



Towards a General Model for Ferrite Growth in Fe-C-X

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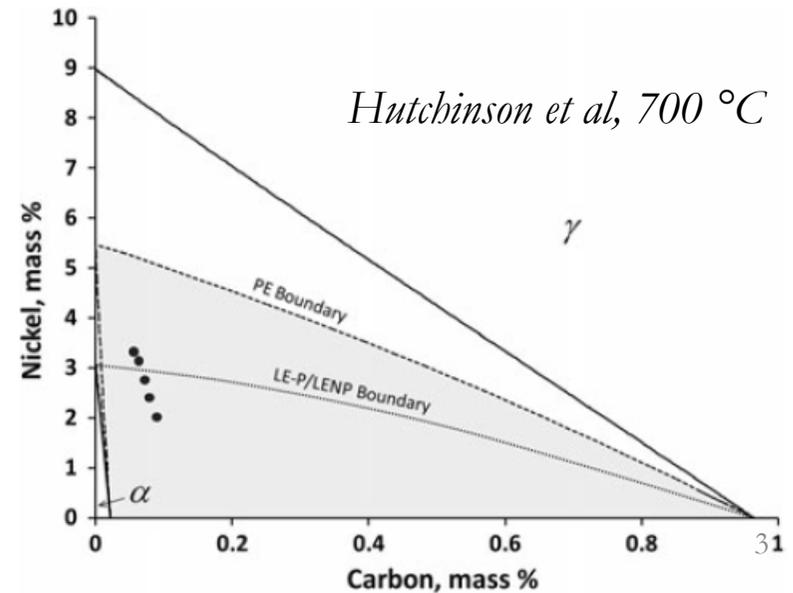
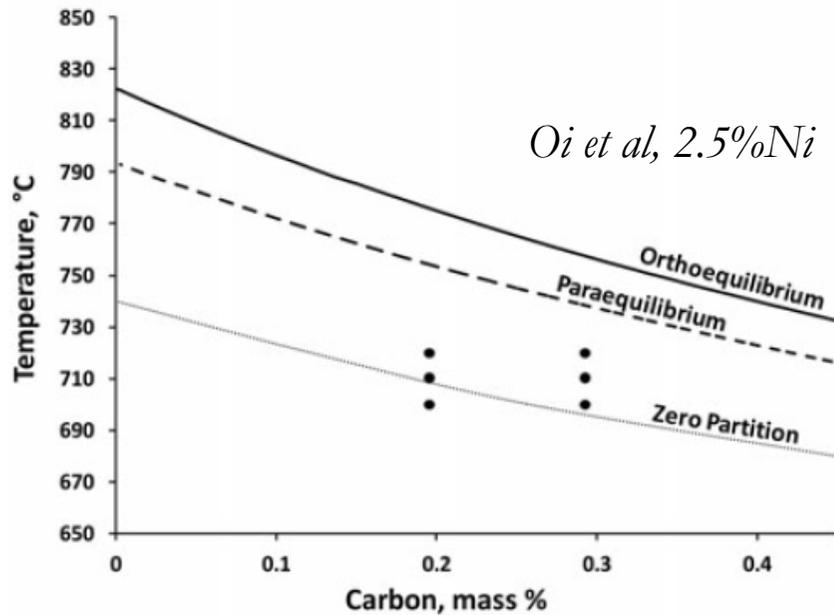
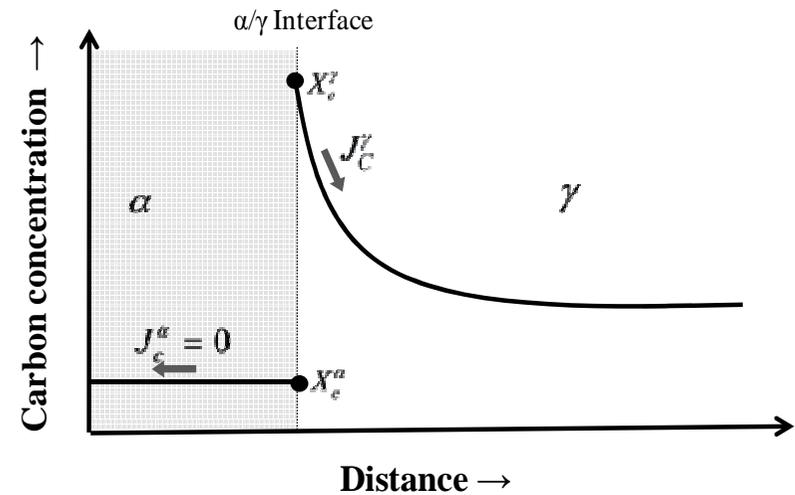
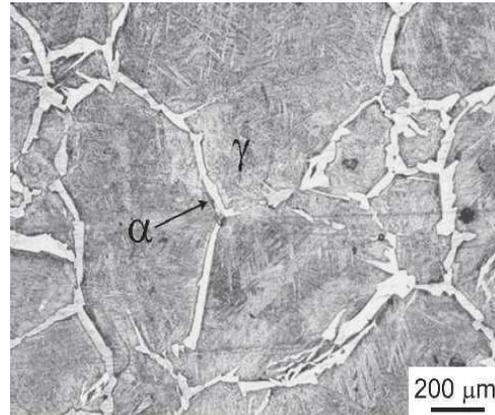
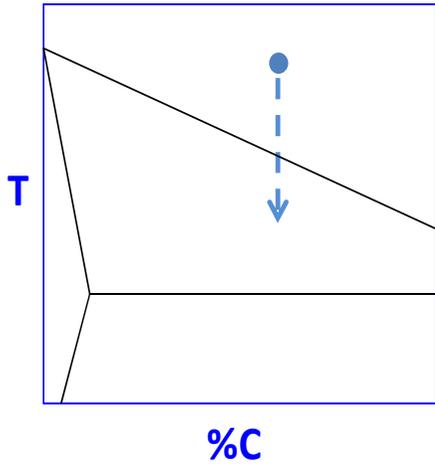
Yves Brechet- INP Grenoble

Outline

- Summary of existing data and need for a general model.
- Development of the model.
- Comparison with precipitation data.
- Comparison with decarburization data.
- Conclusions.

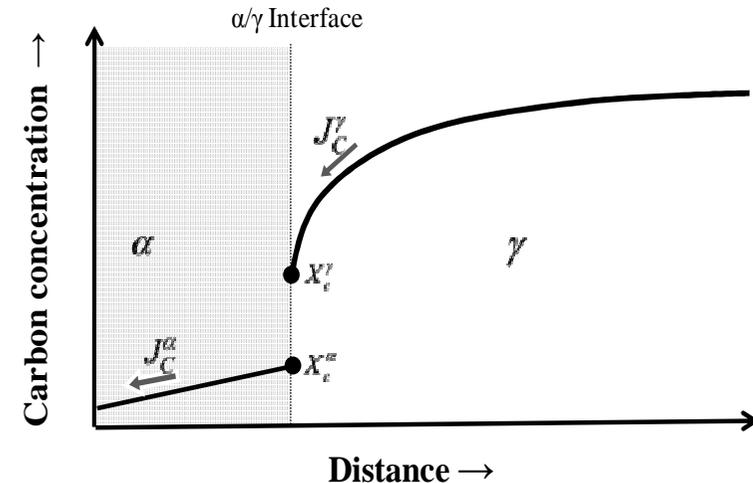
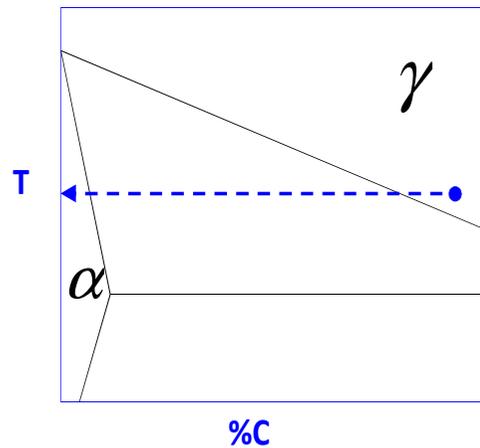
Classical Precipitation

Summary of Prior Experimental Results



Decarburization Experiments

Summary of Prior Experimental Results



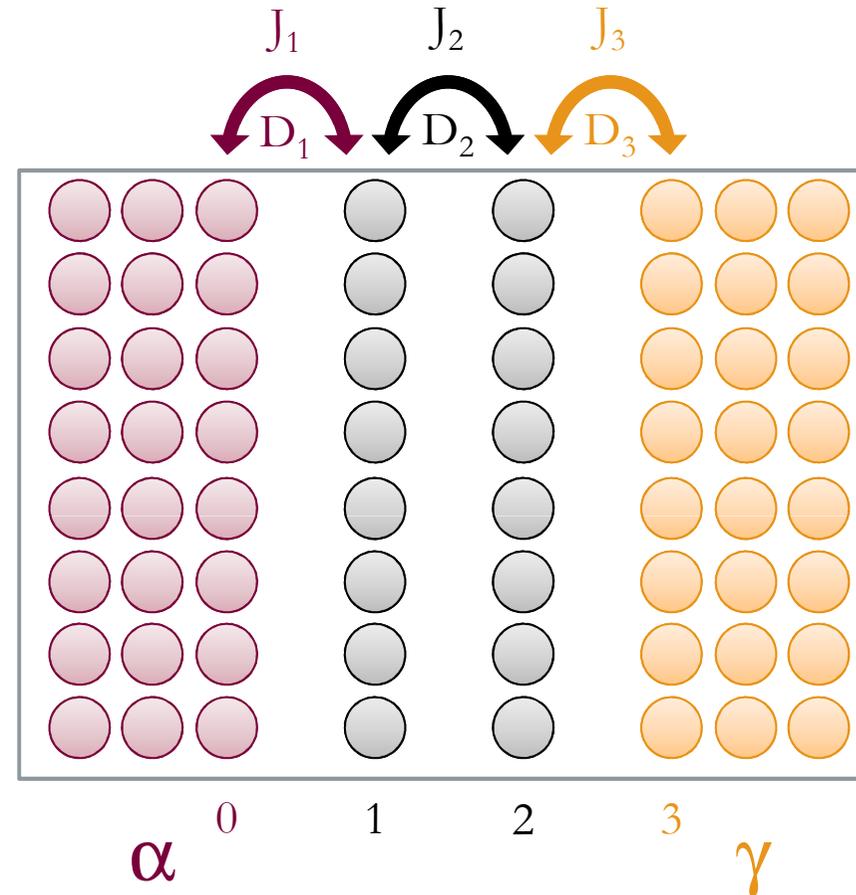
System	Observations	Implications/difficulties
Fe-C-Ni	LENP kinetics	Full spike present.
Fe-C-Mn	LENP at “low” temperatures, PE at “high” temperatures.	Interface Capacity concept.
Fe-C-Si	Slower than LENP	Constant dissipation could fit the data.
Fe-C-Mo	(important contribution due	
Fe-C-Cr	to dissipation)	

New Generalized Approach

- Four key steps similar to *Odqvist et al.*
 - 1) Assuming steady-state, the **X concentration profile across the interface** is computed as a function of v .
 - 2) **The dissipation associated with solute diffusion** is calculated as a function v .
 - 3) **The carbon concentration on both ferrite and austenite sides** is calculated as a function of v .
 - 4) Model interface motion as a function of time taking into account carbon diffusion in the bulk austenite and ferrite.

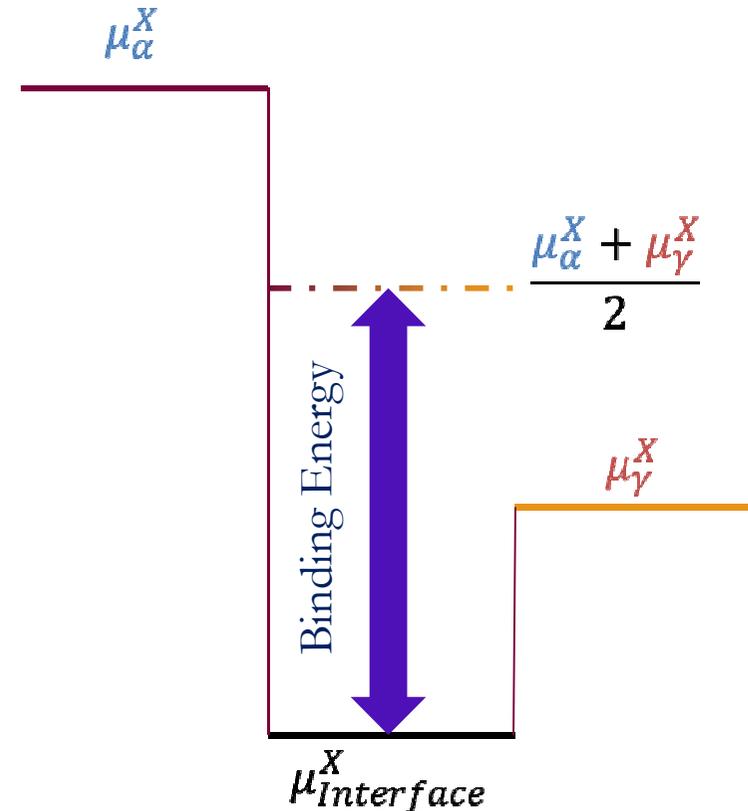
Step 1: Solute profile across the interface

- Discrete three jump model across the interface (Lucke and Stuwe).
- Convection is taken into account using the classical approach.
- Both Steady-state and non-steady state calculations were performed.



Step 1: Solute profile across the interface

- Discrete three jump model across the interface (Lucke and Stuwe).
- Convection is taken into account using the classical approach.
- Both Steady-state and non-steady state calculations were performed.
- The free energy of the interface is created by modifying the free energy of austenite.
- The tendency of the solute to segregate to the interface is introduced through the parameter: $L(\text{bou}, \text{Fe}, \text{X}; \text{Va}; 0)$

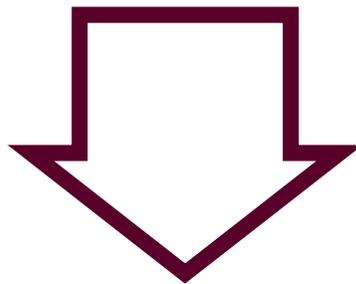


$$D_1 = D_\alpha \quad D_2 = \sqrt{D_\alpha D_\gamma} \quad D_3 = D_\gamma$$

Step 2: Dissipation Calculations

- Dissipation is calculated using a discrete version of Hillert's Equation.
- Calculations are carried out over the interface only (spike is not included).

$$\Delta G^{dissipated} = -\frac{V_m}{v} \int_{-\delta}^{+\delta} J_M \cdot \frac{d(\mu_M - \mu_{Fe})}{dy} \cdot dy$$



$$\Delta G^{dissipated} = \sum_{i=1}^{i=3} -\frac{V_m}{v} \cdot J_X^i \cdot \left[(\mu_X^i - \mu_X^{i-1}) - (\mu_{Fe}^i - \mu_{Fe}^{i-1}) \right]$$

Step 3: Carbon Concentrations

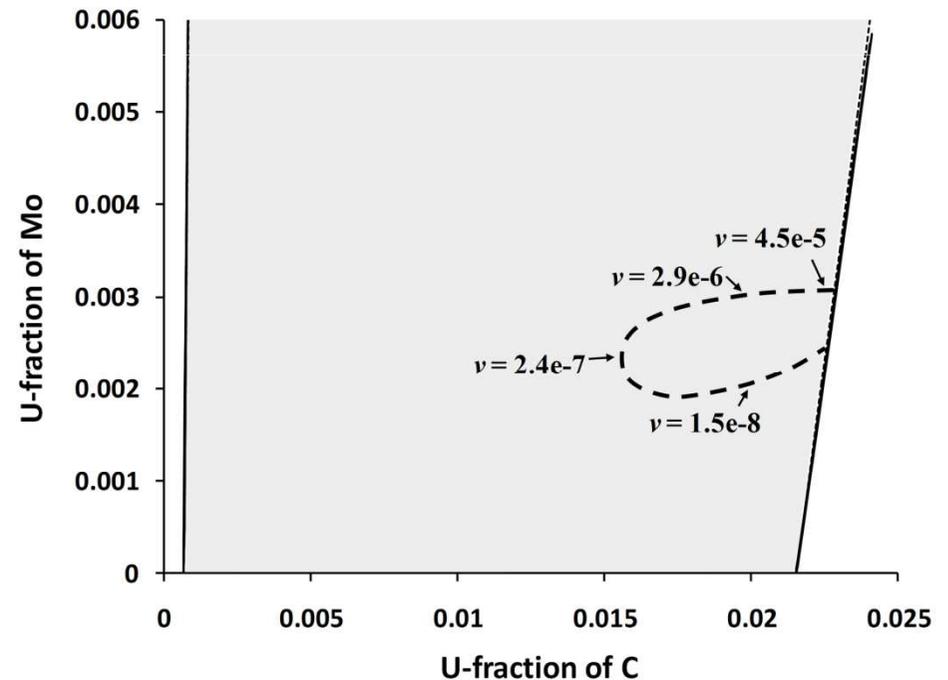
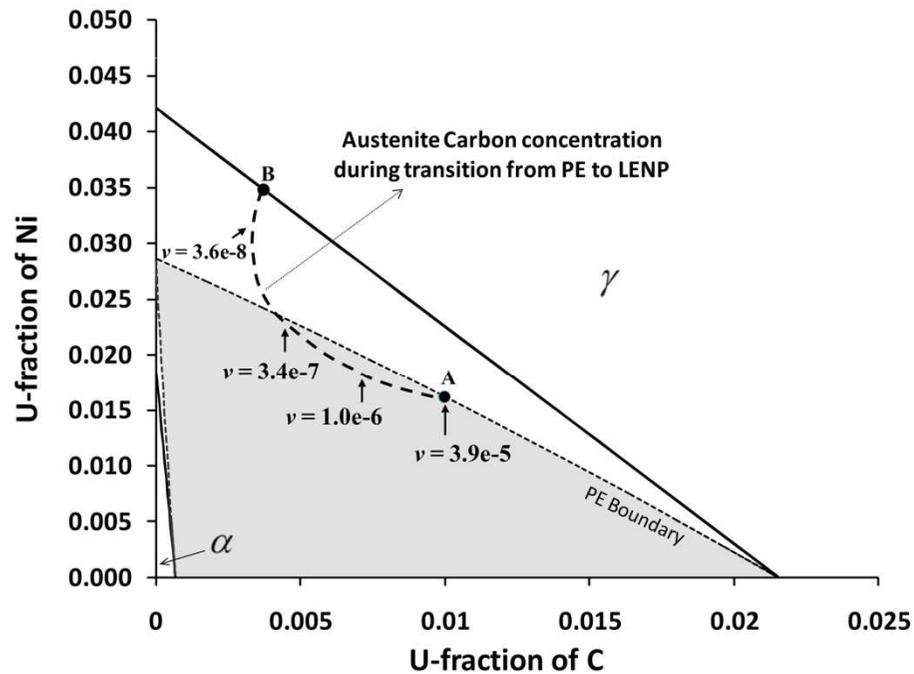
- We solve for the carbon concentration assuming:
 - The chemical potential of carbon is constant across the interface.
 - The sum of driving force and dissipation equals zero.

$$\Delta G^{DF} - \Delta G^{dissipated} = 0$$

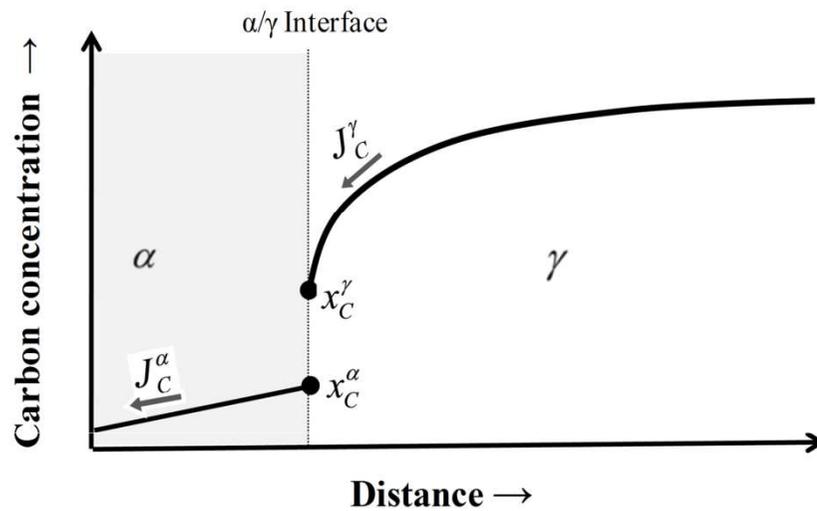
$$\Delta G^{DF} = \frac{(U_M^{fcc} + U_M^{bcc})}{2} \cdot (\mu_M^{fcc} - \mu_M^{bcc}) + \frac{(U_{Fe}^{fcc} + U_{Fe}^{bcc})}{2} \cdot (\mu_{Fe}^{fcc} - \mu_{Fe}^{bcc})$$

Step 3: Carbon Concentrations

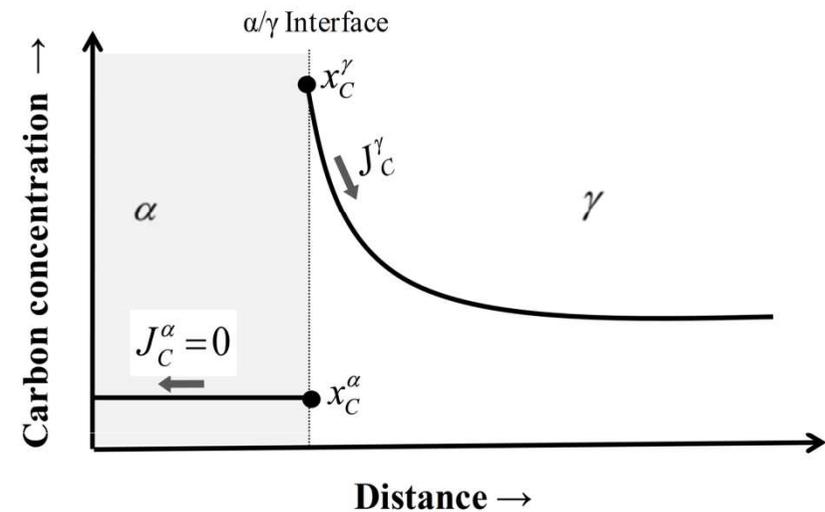
- We solve for the carbon concentration assuming:
 - The chemical potential of carbon is constant across the interface.
 - The sum of driving force and dissipation equals zero.



Step 4: Time Evolution Subject of Carbon Diffusion in Bulk Phases



$$v = \frac{J_C^\alpha - J_C^\gamma}{x_C^\alpha - x_C^\gamma}$$



$$v = \frac{J_C^\alpha - J_C^\gamma}{x_C^\alpha - x_C^\gamma}$$

- Diffusion in austenite is modeled using an explicit finite-difference Murray-Landis algorithm.
- Spherical geometry is used for precipitation, planar for decarburization.

Results:

- Precipitation and decarburization results were satisfactorily modelled using the following parameters:

Binding Energies (kJ/mol)

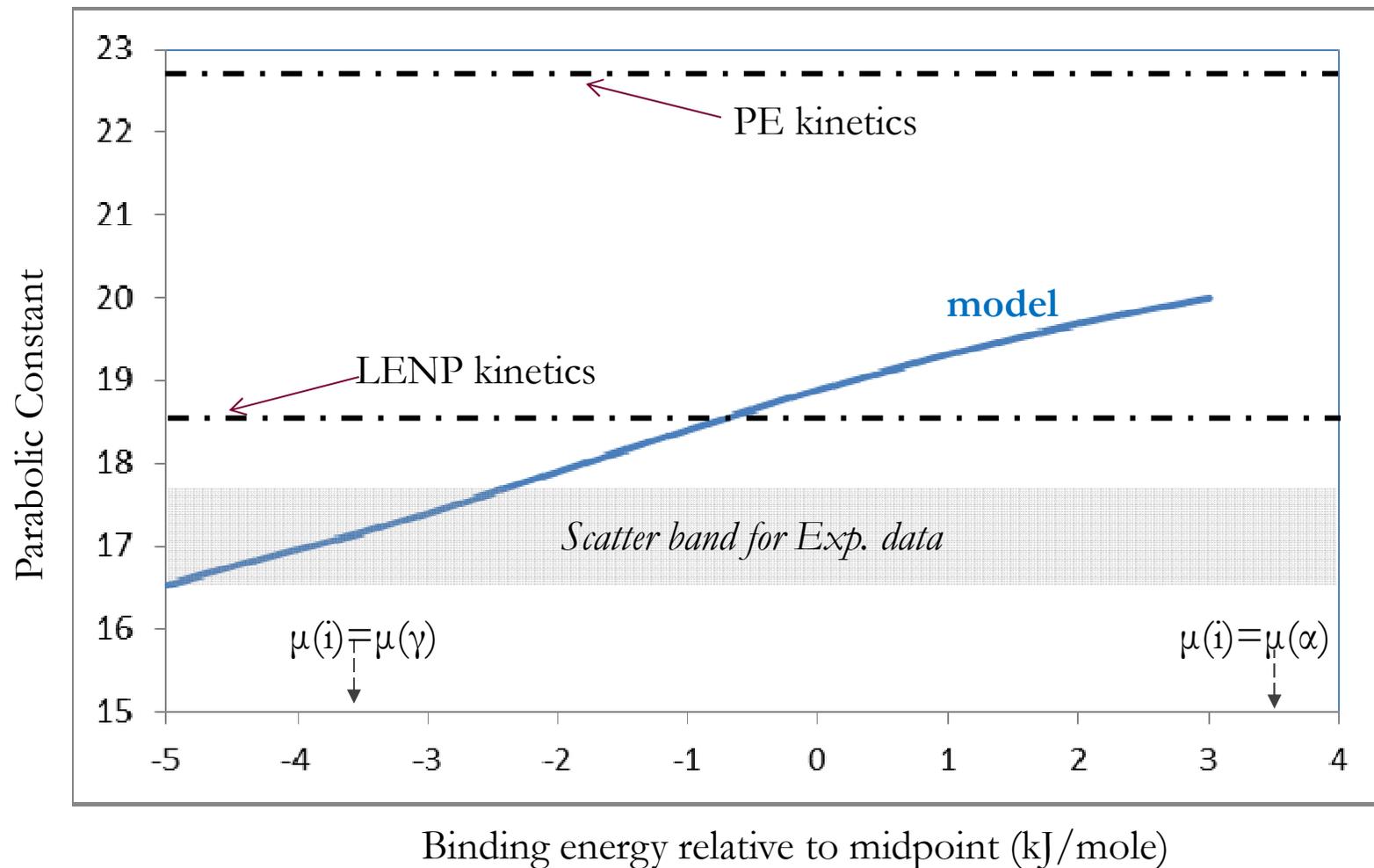
Diffusion Coefficients

Fe-Ni-C:	+1.5	fga
Fe-Cu-C:	-1	fga
Fe-Cr-C:	-1.5	f a a
Fe-Co-C:	-2	fga
Fe-Mn-C:	-2.5	fga
Fe-Si-C:	-9	f a a
Fe-Mo-C:	-15	fga

f=ferrite bulk, g=geometric average, a=austenite bulk

Results:

- Precipitation and decarburization results were satisfactorily modelled using the following parameters:



Fe-0.94%Mn-0.57%C decarburized at 755C

Precipitation Volume Fractions

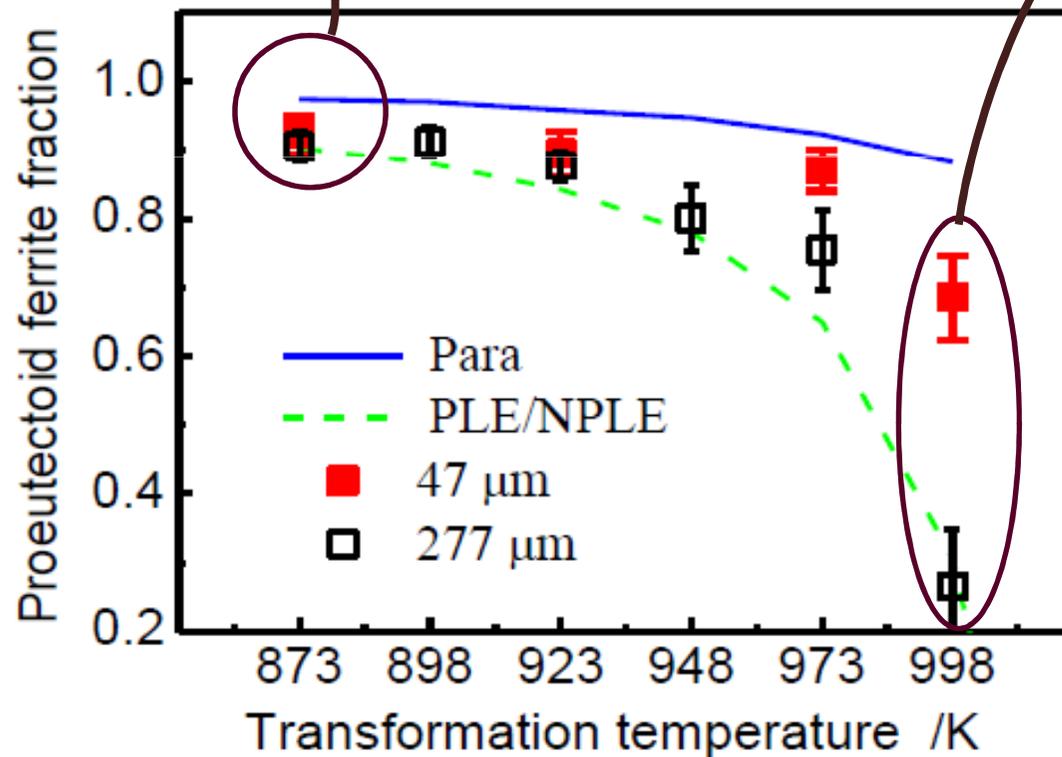
We can predict the **critical limits** for partitionless growth as a function of temperature (Oi et al) and as a function of composition (Hutchinson et al).

Alloy	Temperature K (°C)	Measured, V_f	Calculated, V_f
2.66%Ni-0.196%C	973 (700)	47%	34%
	983 (710)	n/a	20%
	992 (720)	3%	0%
2.42%Ni-0.293%C	973 (700)	21%	18%
	983 (710)	<1%	0%
	993 (720)	0%	0%
2.02%Ni-0.088%C	973 (700)	82%	81%
2.41%Ni-0.078%C		77%	79%
2.76%Ni-0.071%C		66%	76%
3.14%Ni-0.062%C		<10%	26%
3.33%Ni-0.055%C		<10%	22%
2.08%Mn-0.095%C	943 (670)	67%	35%
	973 (700)	23%	32%
	983 (710)	3%	4%
	993 (720)	n/a	0%
	1003 (730)	0%	0%
2.17%Mn-0.217%C	943 (670)	18%	6%
	973 (700)	0%	0% ¹⁴

Precipitation

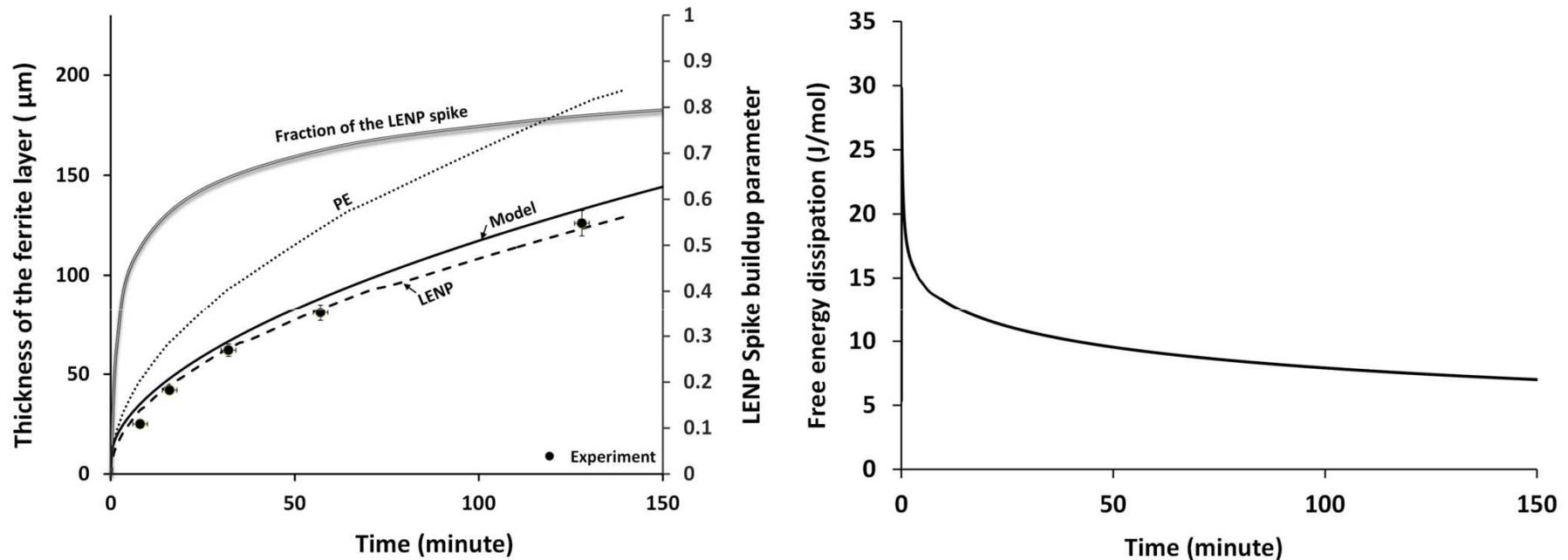
Effect of Grain-Size

Model correctly predicts essentially constant volume fraction of ferrite for grain size from 5 to 500 μm



Model shows dependence on grain-size.

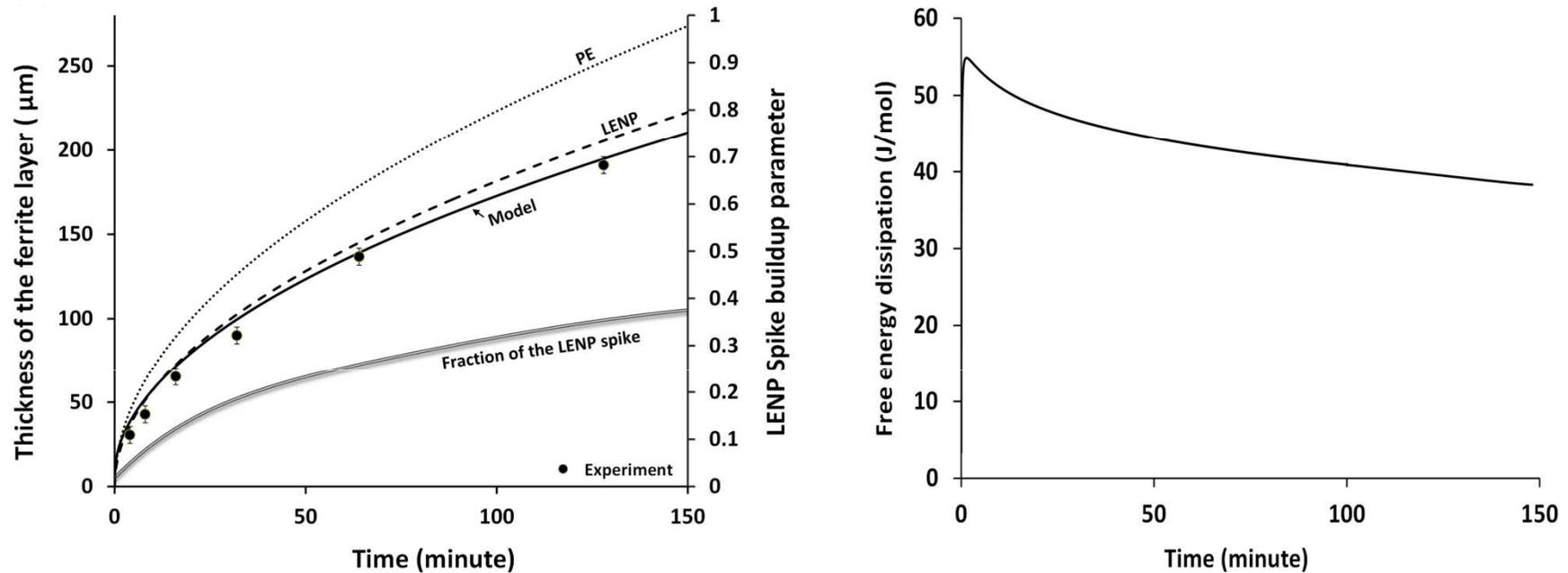
Decarburization: LENP observations revisited



Fe-0.94%Mn-0.57%C- 825C

- Data is very close to LENP. Model predicts that there is a spike.
Everything is consistent.

Decarburization: LENP observations revisited



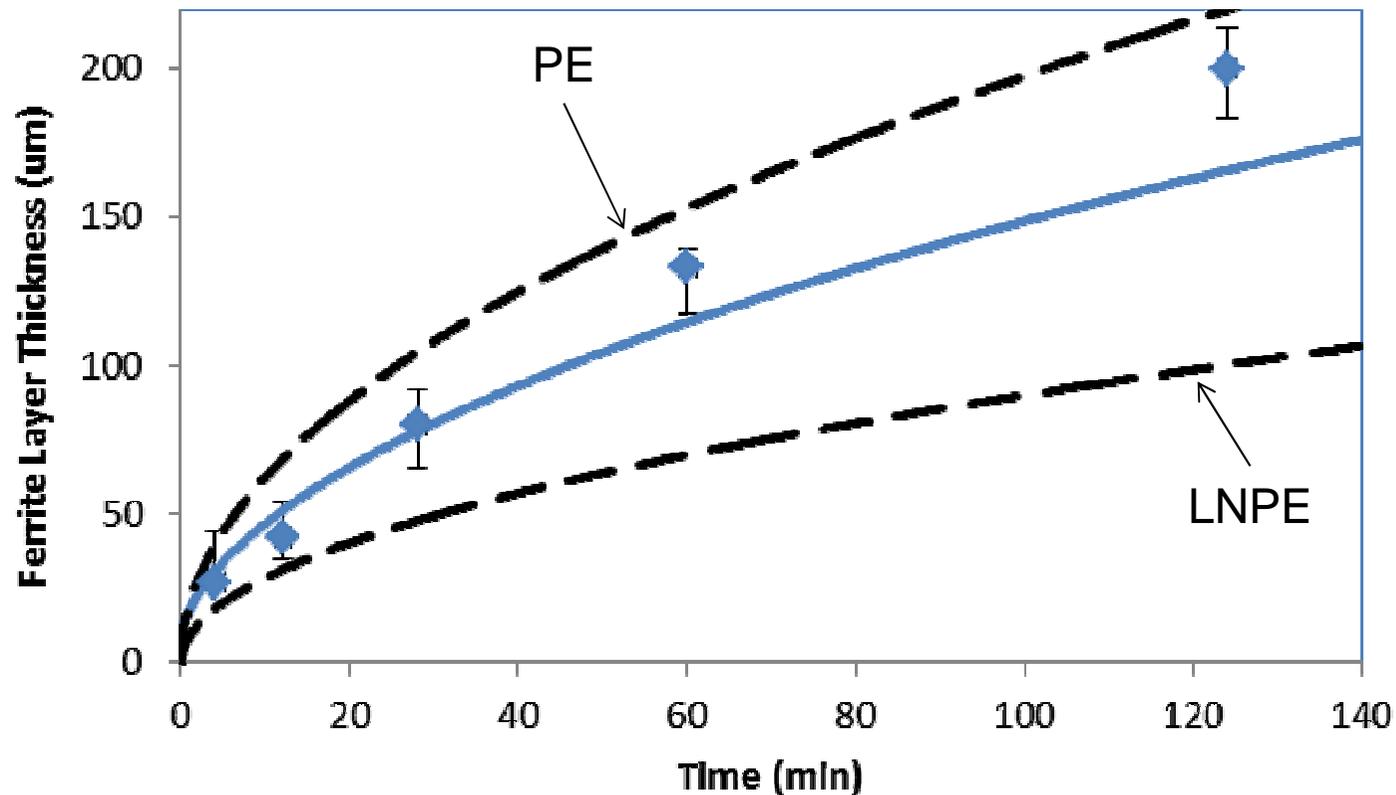
Fe-0.94%Mn-0.57%C- 755C

-Data is very close to LENP, but there is not a spike. In this case the magnitude of dissipation is such that the overall kinetics are close to LENP.

- To confirm this we performed new experiments on Fe-Ni-C and Fe-Mn-N

Decarburization:

LENP observations revisited



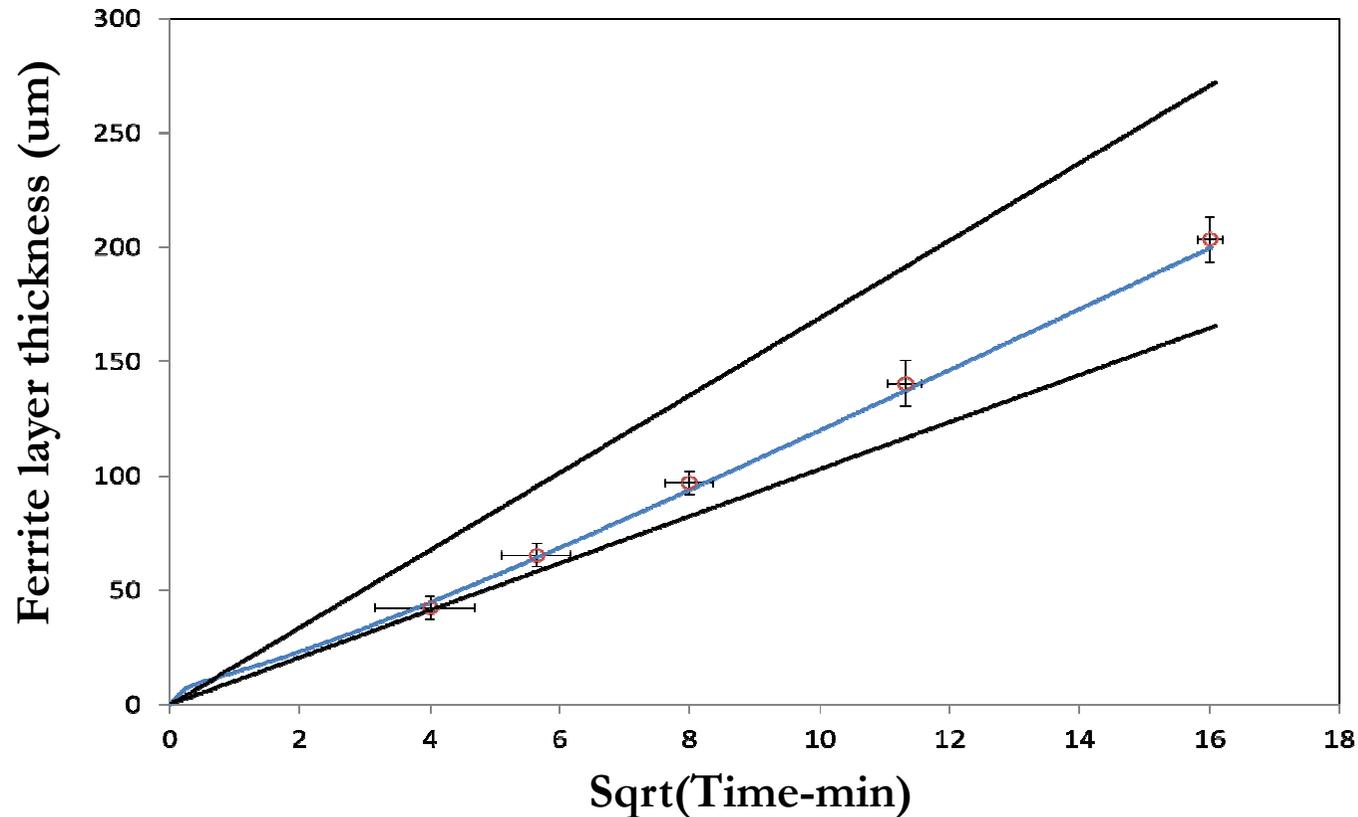
Fe-1.43%Mn-1.4%N- 750C

-Similar temperature that in which Fe-Mn-C showed kinetics close to LENP.

-In this case, the observed kinetics do not coincide with LENP.

Decarburization:

LENP observations revisited



Fe-1.46%Ni-0.76%C- 775C (work by Cong @ Monash)

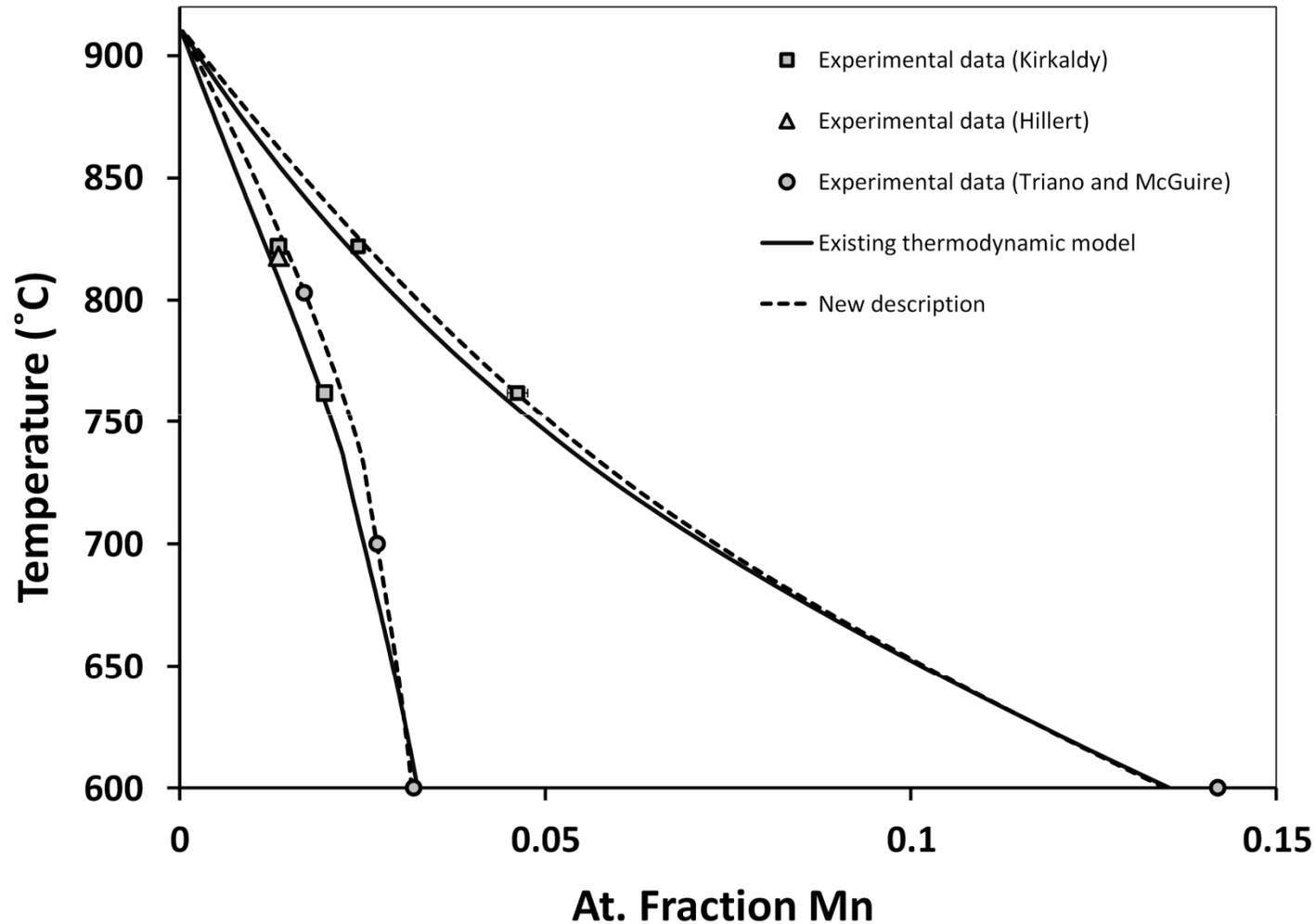
-One can find conditions in which the Fe-Ni-C data is not LENP.

Decarburization:

PE @ High Temperatures

- The observation of PE at high temperature could not be explained using the present model no matter what values of diffusion coefficients and binding energies are used.
- It is possible that there is new physics that we don't yet understand (eg. Interface capacity).
- Another possibility is that the thermodynamics of the Fe-Mn-C system are not sufficiently accurate in the temperature range of interest.

Decarburization: PE @ High Temperatures



$$L(\text{BCC,Fe,Mn:Va;0})_{\text{new}} - L(\text{BCC,Fe,Mn:Va;0})_{\text{TCFE2}} = 4007.8 - 4.44 T(\text{K}) \text{ J/mol}$$

Decarburization:

PE @ High Temperatures

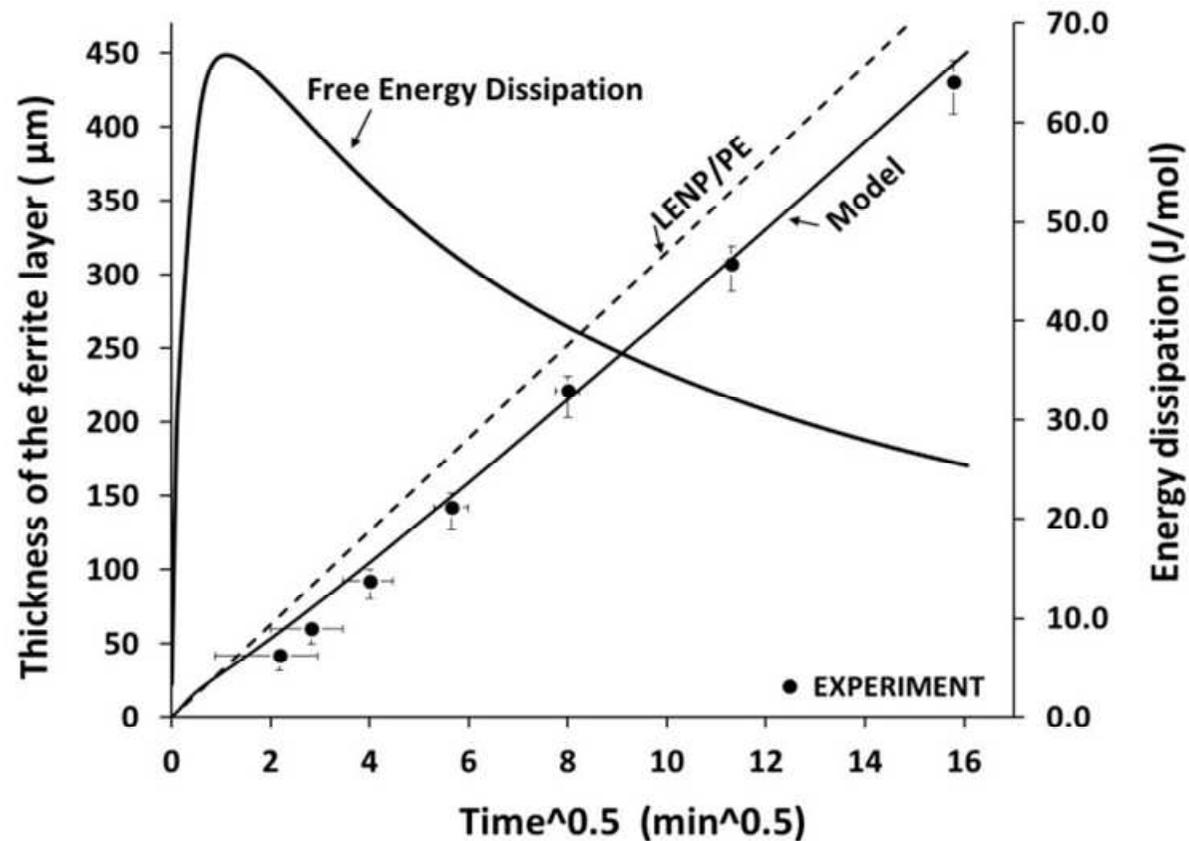
- The observation of PE at high temperature could not be explained using the present model no matter what values of diffusion coefficients and binding energies are used.
- It is possible that there is new physics that we don't yet understand (eg. Interface capacity).
- Another possibility is that the thermodynamics of the Fe-Mn-C system are not sufficiently accurate in the temperature range of interest.
- If we make the above change, all of the Fe-Mn-C results can be fit using the present model. There is no need to introduce any new concepts.

Decarburization:

“Constant” Dissipation

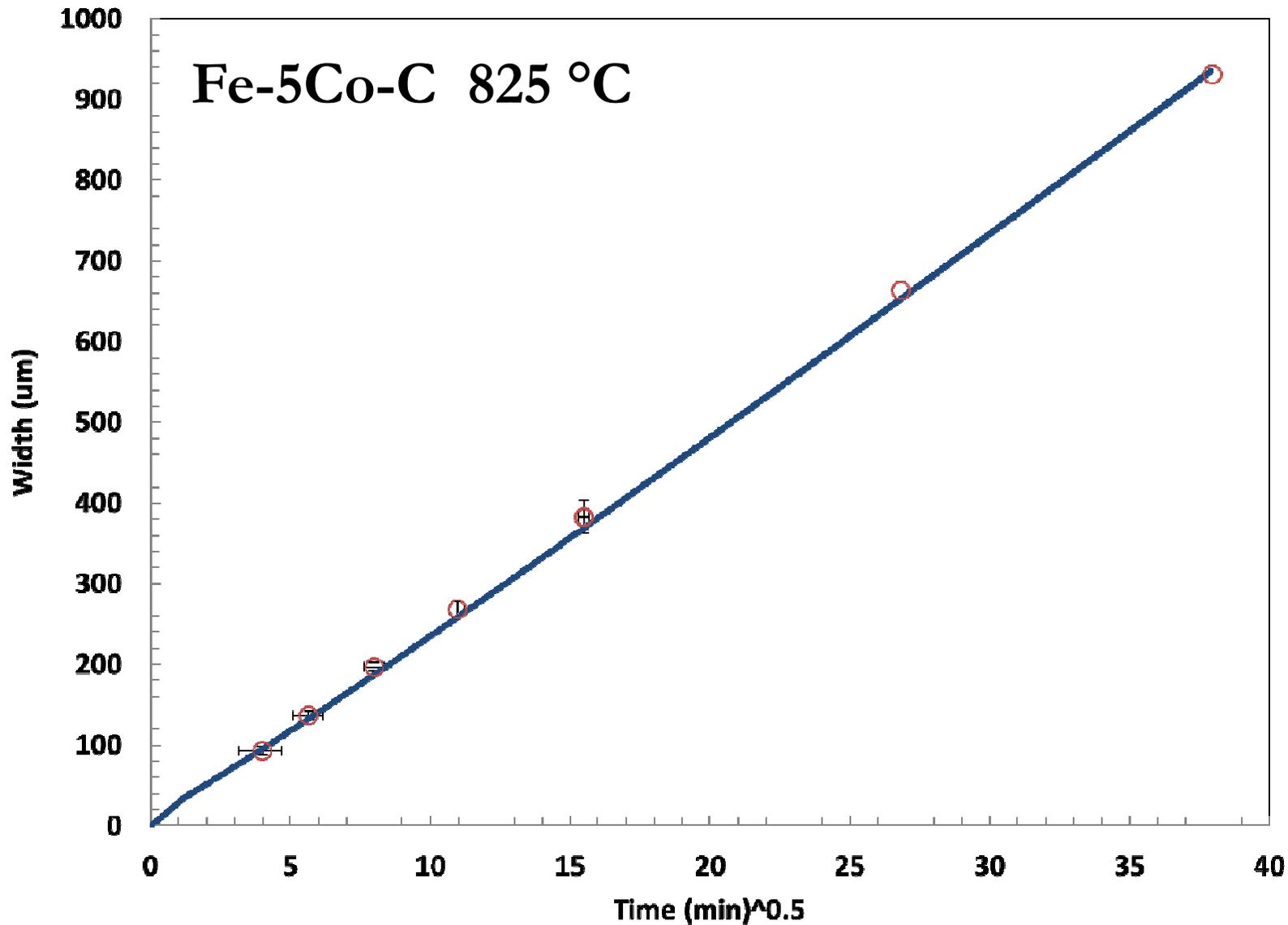
- In the past we noted that the Fe-Mo-C data was slower than PE/LENP predictions.
- The data could be described using a constant dissipation. This was puzzling because dissipation should change with v .
- Calculations with the new model show that over the times of interest, the dissipation does not change quickly enough. This might explain why a constant dissipation could be used in earlier works.

Decarburization: “Constant” Dissipation

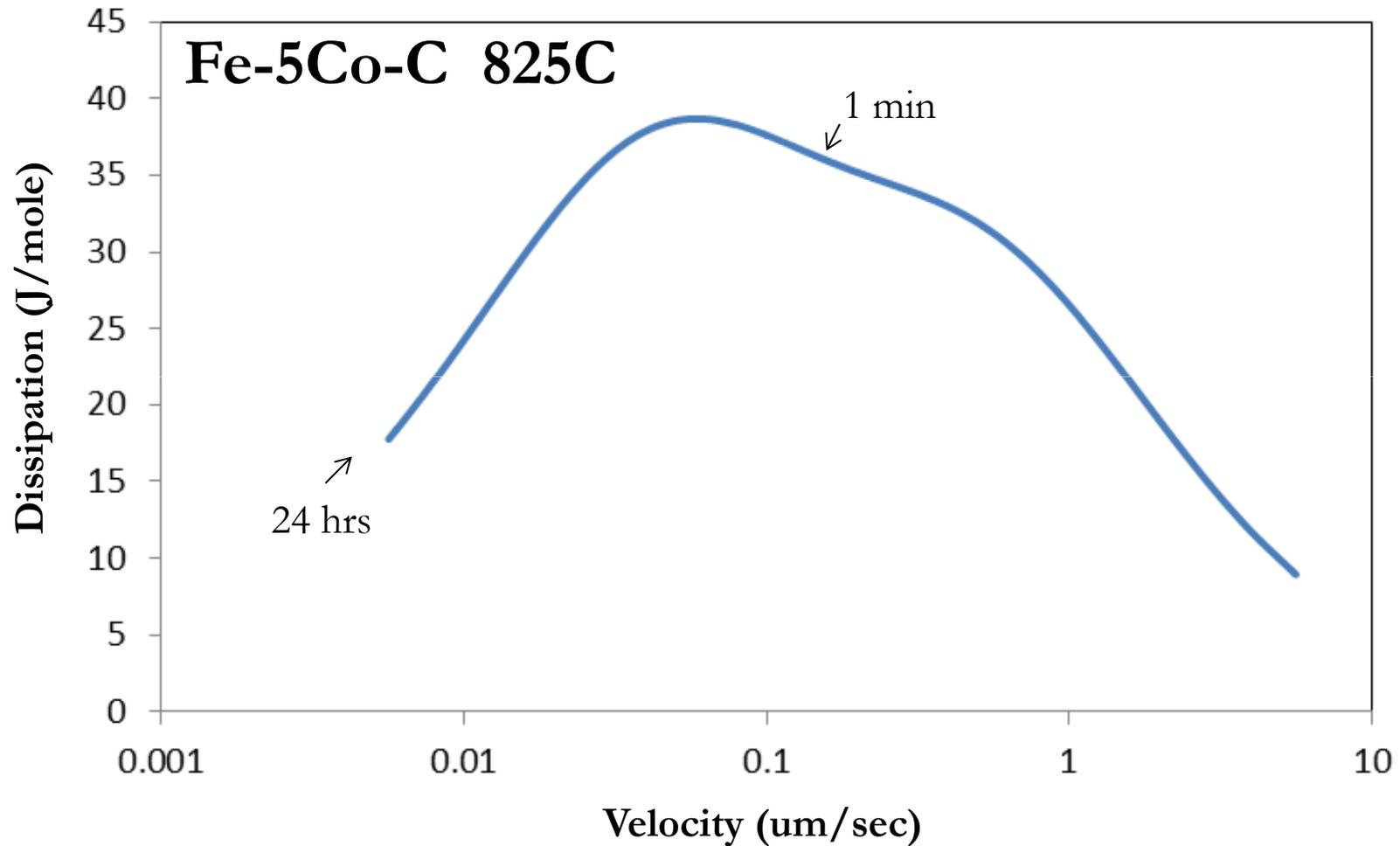


Fe-0.51%Mo-0.54%C @ 775 °C

Decarburization: “Constant” Dissipation



Decarburization: “Constant” Dissipation



Summary

- We have developed a general model for ferrite growth in Fe-C-X alloys which can fit both decarburization and precipitation observations for X=Ni,Mn,Si,Co,Cr,Mo&Cu.
 - Binding energies were estimated and are in reasonable agreement with GB binding energies.
 - Diffusion coefficients across the interface are of the order of the bulk diffusion coefficients.
- LENP observations are often the result of dissipation and not necessarily due to a full spike.
- PE observations in Fe-Mn at high T are probably due to uncertainties in the Fe-Mn-C thermodynamic assessment.
- Decarburization data can often be fitted using a constant dissipation because the interfacial conditions change very slowly with time.