Solubility of carbon in non-cubic ferrite

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The beginning..

I would like to know the change in the solubility of carbon in ferrite as a function of its lattice parameter. Is that possible to calculate using first principles, or for example by putting a negative pressure in Thermocalc?

Carbon at concentrations much greater than equilibrium seems to remain within bainitic ferrite, in solid solution and in the presence of nearby austenite. This is unexplained.

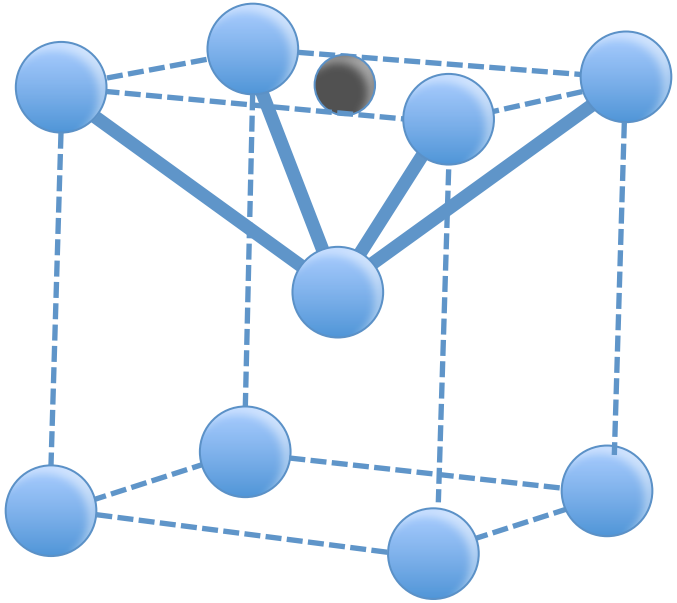
In the first principles method, one could also try and see what happens if the ferrite unit cell is made tetragonal.

Of course, when we talk about solubility, it is always with respect to a particular other phase. So it would be necessary to put any first principles results into thermocalc to allow austenite and ferrite to coexist.

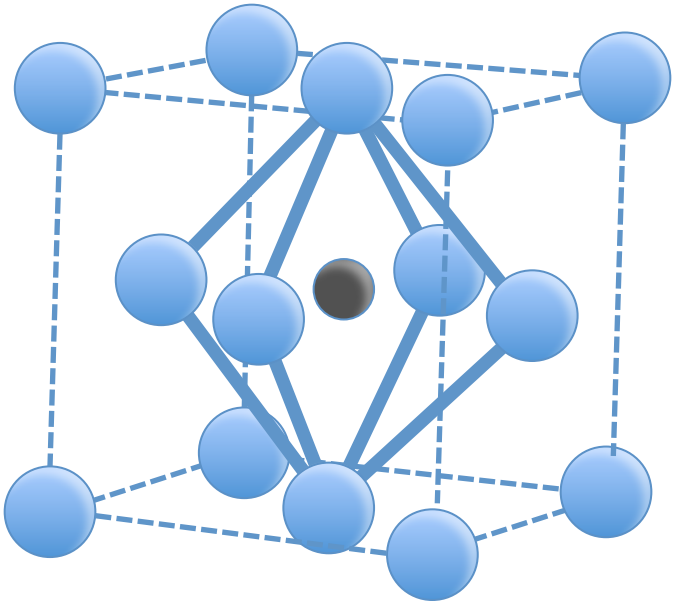
Best wishes, Harry

7th May, 2012

Carbon in iron



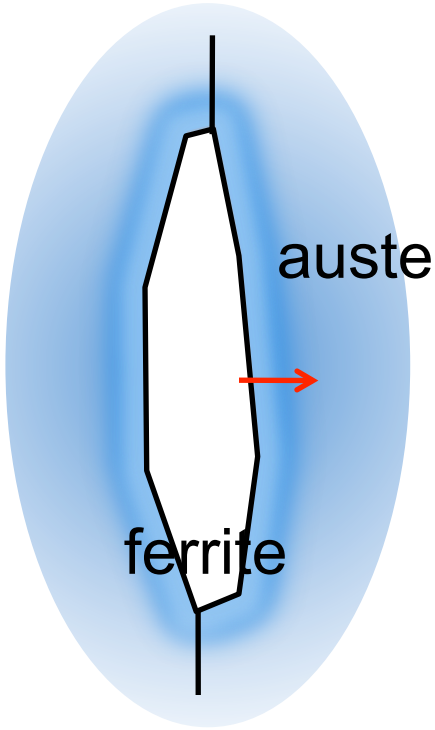
ferrite

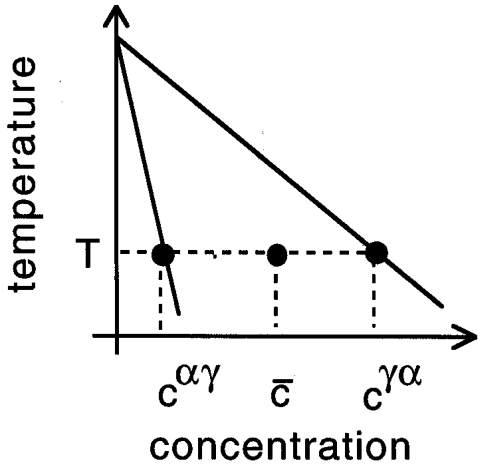


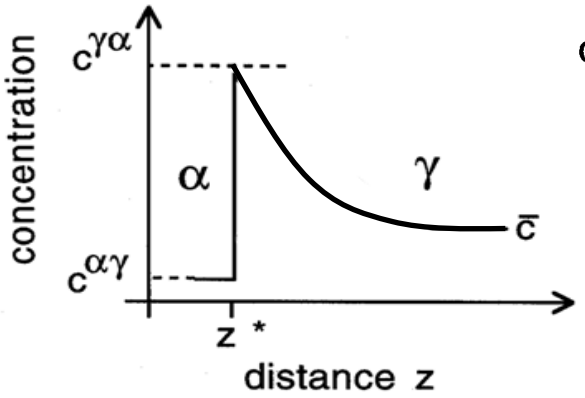
austenite

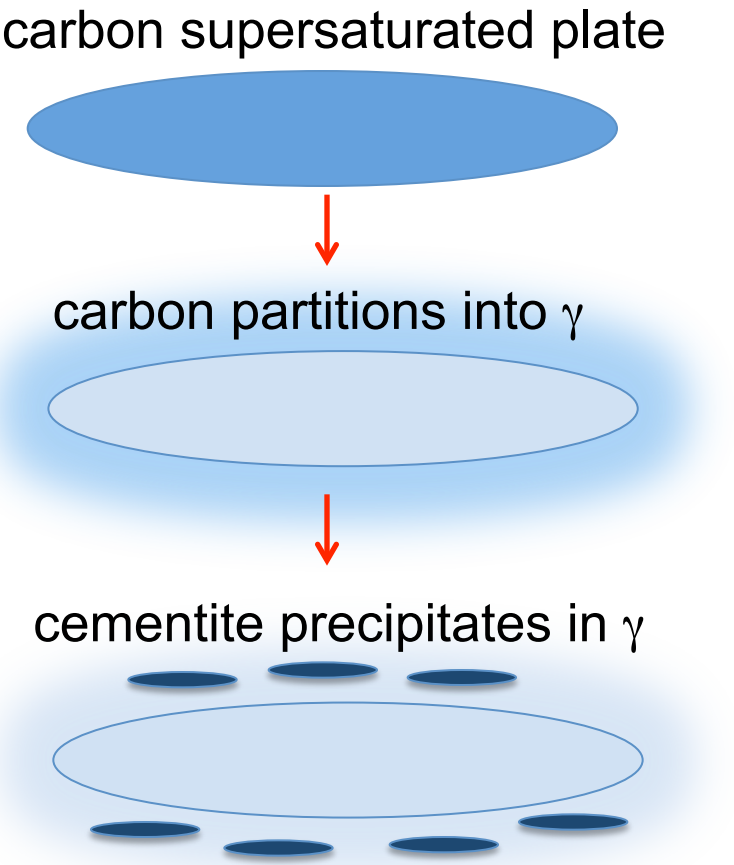
- Carbon in octahedral site of the iron lattice
- ~ 0.4 Å in ferrite, ~ 1 Å in austenite (atomic diameter of C ~ 1.54 Å)
- Much smaller solubility in ferrite than austenite
- Carbon in ferrite contributes to hardening but little hardening in austenite

Movement of carbon in transformation

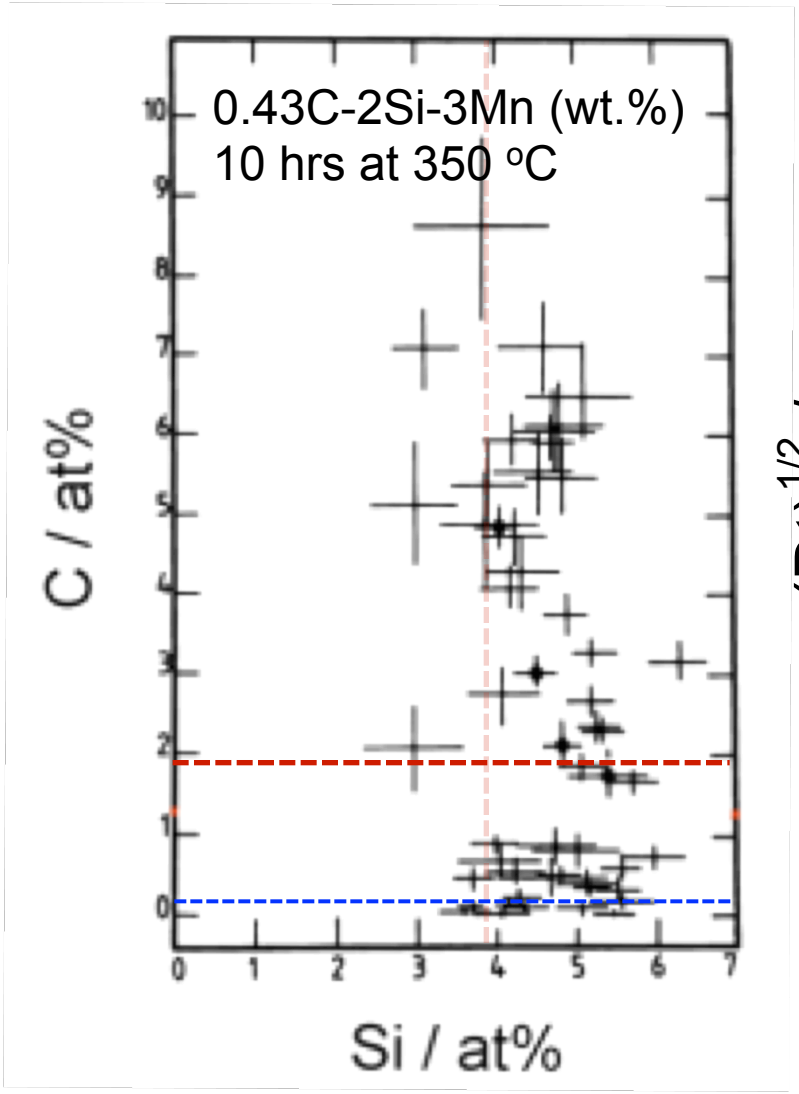


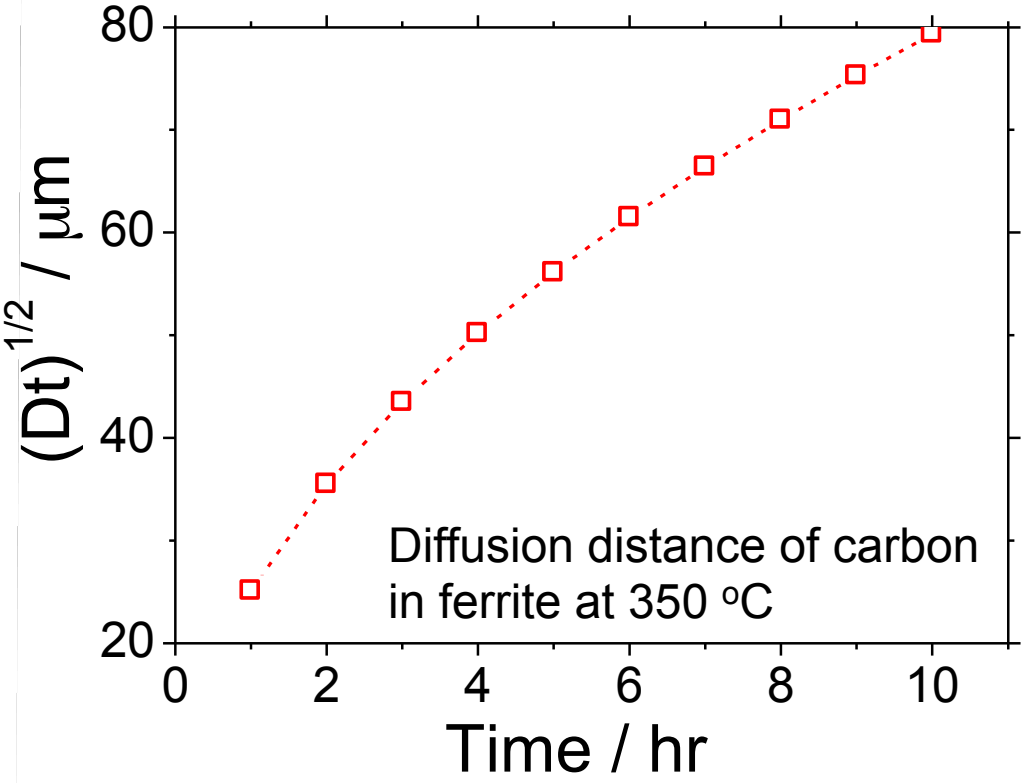






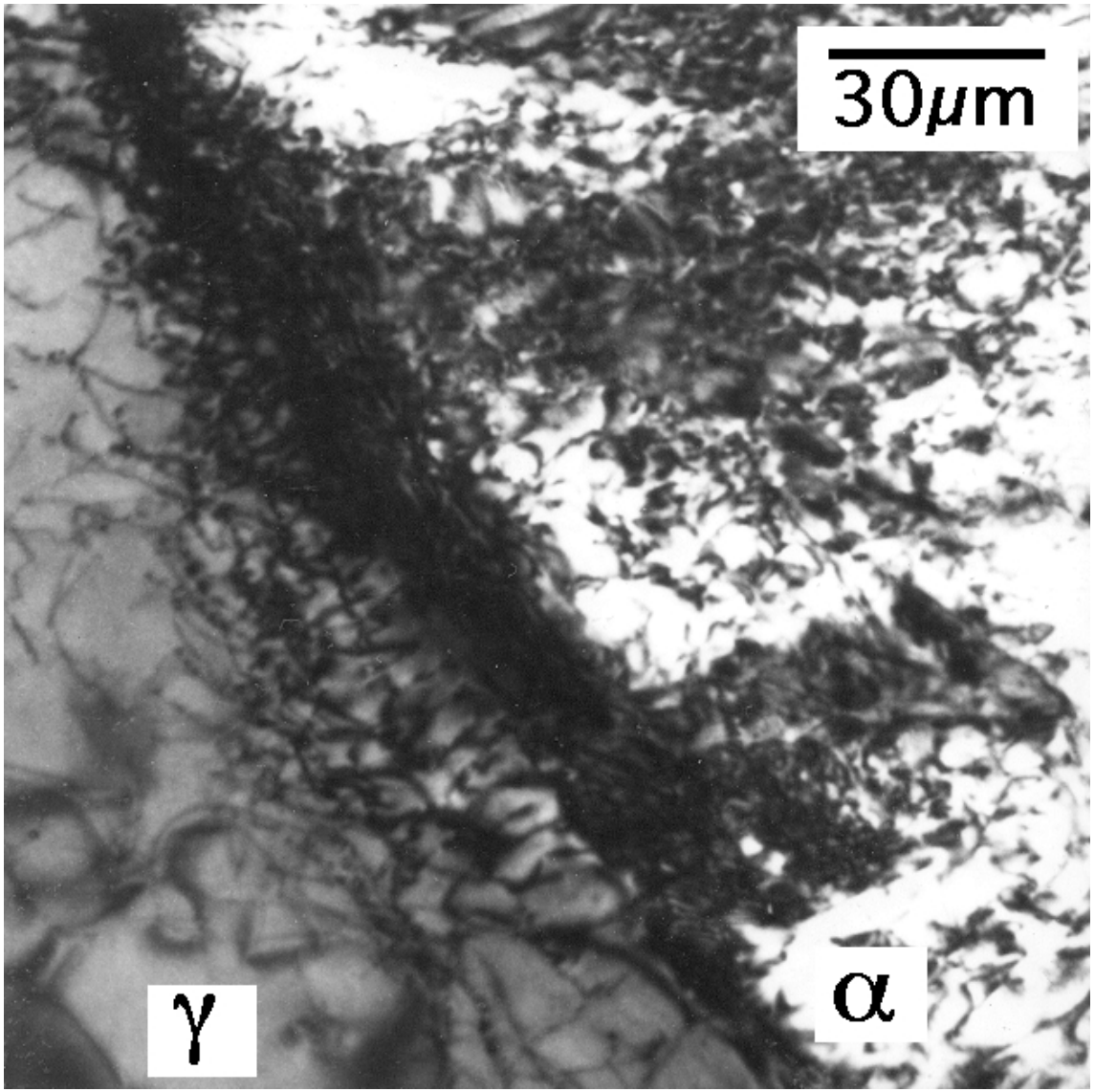
Carbon in bainitic ferrite





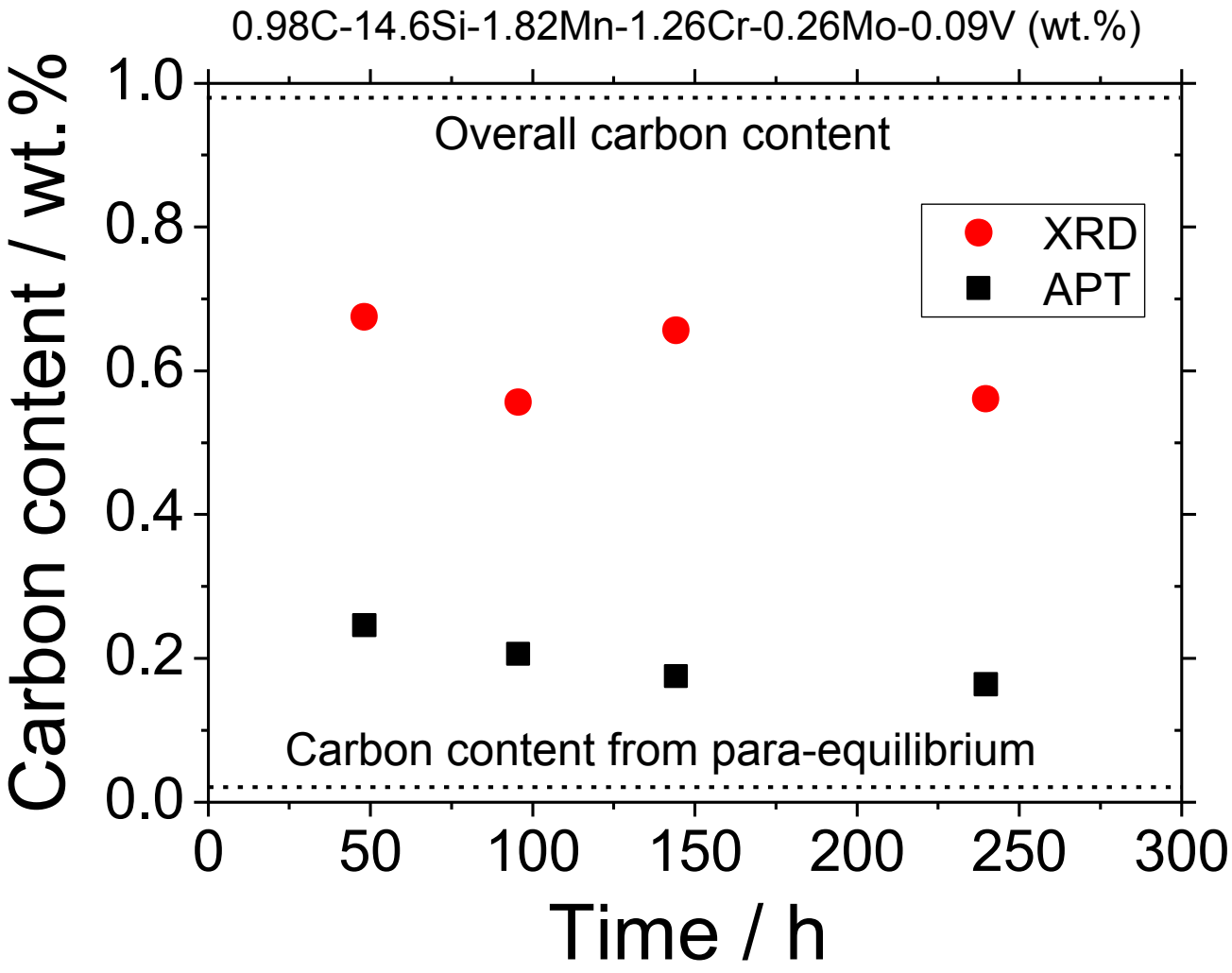
Waugh, Bhadeshia.
Acta Metall., (1981)

Carbon in bainitic ferrite



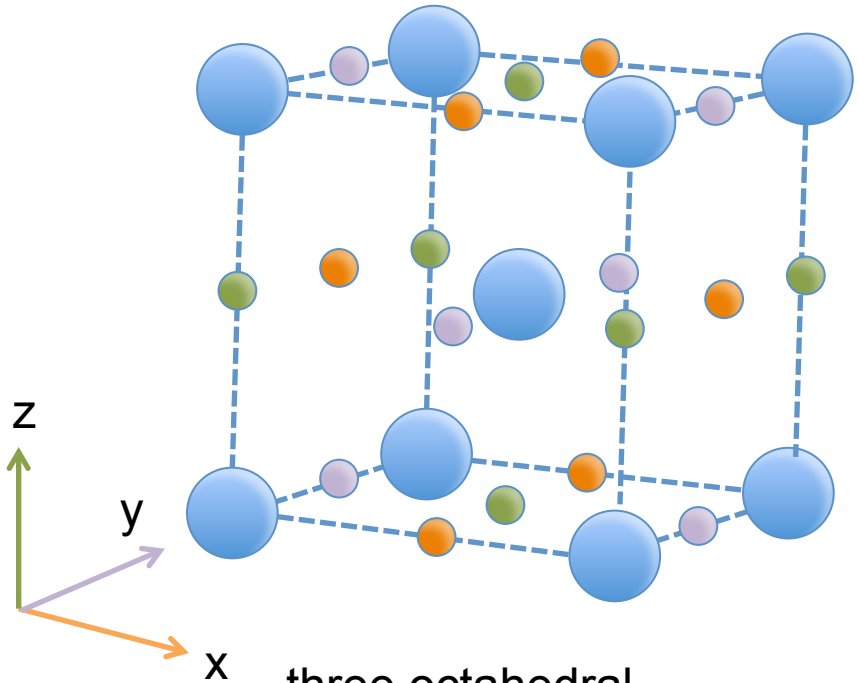
Bhadeshia, Edmonds
Metall. Trans. (1979)

Recent analysis on carbon content

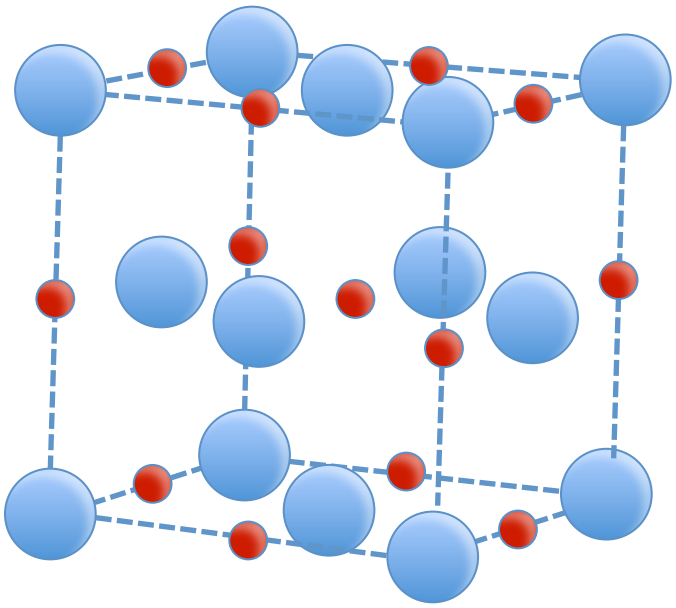


Adapted from Caballero, Miller, Mateo, Cornide.
J. Alloys & Compounds, (2012)

Available octahedral site in α and γ



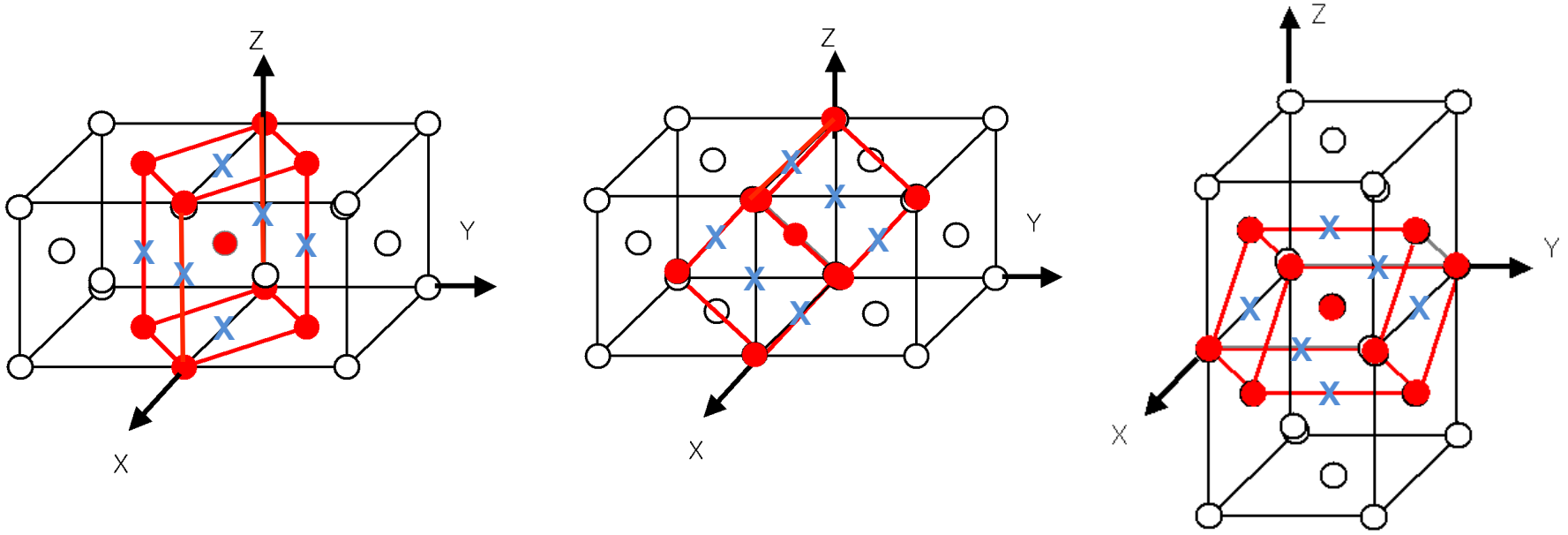
three octahedral interstices per iron atom in ferrite



one octahedral interstice per iron atom in austenite

During displacive transformation, all of the carbon in austenite is inherited into one of three subsets of octahedral sites in ferrite depending on the direction of Bain deformation

Tetragonality by displacive transform.



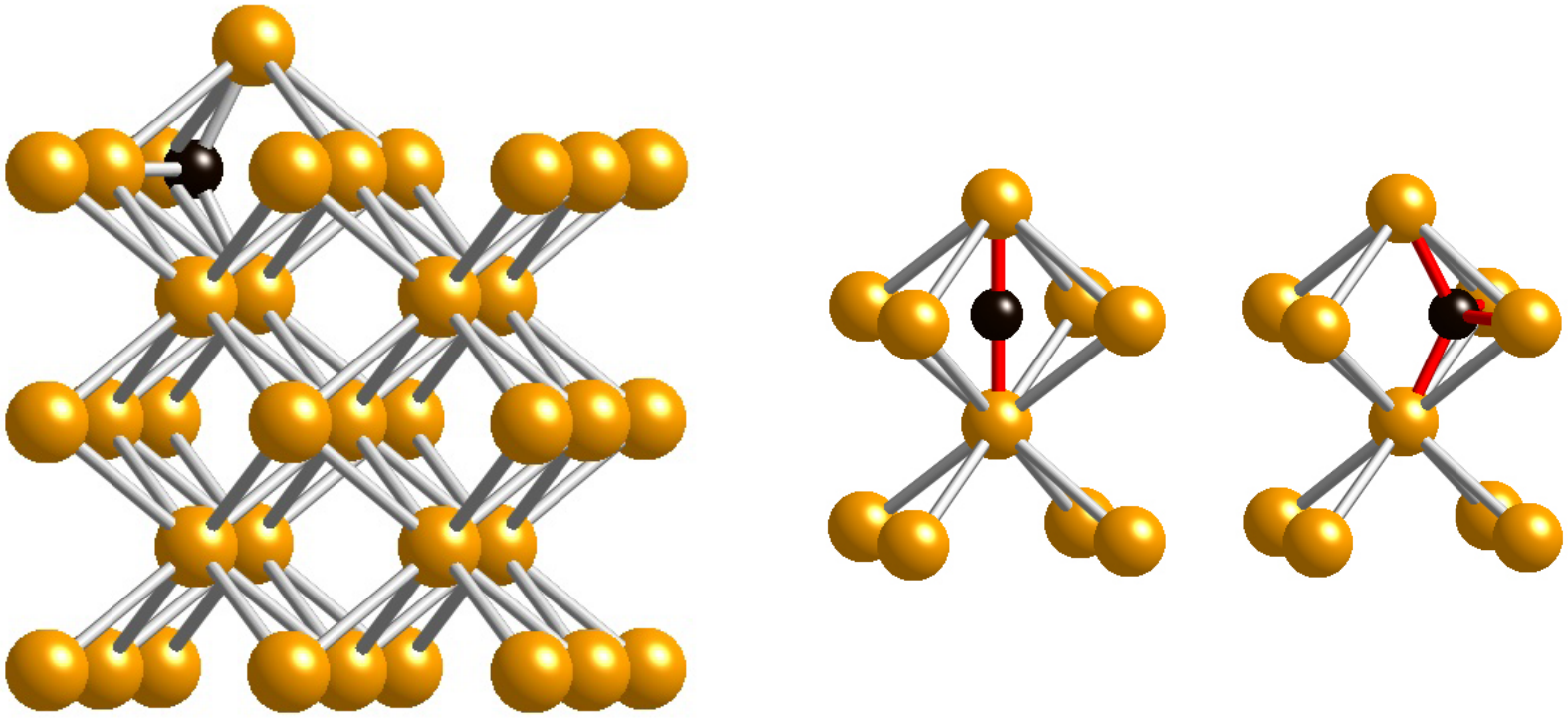
- Consider BCT lattice in austenite
- X indicates the location of carbon in octahedral site in austenite lattice
- During Bain deformation, the carbon resides at the octahedral site in BCT lattice, which makes it tetragonal

- A diffusionless transformation will necessarily lead to a body-centered tetragonal ferrite*.

- Does the tetragonality of ferrite have an influence on the partitioning of carbon from bainitic ferrite into austenite?

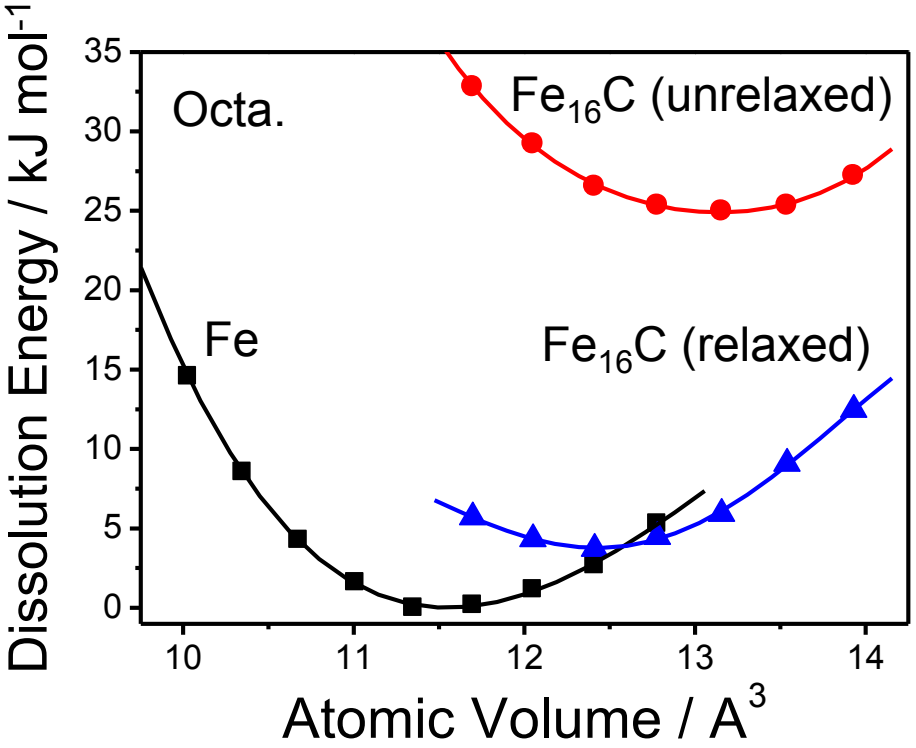
*C. N. Hulme-Smith et al. Scripta Mater. (2013)

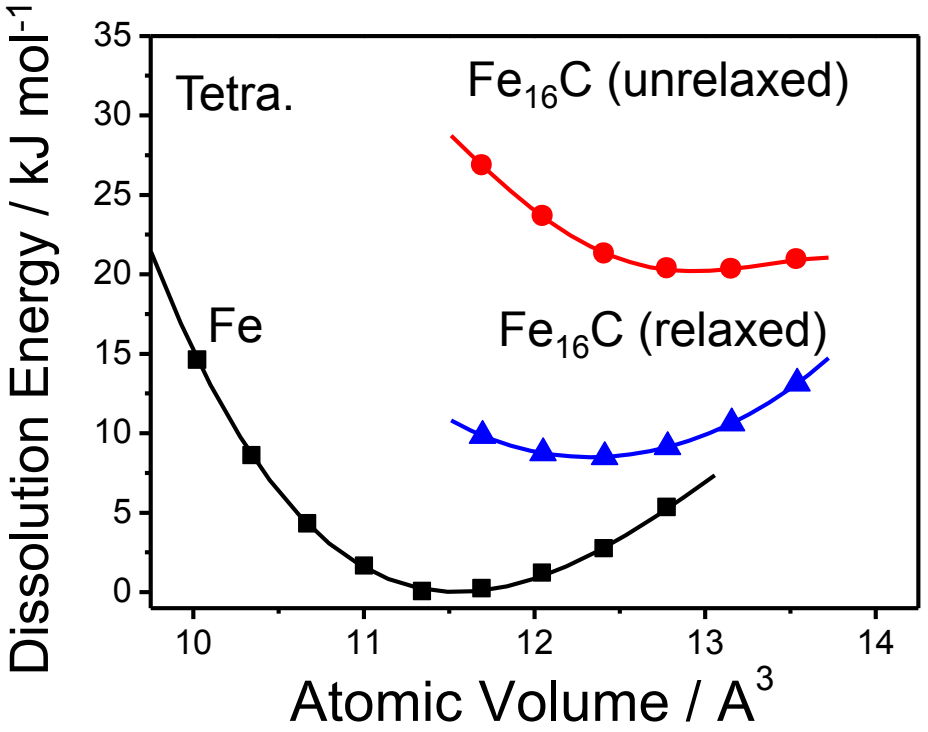
Computational setting



- A 2 x 2 x 2 supercell of ferrite unit cell are used.
- Carbon is located both at octahedral and tetahedral interstices.
- The concentration of carbon is set to 1/17 at. fraction (~1.3 wt.%)
- Total energy all-electron full-potential linearized augmented plane-wave method (FLAPW).

Dissolution energy of carbon





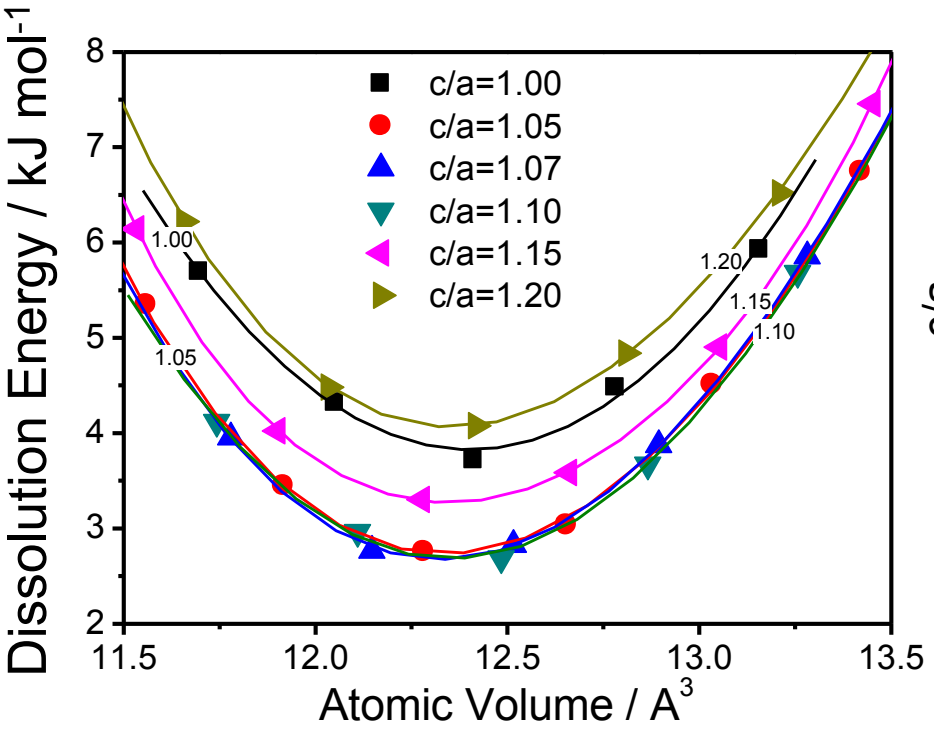
$$\Delta H = \frac{E(\mathrm{Fe_{16}C}) - 16 \times E(\mathrm{Fe}) - E(\mathrm{C})}{17}$$

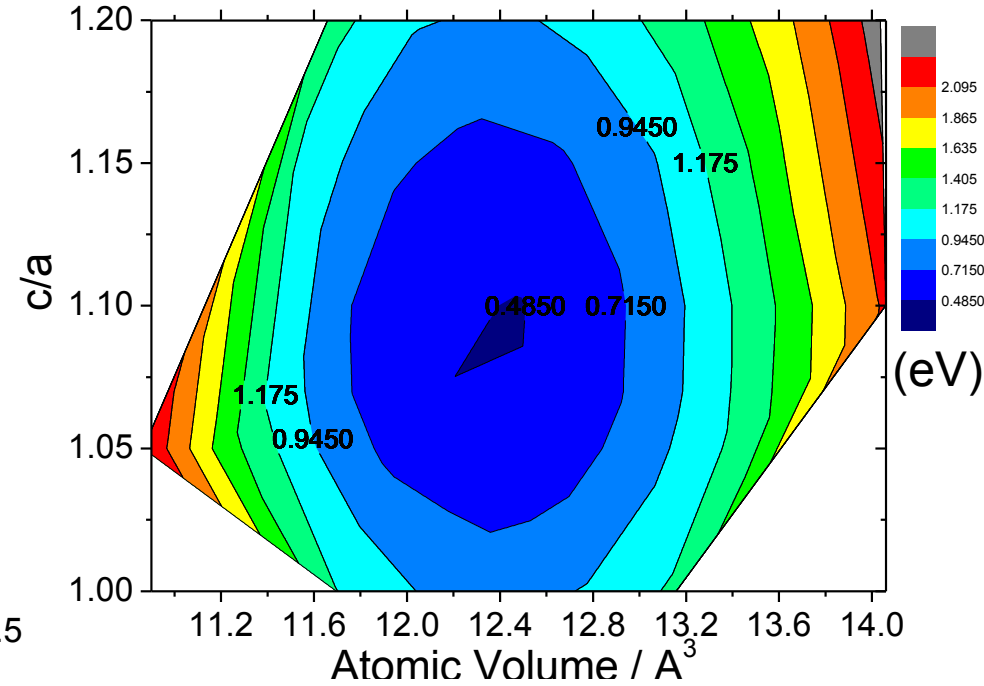
	Atomic volume / Å^3		ΔH_s / kJ mol^{-1}	
	unrelaxed	relaxed	unrelaxed	relaxed
Octa	13.15	12.43	24.89	3.77
Tetra	12.93	12.32	20.19	8.49

- Since the unrelaxed tetrahedral site has a larger interstitial radius, the dissolution energy is smaller compared with that for octahedral interstice.

- The dissolution energy for the atomic position relaxed octahedral interstice is smaller, because the main deformation due to the location of carbon occurs along one of the <100> axes.

Dissolution energy with tetragonality



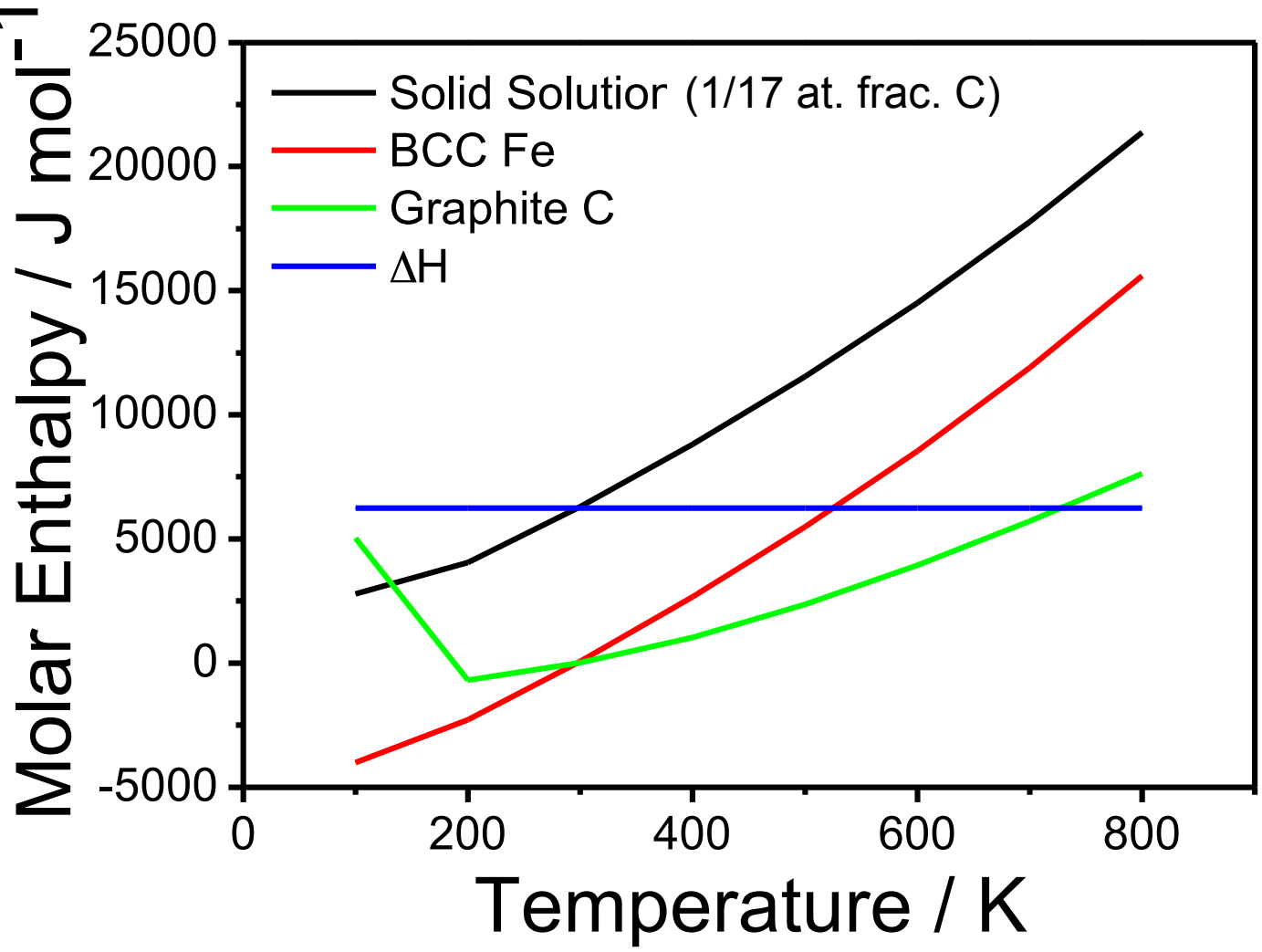


An optimum lattice parameter ratio *c/a* exists in minimizing the dissolution energy.

For *c/a*=1.00, the dissolution energy is 3.77 kJ/mol and decreases to 2.76 kJ/mol until the ratio reaches to 1.07.

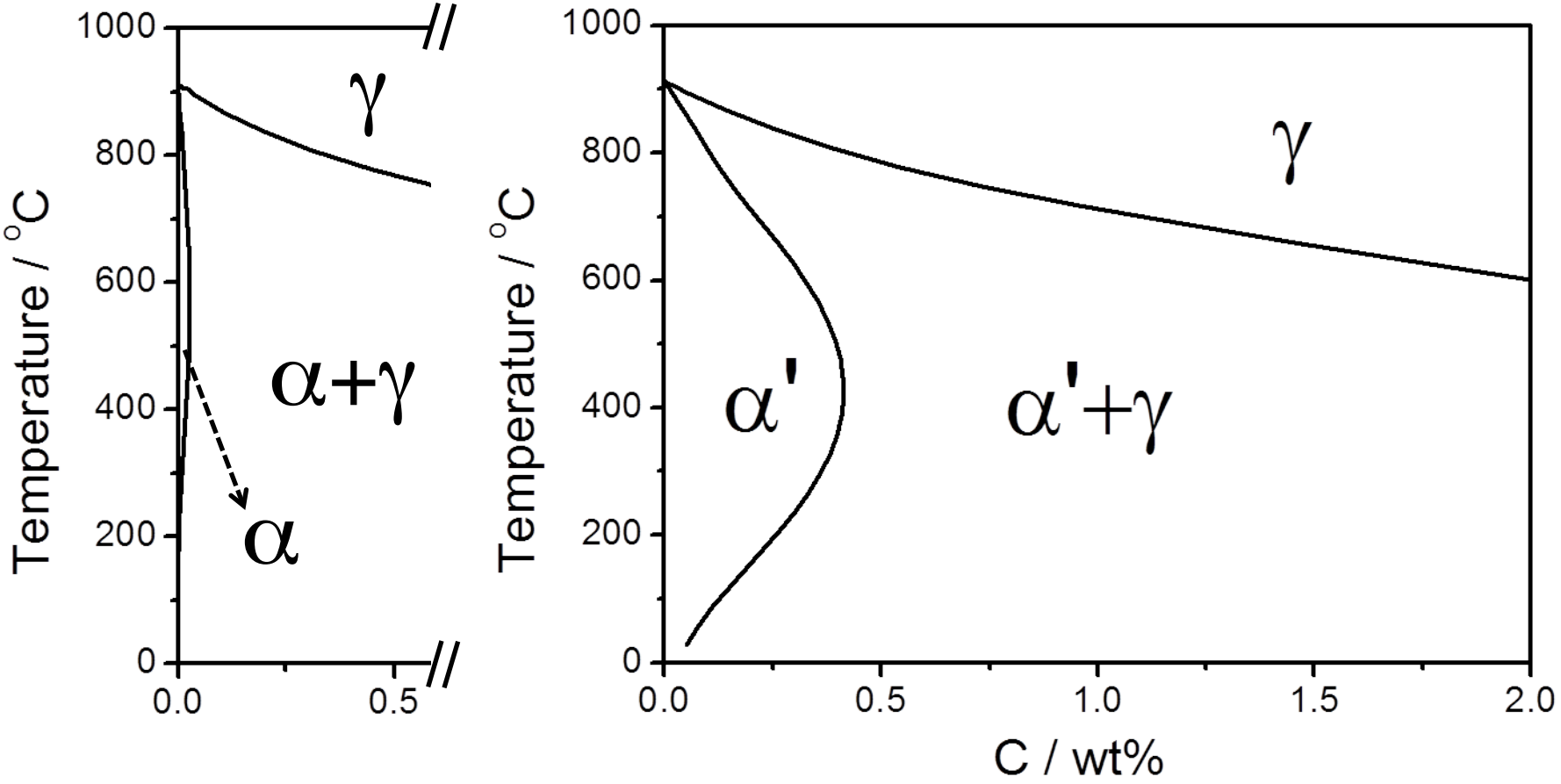
The ratio of 1.07 agrees well with the value of 1.06 obtained from the experiments in 1.3 wt.% carbon steel.

Implementation



Dissolution energies of carbon in ferrite are ~ 6.24 kJ/mol in TCFE2000 Database in the temperature range from 100K to 800K.

Ferrite equilibrium with austenite

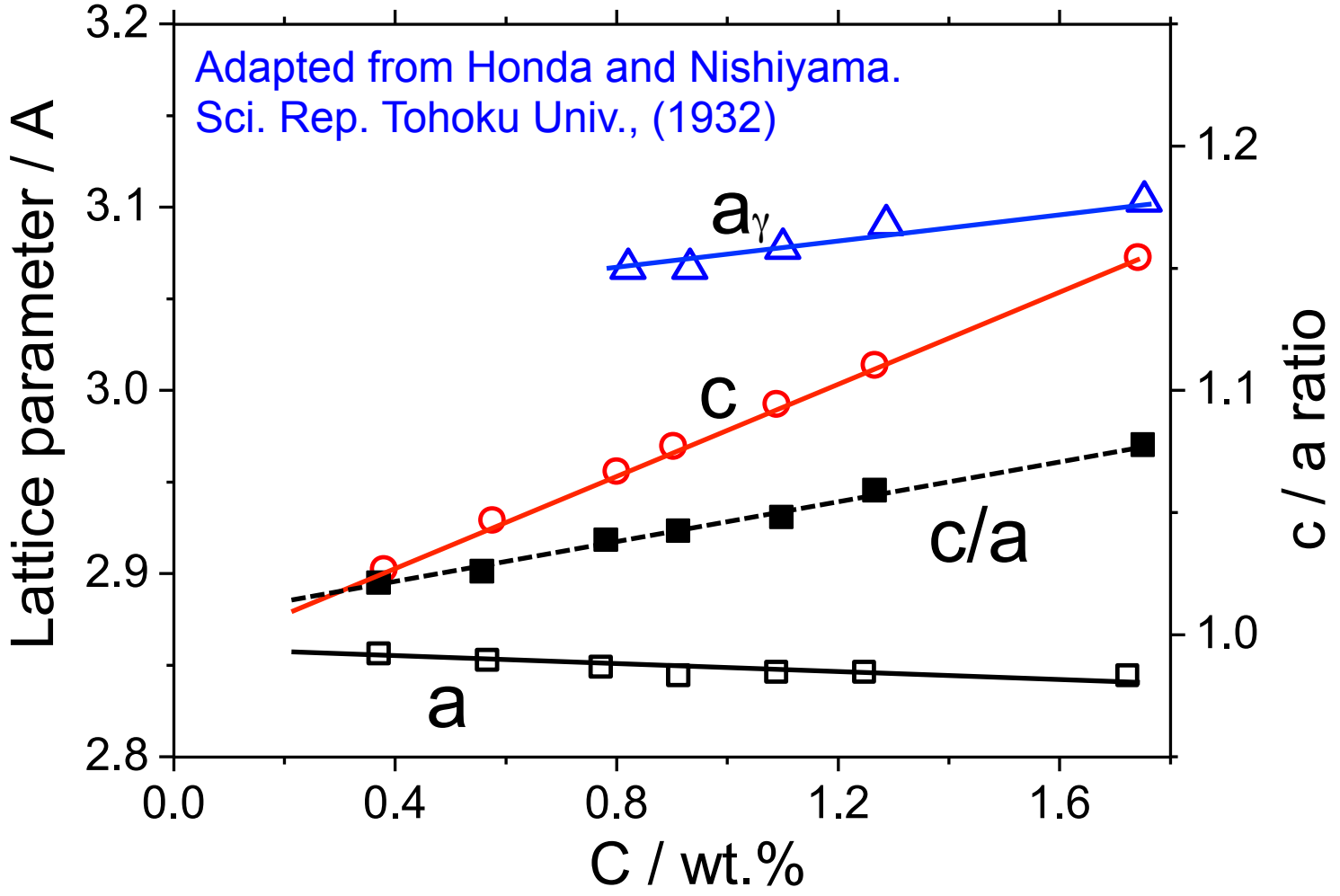


Cubic ferrite

Tetragonal ferrite

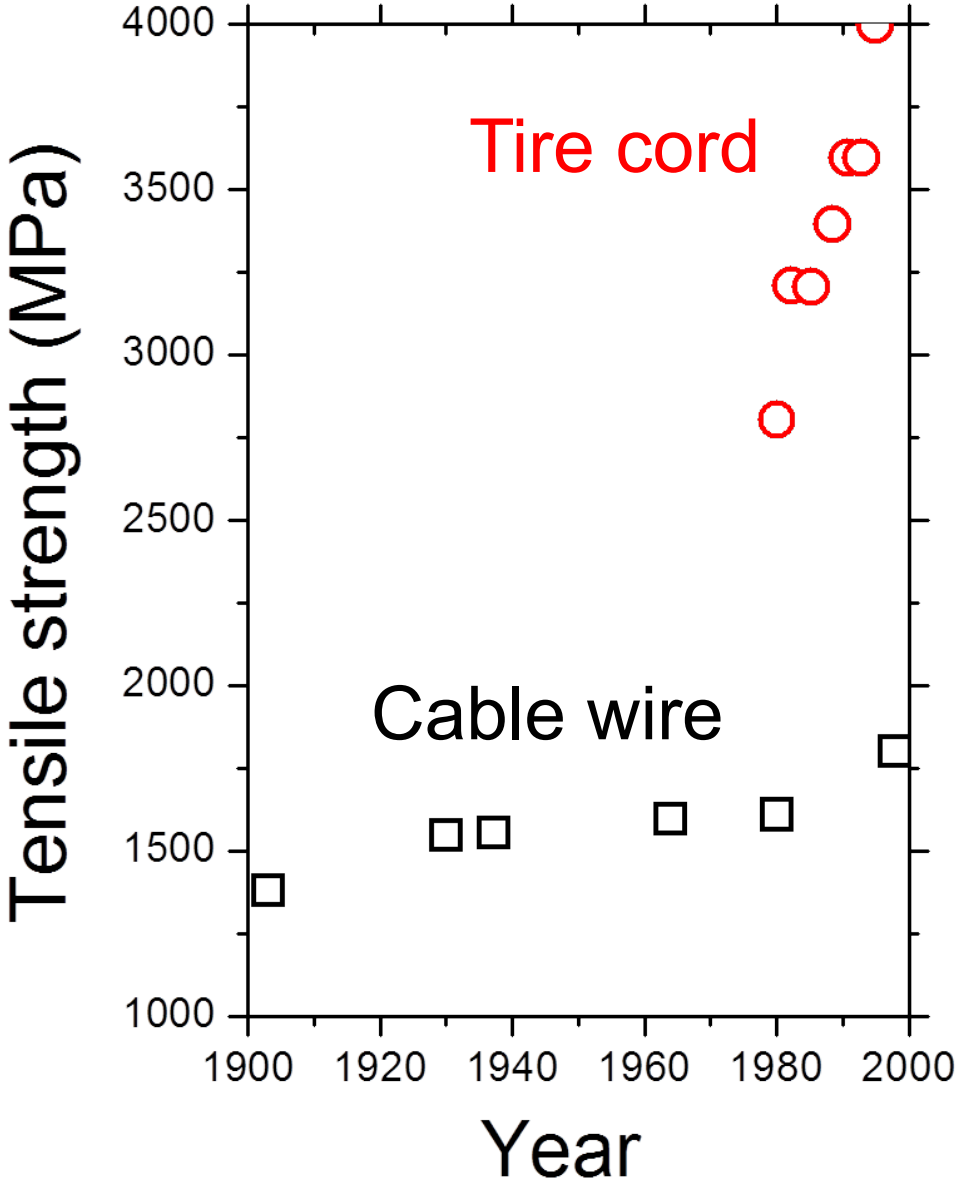
Jang et al. Scripta Mater. (2013)

Influence of carbon concentration



In low carbon steels, it may be difficult to observe the effect of tetragonality in bainitic ferrite because of lower Zener ordering temperature

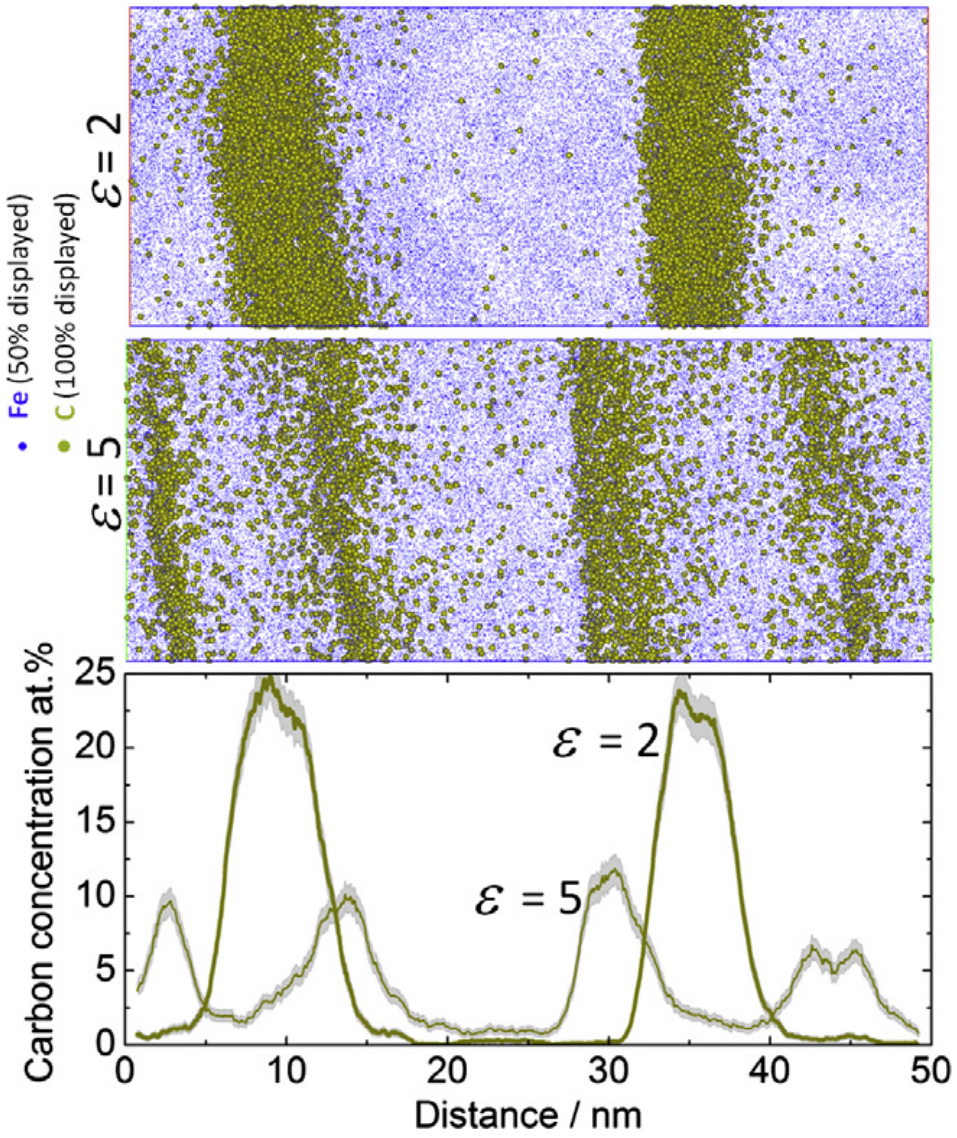
Tetragonality by deformation



- Currently, strength level increases to around 6GPa
- During wire drawing, strong texture is developed
- Elastic strain ~ 3 %

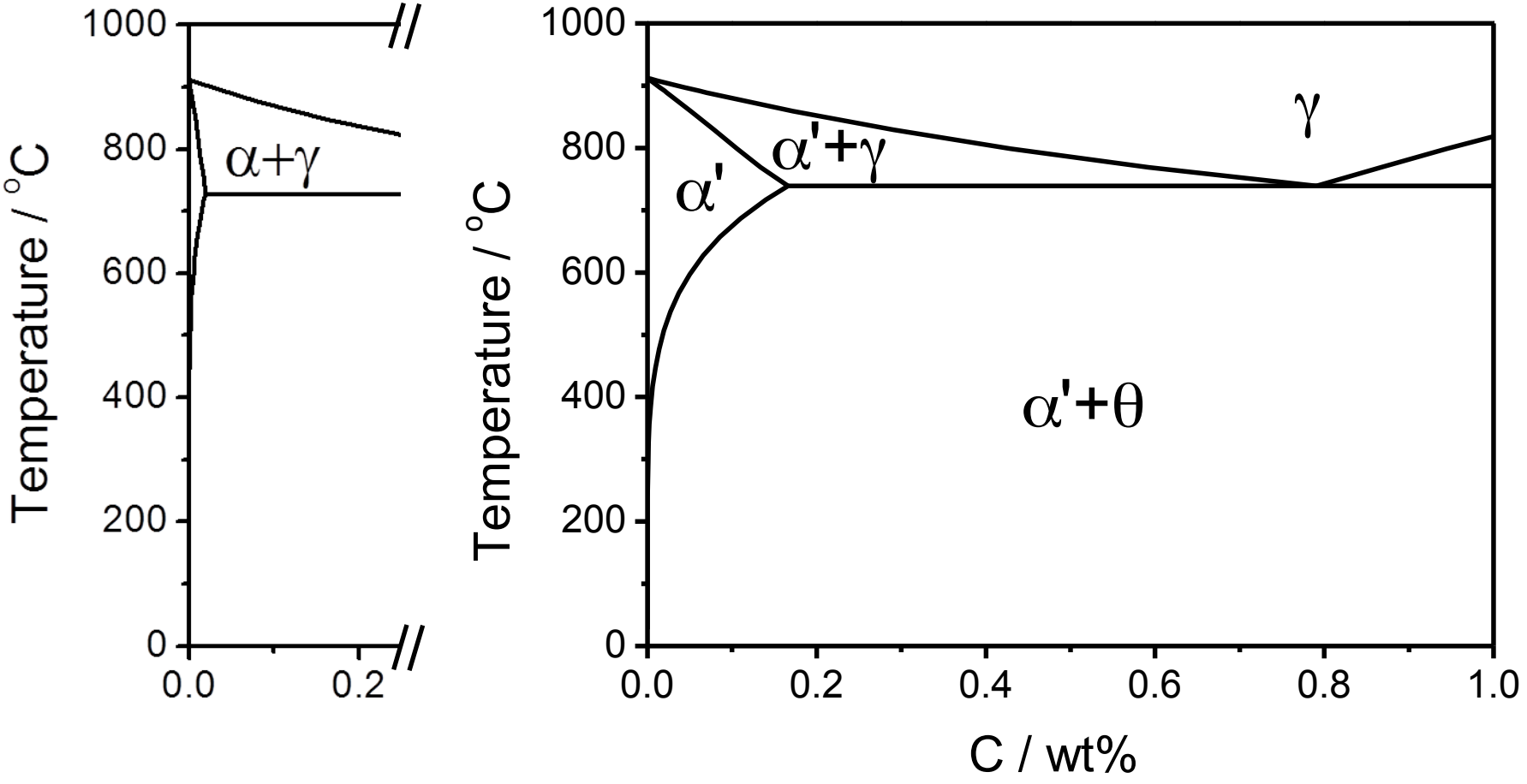
Adapted from Raabe et al. MRS Bulletine, (2010)

Dissolution of cementite



Li et al. Acta Materialia, (2011)

Ferrite equilibrium with cementite

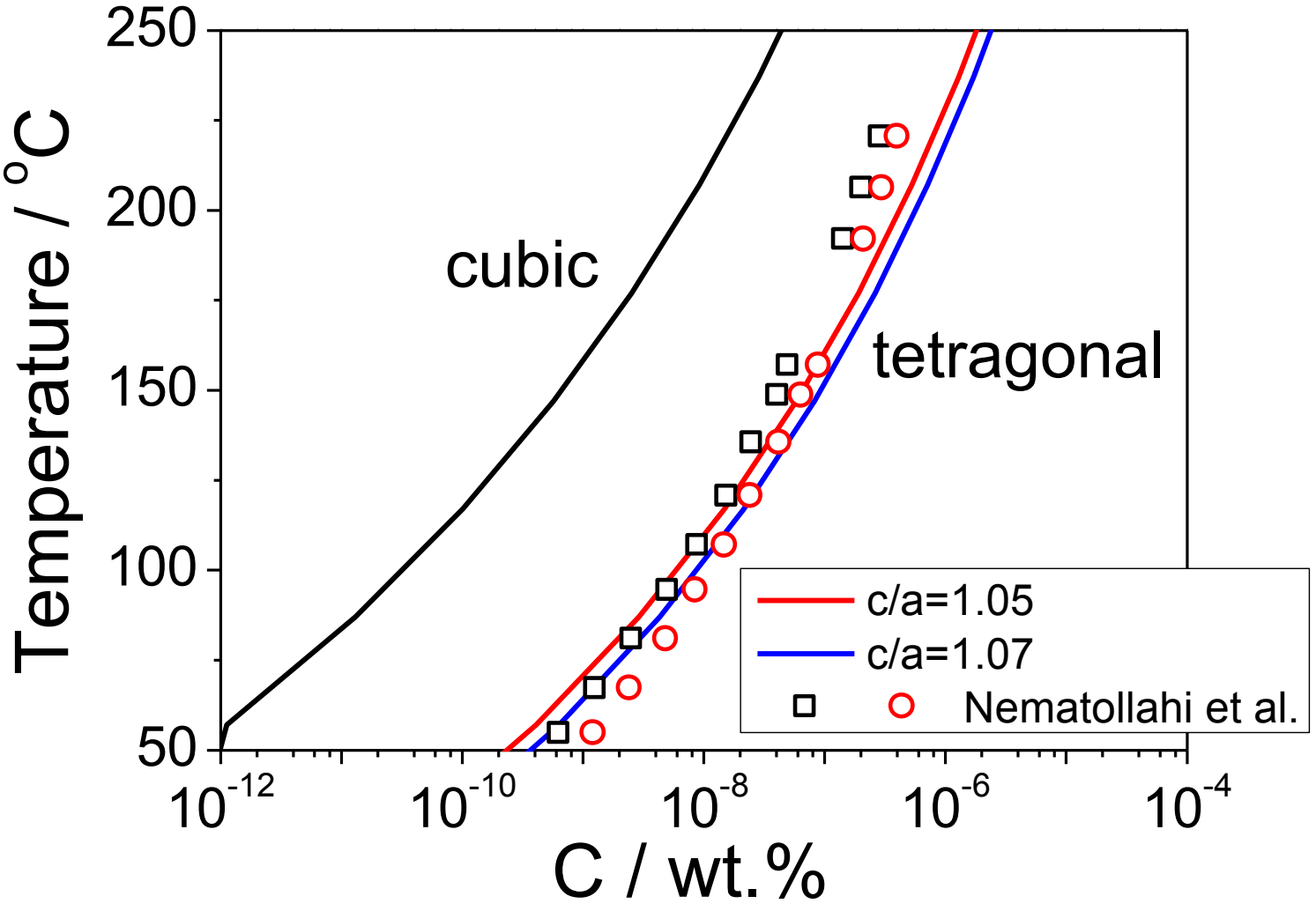


Cubic ferrite

Tetragonal ferrite

Jang et al. Unpublished work

Ferrite equilibrium with cementite



Nematollahi et al. Acta Materialia, (2013)

Summary

- Some calculations suggest a role of non-cubicity of ferrite in increasing the solubility of carbon