Simpified Modelling of the PE / LENP transition

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Growth of ferrite

- Models
  - Based on carbon diffusion in austenite
    - Finite difference scheme
  - 2 thermodynamic bounds possible
    - LENP
    - Para-equilibrium
    - Mixed mode + dissipation in interface
  - Spherical geometry
  - Initial system
    - Austenite homogeneous carbon rich
    - Radius determine by the size of the system and the fractions
      - Radius = 0.5 * distance between centers of 2 ferrite grains~4µm

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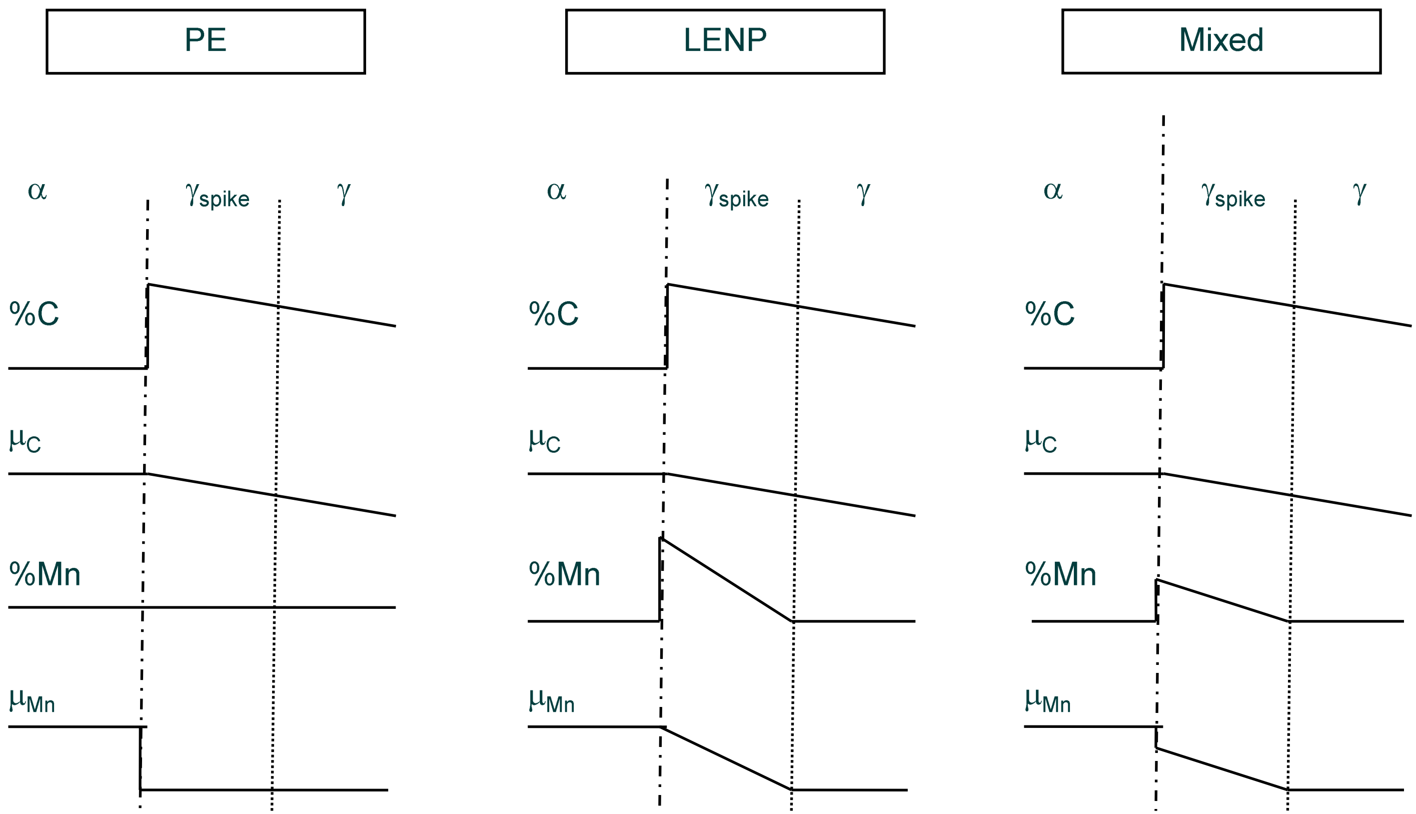
- Development of a mixed mode model : comparison PE, LENP, mixed mode



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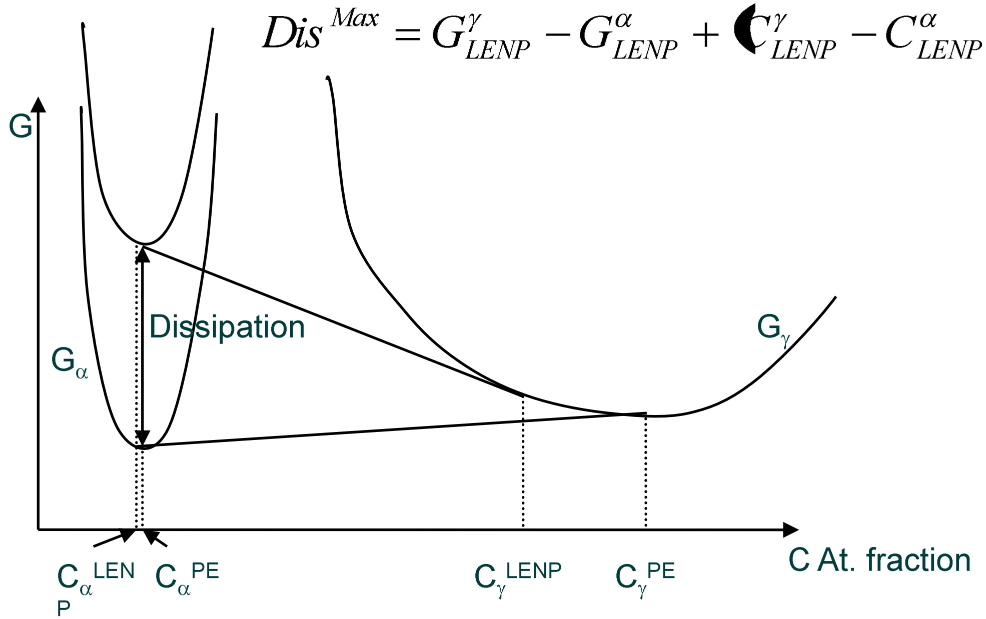
- Condition at interface

$$Dis^{Max} = G^{\gamma}_{LENP} - G^{\alpha}_{LENP} + \left(C^{\gamma}_{LENP} - C^{\alpha}_{LENP}\right) \cdot \left(\mu^{\gamma}_{Fe*,LENP} - \mu^{\gamma}_{C,LENP}\right)$$



- LENP = PE + dissipation of energy in the spike
- Idea: dissipation in the spike can vary between 0 and the LENP value

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- Flux through the interface

$$-L_{\text{int}} \cdot \left(\Delta\mu\right)^{\text{int}} = \frac{v}{V_m} \cdot \left(y_k - y_k^{\alpha}\right) = J_{\text{int}}$$

- Driving force for jump of 1 mole through the interface

$$\Delta\mu_{jn} = \left(\mu_j - \mu_n\right) - \left(\mu_j^{\alpha} - \mu_n^{\alpha}\right)$$

- Hypothesis:
  - no accumulation in interface in function of time
  - Dissipation = Dissipation spike + dissipation interface

$$J = J_{\text{int}} = J_{spike}$$

$$\Delta\mu = \left(\Delta\mu\right)^{\text{int}} + \left(\Delta\mu\right)^{spike}$$

→

$$J = -L \cdot \Delta\mu$$

$$\frac{1}{L} = \frac{1}{L_{\text{int}}} + \frac{1}{L_{spike}}$$

- Extreme cases
  - PE: dissipation = 0 <->L_{int}~∞
  - LENP: dissipation=dissipation LENP

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- LENP case
  - Lint~0

$$Dissipation = -\frac{V_m}{v}\cdot\left(L_{spike}\cdot(\Delta\mu)^{spike}\right)$$

$$Dissipation = -\frac{V_m}{v}\cdot\left(-L_{spike}\cdot(\Delta\mu)\right)(\Delta\mu) = \frac{V_m}{v}\cdot\frac{v}{V_m}\cdot\left(y_k - y_k^{\alpha}\right)(\Delta\mu)$$

$$L_{spike} = -\frac{v}{V_m}\cdot\frac{\left(y_k - y_k^{\alpha}\right)}{(\Delta\mu)^{spike}}$$

$$\frac{Dis^{LENP}}{(\Delta\mu)^2} = \frac{\left(y_k - y_k^{\alpha}\right)}{(\Delta\mu)}$$

Assumed to be constant

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- Mixed case

$$Dis = \frac{V_m}{v} \cdot \left(\frac{1}{L_{\text{int}}} + \frac{1}{\frac{v}{V_m} \cdot \left(\frac{Dis^{LENP}}{(\Delta\mu)^2} \right)} \right)^{-1} \cdot (\Delta\mu)^2$$

or

$$Dis = \frac{L_{\text{int}} \cdot Dis^{LENP}}{L_{\text{int}} + \frac{v}{V_m} \cdot \frac{Dis^{LENP}}{(\Delta\mu)^2}}$$

V>> -> PE

V<< -> LENP

Transition from PE to LENP function of Lint and v

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Estimation for Lint

- Lint
  - Assumption: related to grain boundary diffusion

$$J = -D \cdot \frac{\partial C}{\partial x}$$

or

$$J = -D \cdot \frac{dC}{d\mu} \frac{\partial \mu}{\partial x}$$

$$L_{\text{int}} = \lambda \frac{D_{Ni}^{GBfcc}}{a} \cdot \frac{dC}{d\mu}$$

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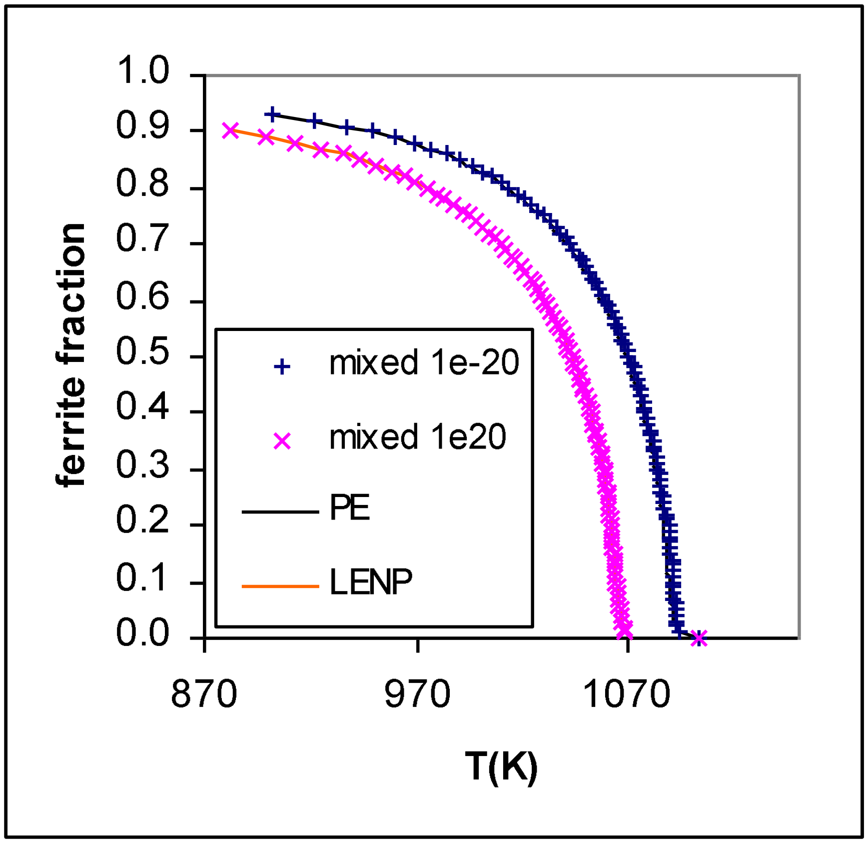
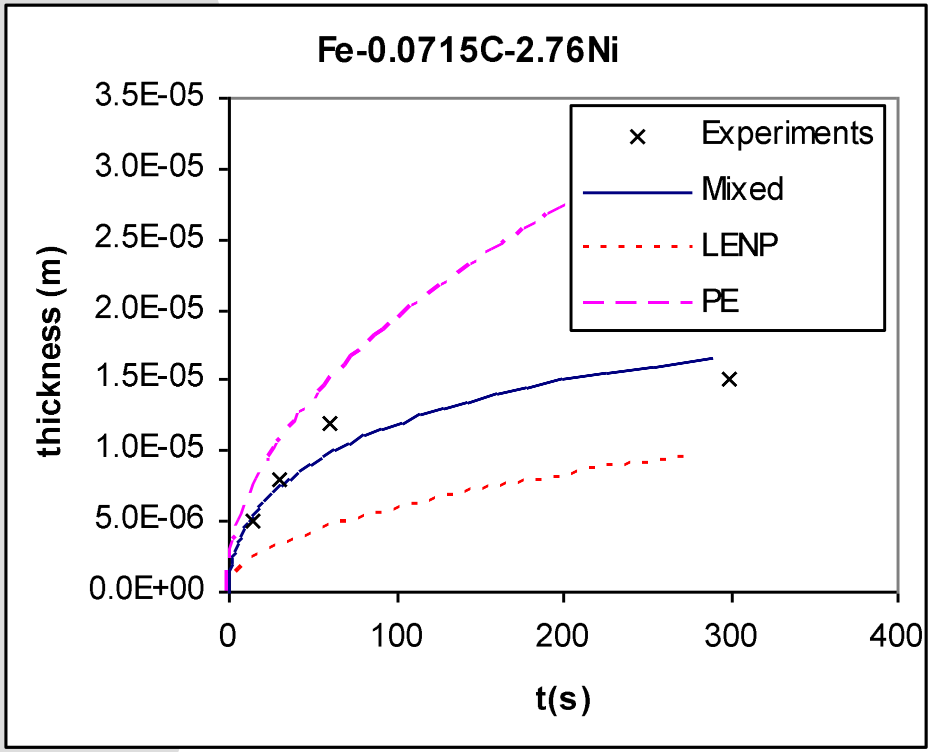
Examples

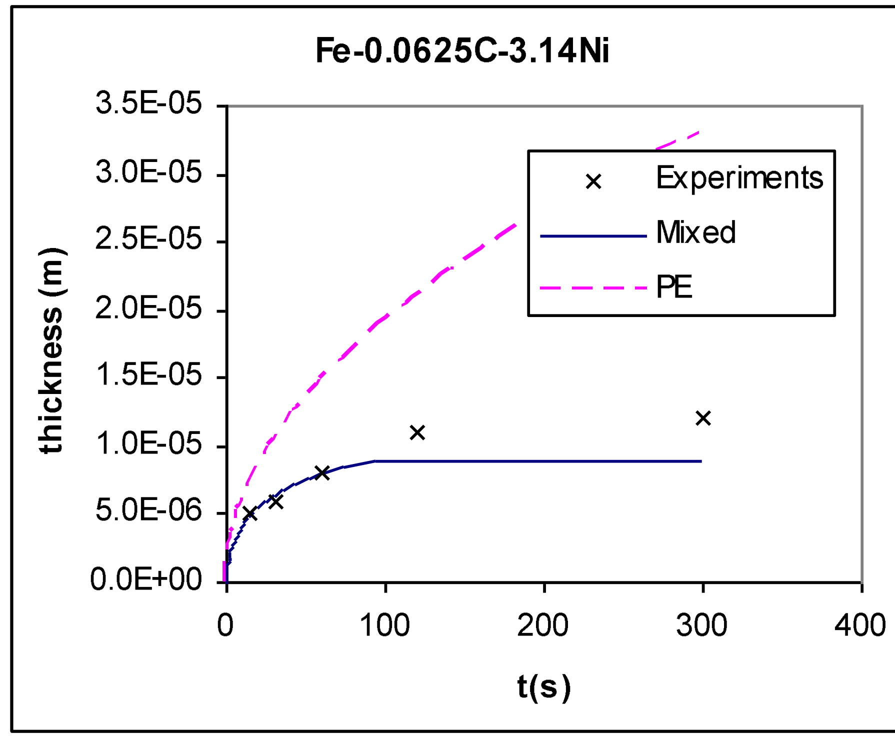
- 0.1%C, 1%Mn, R=10µm, 1°C/s, 3D



Comparison with work of C. Hutchinson (2003)

- Lambda~100





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- Estimation from intercritical annealing (RFCS project)

Steel	C	Mn	Si	Cr	Mo
1	0.09	1.4	0.15	0.75	/
2	0.14	1.46	0.45	0.2	0.07

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- Comparison with experimental results (martensite fraction)

Composition	Holding T (°C)	Quench Temperature (°C)	Cooling rate (°C/s)	Measured	LENP	PE a	Mixed mode
1	800	800	WQ	**55**	/	/	/
1	800	675	10	**15**	25	**11**	**20**
1	800	550	10	**10**	**13**	5	**7**
1	800	675	25	**23**	31	11	**18**
1	800	550	25	**11**	**14**	5	**8**
1	800	675	90	**19**	43	**16**	32
1	800	675	90	**17**	25	7	**13**
2	810	810	WQ	**50**	/	/	/
2	810	700	3	**19**	41	**19**	29
2	810	600	3	**13**	17	10	**15**
2	810	20	3	**14 (*)**	**14**	10	10
2	840	840	WQ	**100**	/	/	/
2	840	730	10	**82**	96	32	**74**
2	840	640	10	**14**	38	**13**	20
2	840	540	10	**11**	22	8	**11**

Better description with the mixed mode than with LENP or PE hypothesis

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Conclusion

- Simplified mixed mode model has been developed, with only computation of carbon diffusion
- Fitting of the interface condition is based on grain boundary conditions
- Possibility to reproduce with a good agreement the experimental results of C.Hutchinson between LENP and PE.

- Perspective
  - Determination of the size of the cell remains the key parameter to master the phase transformation kinetics.

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