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# Thermodynamic effects of substitutional elements on the CPE interface conditions in Q&P steels

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## Introduction

Carbon partitioning from martensite to austenite is a key phenomenon which occurs during the Q&P process. Its kinetics is governed by bulk carbon diffusion in both phases and by the interface conditions at martensite/austenite interface. In the literature, it is often assumed to be governed by a Constrained Para-Equilibrium (CPE). This interface condition encompasses no partitioning of substitutional elements, continuity of carbon chemical potential across the interface, no interface mobility and absence of carbide precipitation [1,2].

Few previous works have proposed thermodynamic calculations describing the CPE condition in binary Fe-C, neglecting the effect of substitutional elements [1,3]. Nevertheless, in practice Q&P steels are often highly alloyed to reach a sufficient hardenability (Mn, Ni, Mo, Cr) or to minimize carbide precipitation (Ni, Al, Si).

To fill this gap, we have investigated the relative effect of substitutional elements on CPE condition using thermodynamic calculations (Thermocalc Version-S TCFe7 database).

## CPE interface condition

In the following, we consider a martensite( $\alpha'$ )/austenite( $\gamma$ ) interface at partitioning temperature. In practice, we have made the rough thermodynamic assumption that martensite behaves as ferrite.

The interface condition in CPE is defined by two equations :

$$\begin{aligned} u_i^{\alpha'} &= u_i^{\gamma} \\ \mu_c^{\alpha'} &= \mu_c^{\gamma} \end{aligned}$$

Where  $u_i = x_i/(1-x_c)$ , with  $x_i$  the atomic concentrations of elements  $i$  ( $i$  is a substitution element) and  $x_c$  the one of carbon,  $\mu_c^{\alpha'}$  and  $\mu_c^{\gamma}$  the carbon chemical potentials in both phases. Figure I illustrates this particular interface condition (in red) compared to the equilibrium common tangent (in blue) in a Gibbs energy map.

If the fraction of martensite is not imposed, the previous set of equations thus lets one degree of freedom, allowing to establish a relationship between the carbon concentration in martensite ( $w_c^{\alpha'}$ ) and austenite ( $w_c^{\gamma}$ ) at the interface.

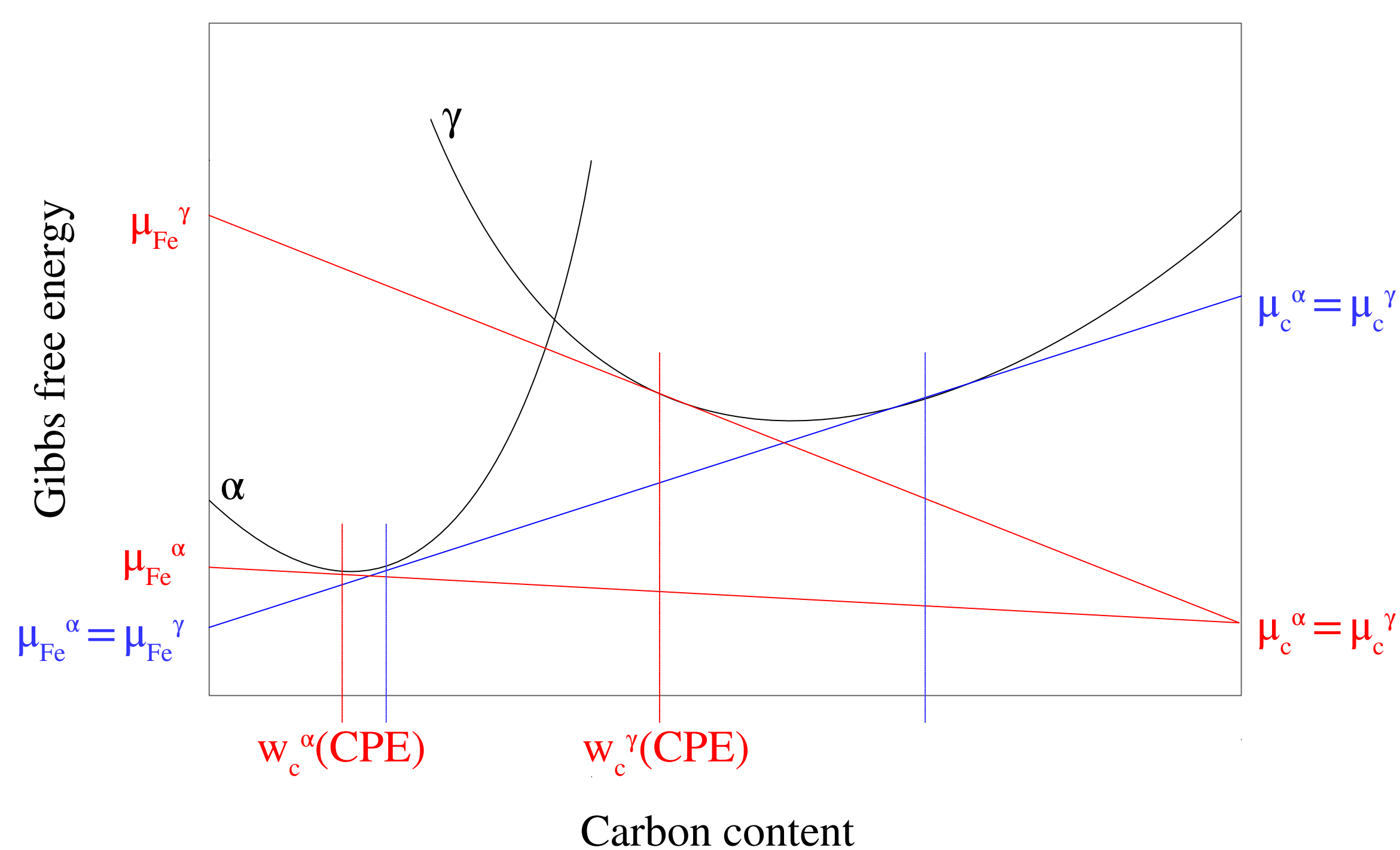


Figure I : Schematic representation of Gibbs free energy as function of carbon content of martensite and austenite for a given temperature. Blue line represents the equilibrium common tangent for the two phase domain and CPE interface condition is represented in red.

## References

- [1] Speer, J., Matlock, D.K., De Cooman, B.C., & Schroth, J.G. Acta mater., 2003, Vol.51(9), pp.2611-2622
- [2] Matlock, D.K., Bräutigam, V.E., & Speer, J.G. Mater. Sci. Forum, 2003, vol.426, pp.1089-1094
- [3] Santofimia, M.J., Zhao, L., & Sietsma, J. Scr. Mater., 2008, Vol.59(2), pp. 159-162

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## Results

Figure II illustrates the relative effect of different substitutional alloying elements on the interface condition for a Fe-X-C steels at 400°C. Only Al and Cr additions affect the CPE interface conditions with antagonist trends. For a given temperature and carbon concentration in martensite, Al increases carbon concentration in austenite while Cr reduces it.

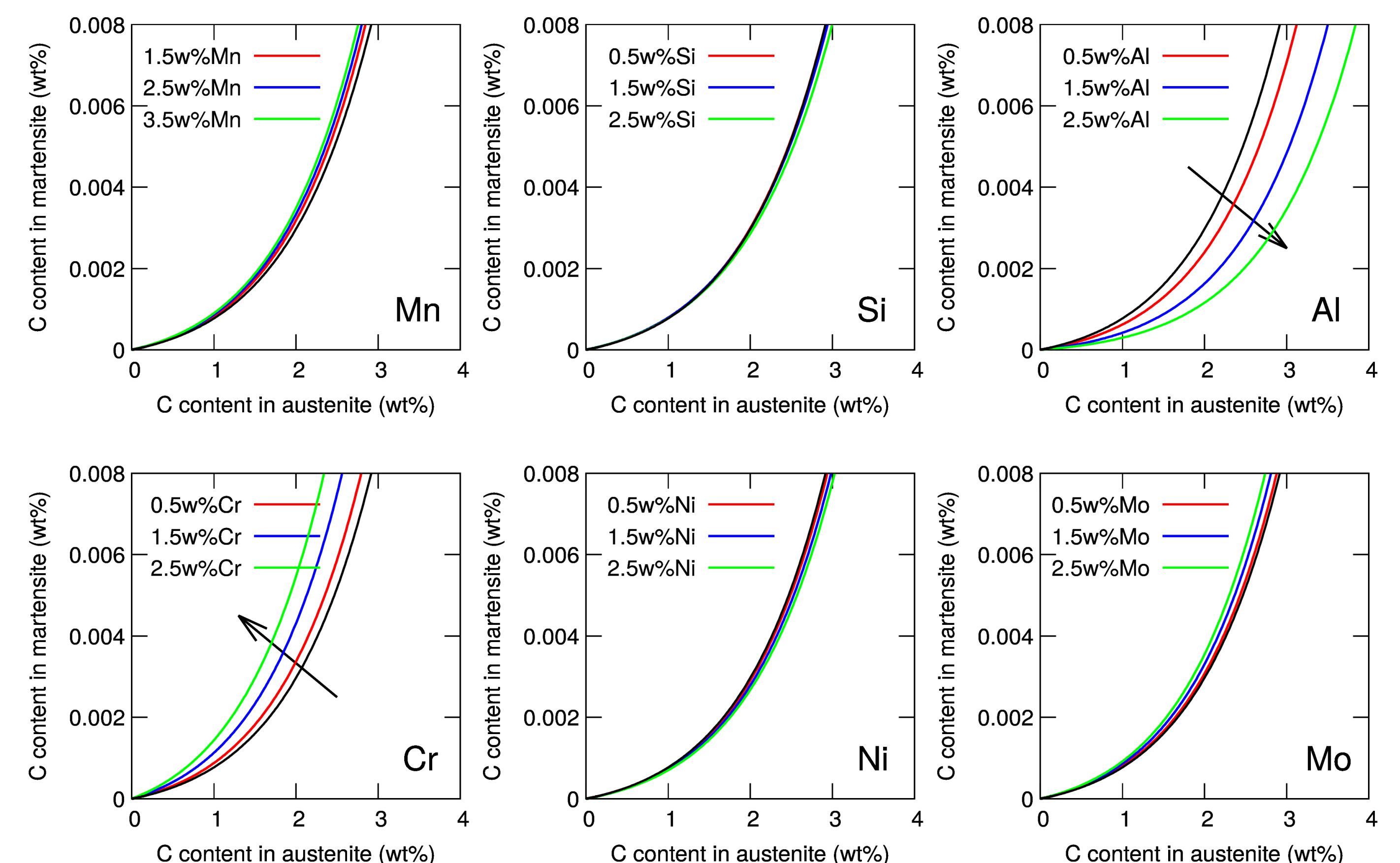


Figure II : Effect of substitutional alloying elements at 673K on the CPE condition. The black curve is the reference of the CPE condition for a binary Fe-C steel.

To assess the consequences of these thermodynamic calculations, the resulting carbon partition between martensite and austenite under CPE for different martensite fraction (after full partitioning) have been calculated, considering Al or Cr additions in a reference alloy (Fe0.3C2.5Mn1.5Si) at 400°C. Figure III(a) shows that below 85% of primary martensitic transformation, there is almost no effect of substitutional alloying elements on austenite enrichment. Above 85%, an influence is expected, but that will be probably hindered in practice by carbide precipitation.

The effects of alloying elements on enrichment kinetics have been assessed thanks to the diffusion-based model proposed by Santofimia et al. [3]. Calculations have been conducted for an initial fraction of martensite of 80% with austenite films of 1  $\mu\text{m}$  thickness. Figure III(b) shows the differences in enrichment kinetics for the same alloys at 350°C and 450°C. It confirms that Al speeds up partitioning process whereas Cr slows it down due to interface conditions only. Nevertheless, the expected effects are weak.

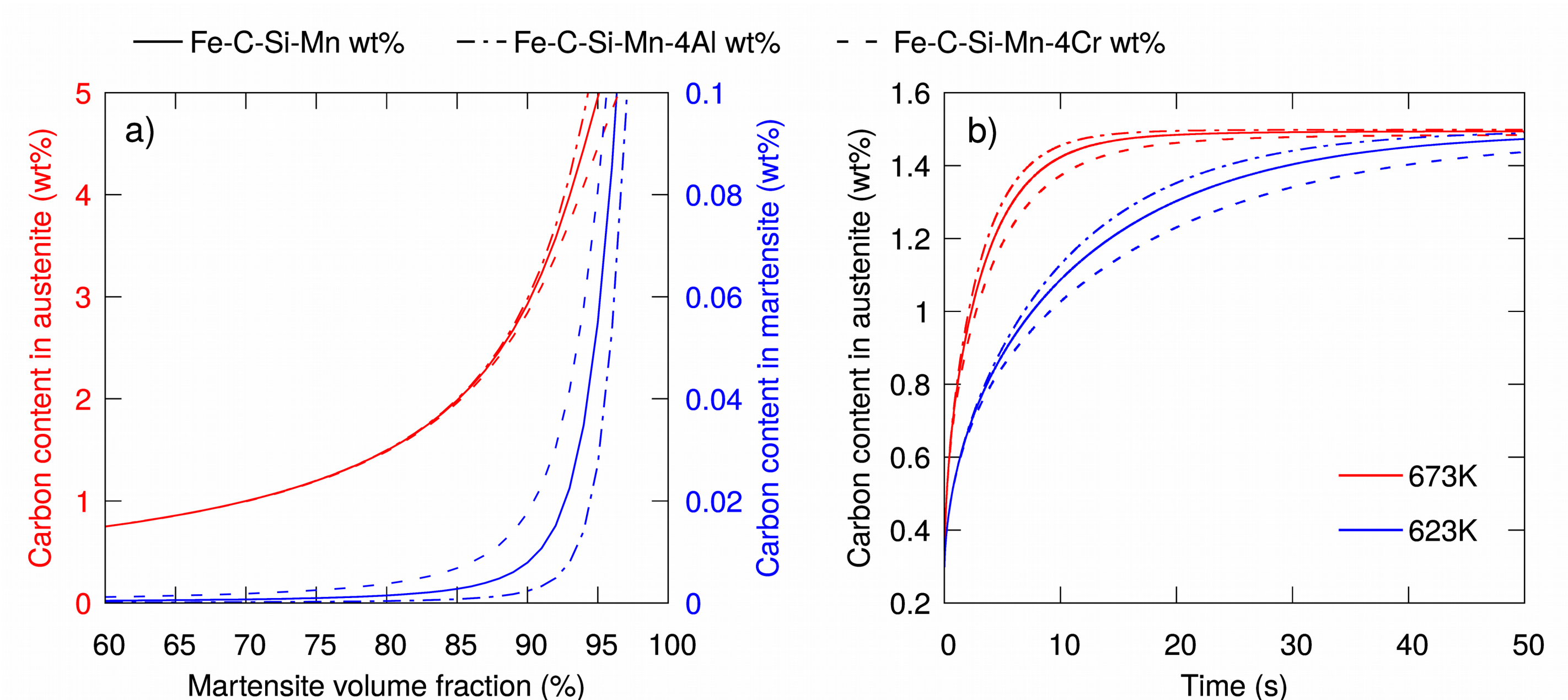


Figure III : (a) Calculated carbon content in austenite and martensite as function of primary martensite fraction after a partitioning at 673K under the CPE (final state) for a Fe-0.3C-1.5Si-2.5Mn-4X wt.% alloy (X = Al or Cr). (b) Calculated enrichment kinetics in austenite for the same alloys at 350°C and 400°C.

## Conclusion

- Except Al et Cr, all investigated elements (Mn, Si, Ni, Mo, P, Co) have a negligible effect on martensite/austenite interface conditions under CPE.
- Aluminum addition speeds up partitioning process but has a negligible effect on final state if CPE conditions are fulfilled and if the primary fraction of martensite is limited.
- Chromium addition will have an antagonist effect on kinetics but also a negligible effect on final state (except increasing carbon solubility in ferrite).
- Calculations can be improved by considering a better thermodynamic description of martensite and by taking into account composition dependent diffusion coefficient for carbon in the kinetics approach.