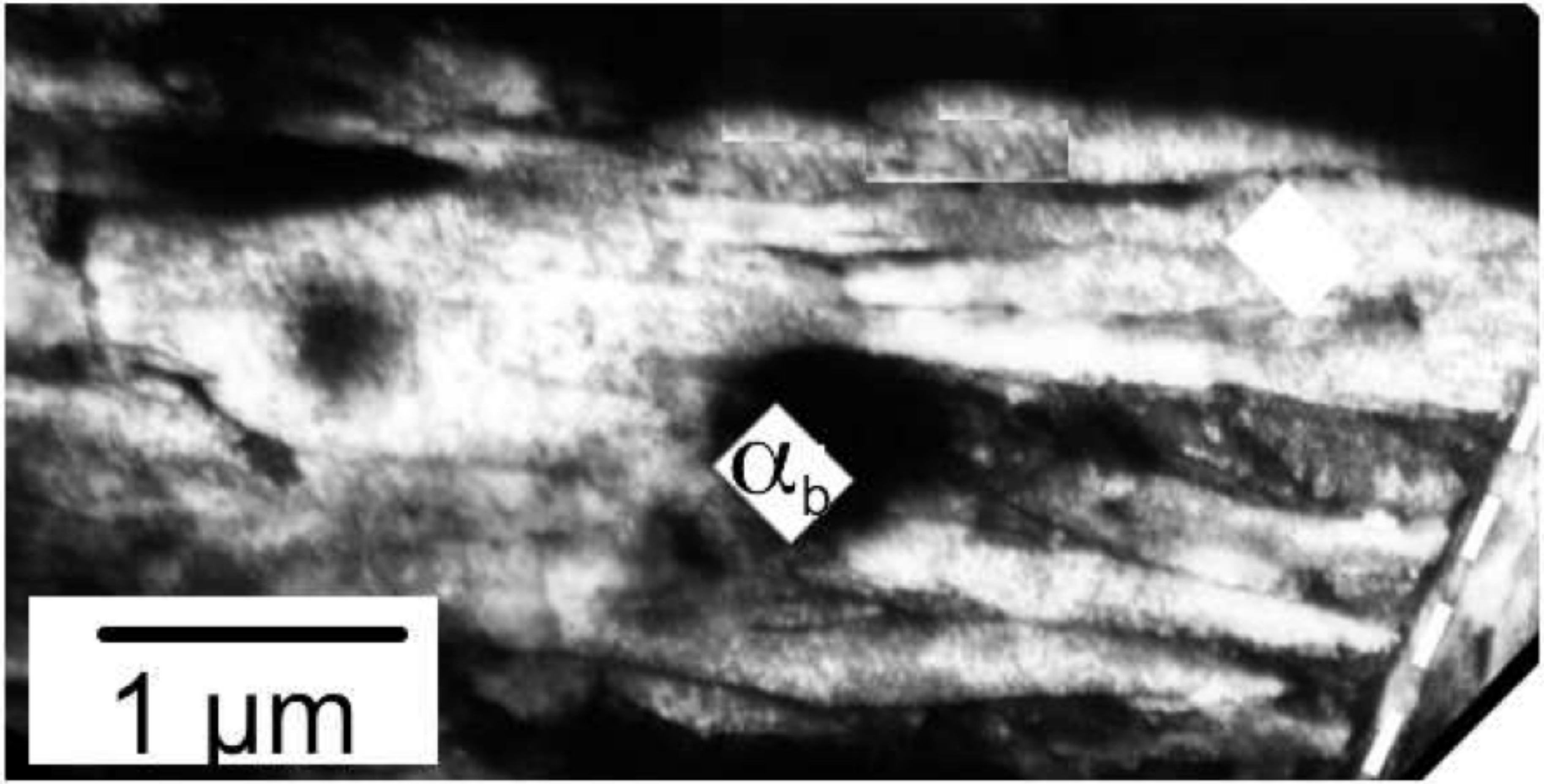
Flash Processing: Fe-0.2C-0.3Si.....



Gary Cola



Temperature / °C
1200
800
400
0
0
5
10
15
Time / s



1464 MPa yield

1658 MPa UTS

10% elongation