PE and LE-NP

Paraequilibrium, and Local Equilibrium-Negligible Partition (proposed boundary conditions for precipitate growth in Fe-C-X);

a review and a discussion

Gary Purdy
McMaster University

McMaster University

Outline:

- Acknowledgments;
- a short history of the development of the two concepts;
- The modeling approach;
- The experimental approach;
- Current findings;
- The future.

Acknowledgements:

Mats Hillert
Jack Kirkaldy
Hub Aaronson

Dieter Weichert
Jim Gilmour
Denton Coates
Paul Wycliffe

Kenji Oi
Christophe Lux

Jinichiro Nakano
Andre Phillion
Hatem Zurob
Chris Hutchinson
Yves Brechet
Hiu Guo
Dmitri Malakhov
Masato Enomoto
Hossein Seyedrezai
Armand Beche

McMaster University

A brief history; some selected early developments:

Hultgren, Trans ASM, 1947;39:915
Hillert, 1953, “Paraequilibrium” Swedish Institute for Metal Research
Kirkaldy, Can. J. Phys., 1958;36:907
Popov, Fiz. Met. Metall., 1958;6:643
Purdy, Weichert, Kirkaldy, TMS-AIME,1964;230:1025
Aaronson, Domian, Pound, TMS-AIME, 1966;237:768
*Kinsman, Aaronson, in “Transformation and Hardenability in Alloy Steels” Climax Molybdenum 1967:39
*Hillert, in “The Mechanism of Phase Transformations in Crystalline Solids” Inst. Metals., 1969:231
Gilmour et al, Met. Trans.,1972;3:3213
Coates, Metall.Trans.,1973;4:1070, 2313

* these anticipated the need to model the interface itself; the others primarily used sharp-interface concepts.

Further selected references 1975-2000

McMaster University

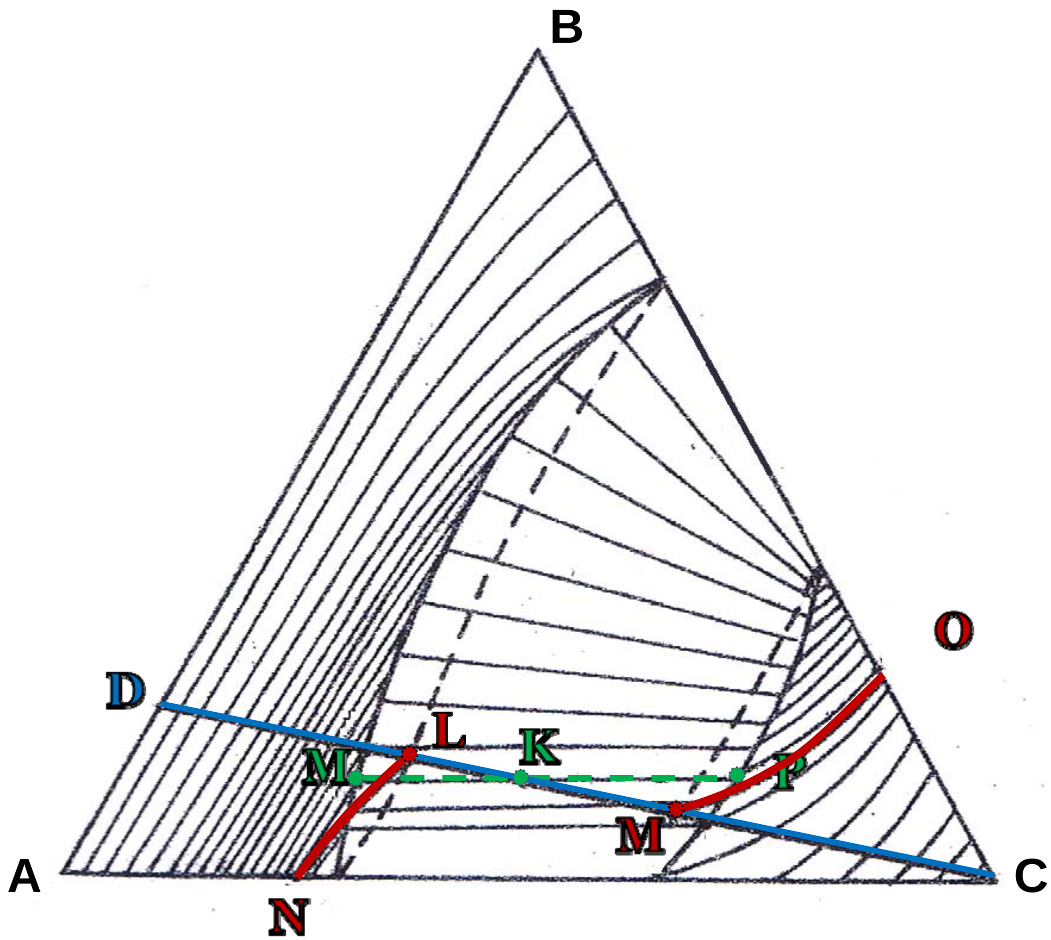
Hillert, Sundman, Acta Met. 1976;24:731, 1977;25:11
Agren, Acta Met., 1989;37:181
Liu, Agren, Acta Met., 1989;37:3157
Purdy, Brechet, Acta Met., Mater., 1995;43:3767
Enomoto, Acta Met., Mater.,1999;47:3533
Liu, Met., Mat., Trans., 1997;28A:1625
Hillert, Acta Mat., 1999;47:4481

Increasing widespread availability of thermodynamic, kinetic databases ↓

2000 +

Oi et al, Acta Mat.,2000;48;2147
Odqvist, Hillert, Agren, Acta Mat. 2002;59:3211
Hutchinson, Fuchsmann, Brechet, MMTA 2004;39A:1211
Hillert, Hoglund, Austenite 2003*
Enomoto, Austenite 2003
Vitek, Babu, Kozeschnik Austenite 2003
Phillion et al, MMTA 2004;35A:1237
Fazeli, Millitzer MMTA 2005;36A:1395
Zurob et al, Acta Mater.,2008;56:2203,2009;57:2781

*Austenite 2003
(Austenite Formation and Decomposition,
Eds; E. B. Damm, M. J. Merwin, ISS and TMS.)



K: Bulk Composition

MP: Equilibrium tie-line

LM: PE tie-line

CD: Component ray of C

NL + MO: Iso-activity lines for C

Mats Hillert, Internal Report, Swedish Inst. for Metals Research (1953)

Mats Hillert 1953
“Paraequilibrium”
Swedish Inst. For
Metals Research

Fig. 3

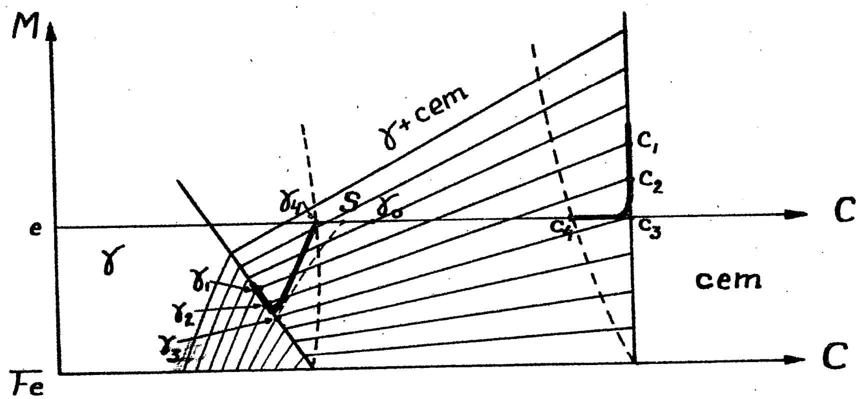
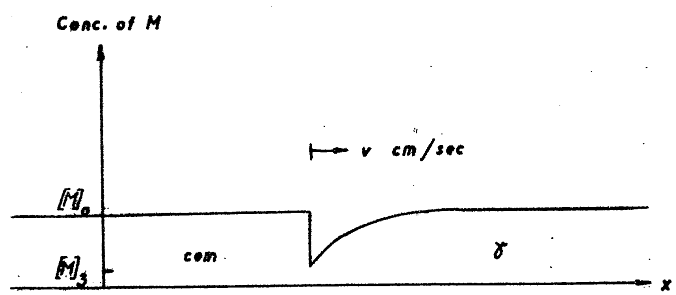
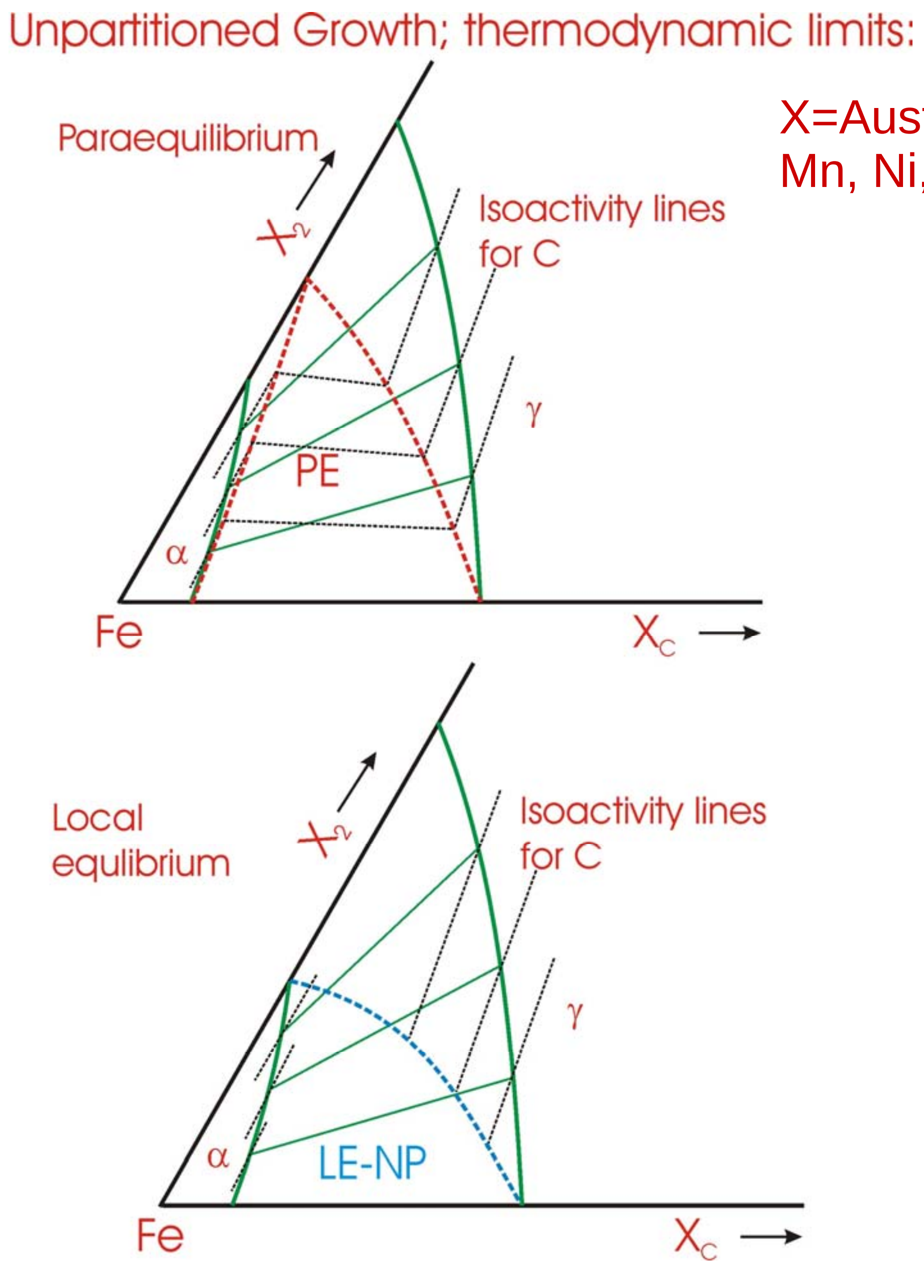
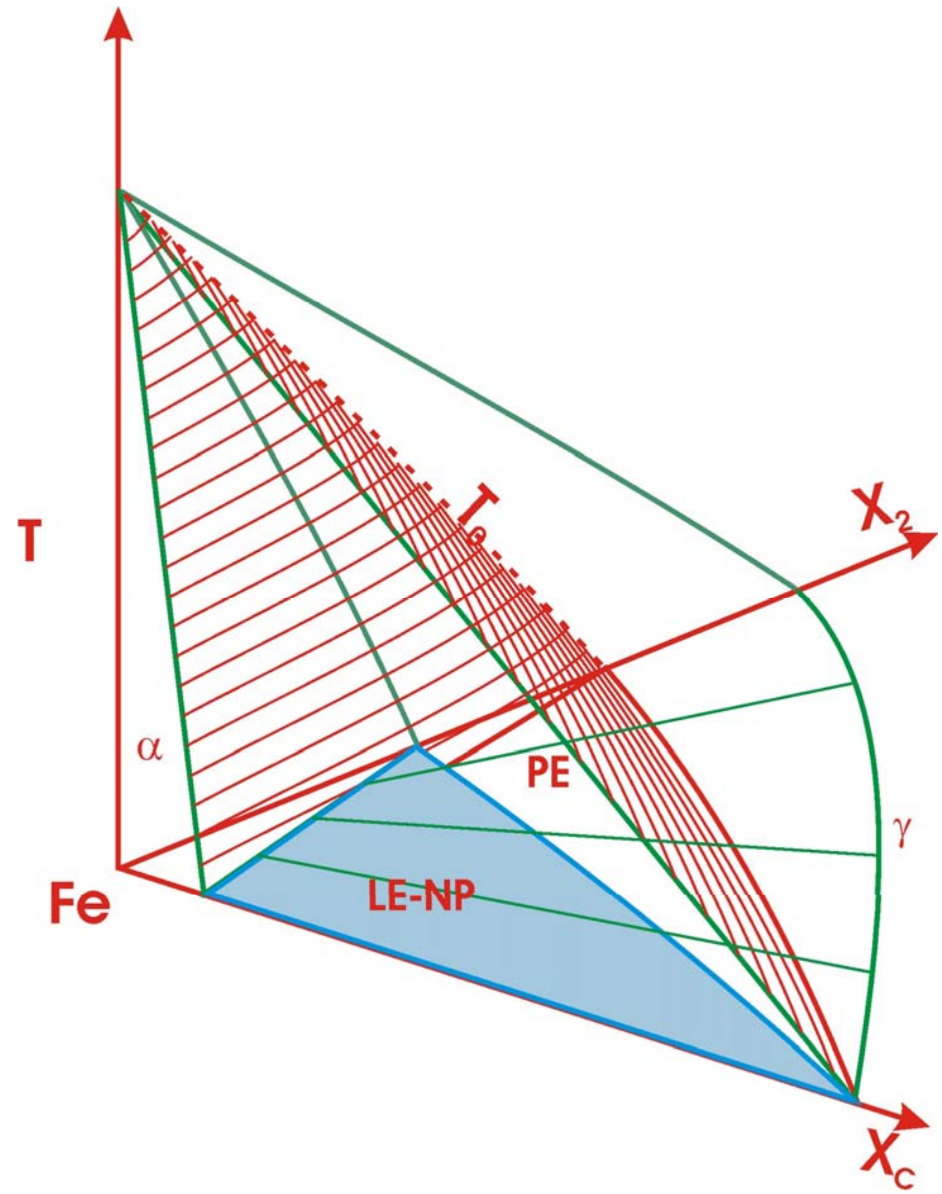


FIG. 4

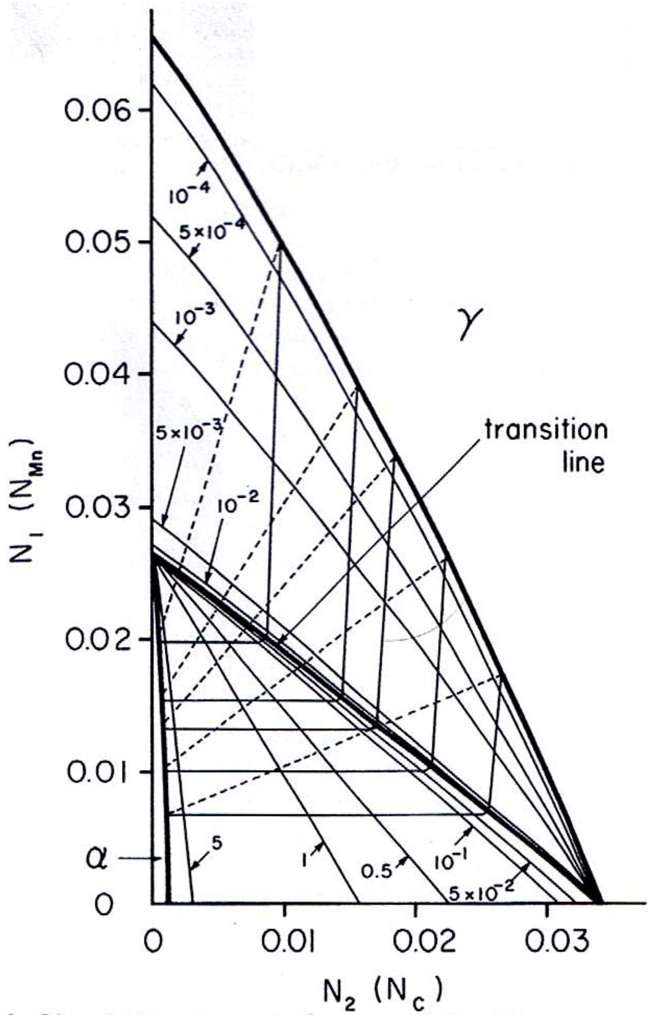


X=Austenite stabilizer
Mn, Ni,…



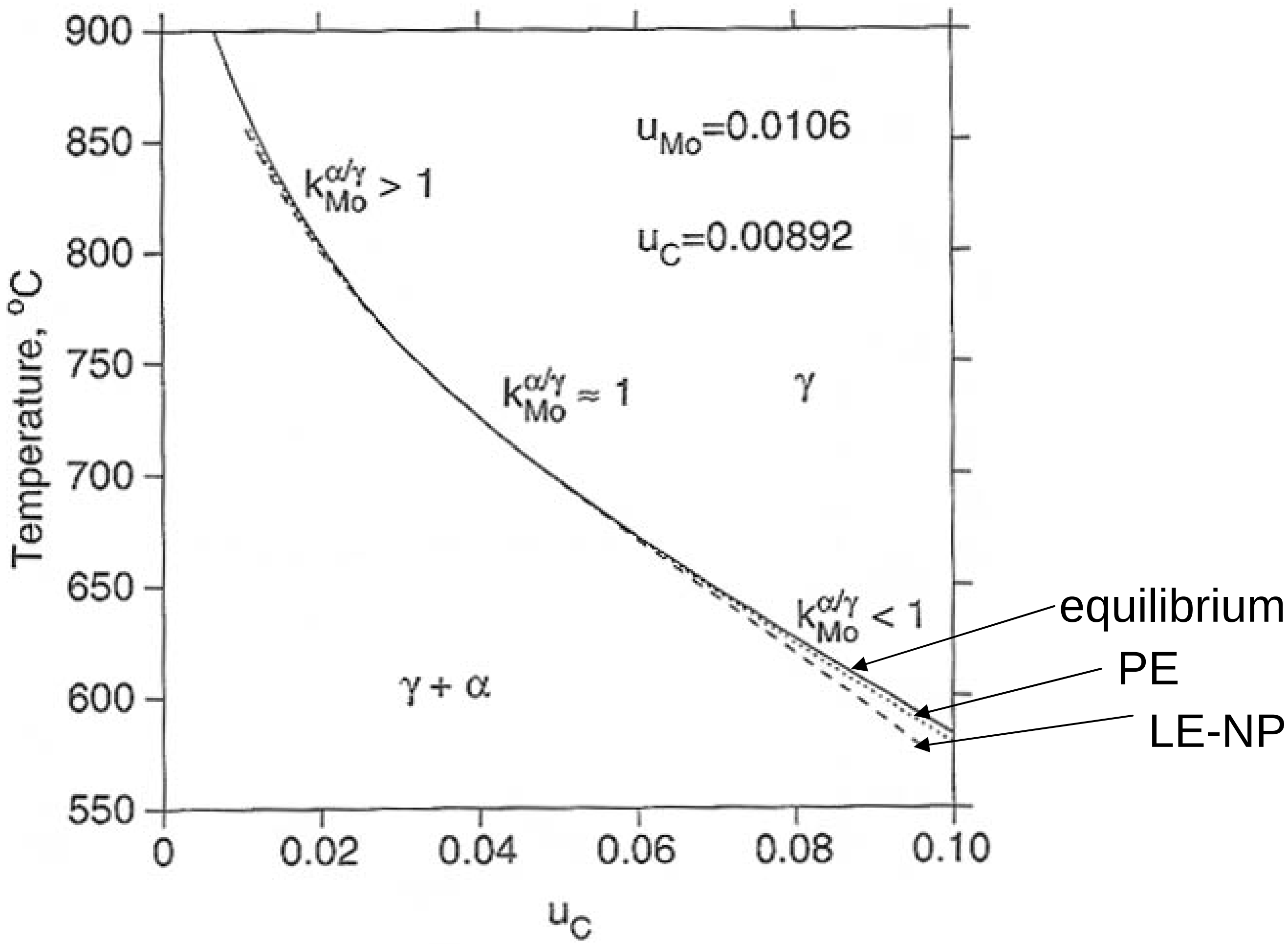


T
X2
α
PE
γ
Fe
LE-NP
Xc

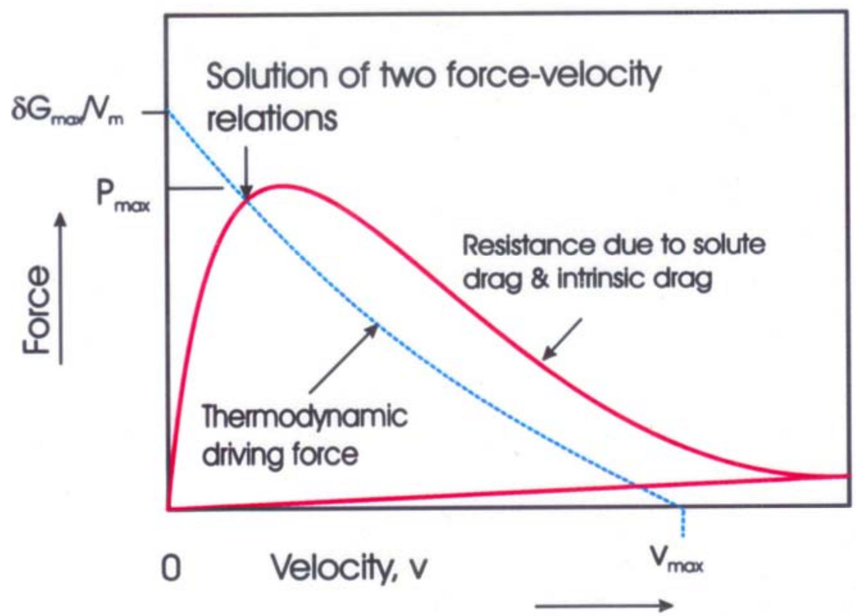


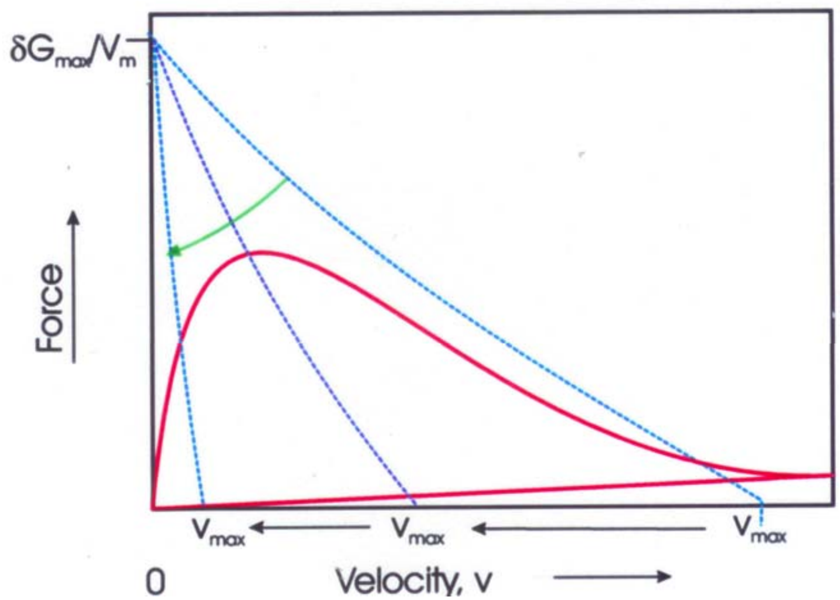
Coates, Met. Trans., 1973;4:1070

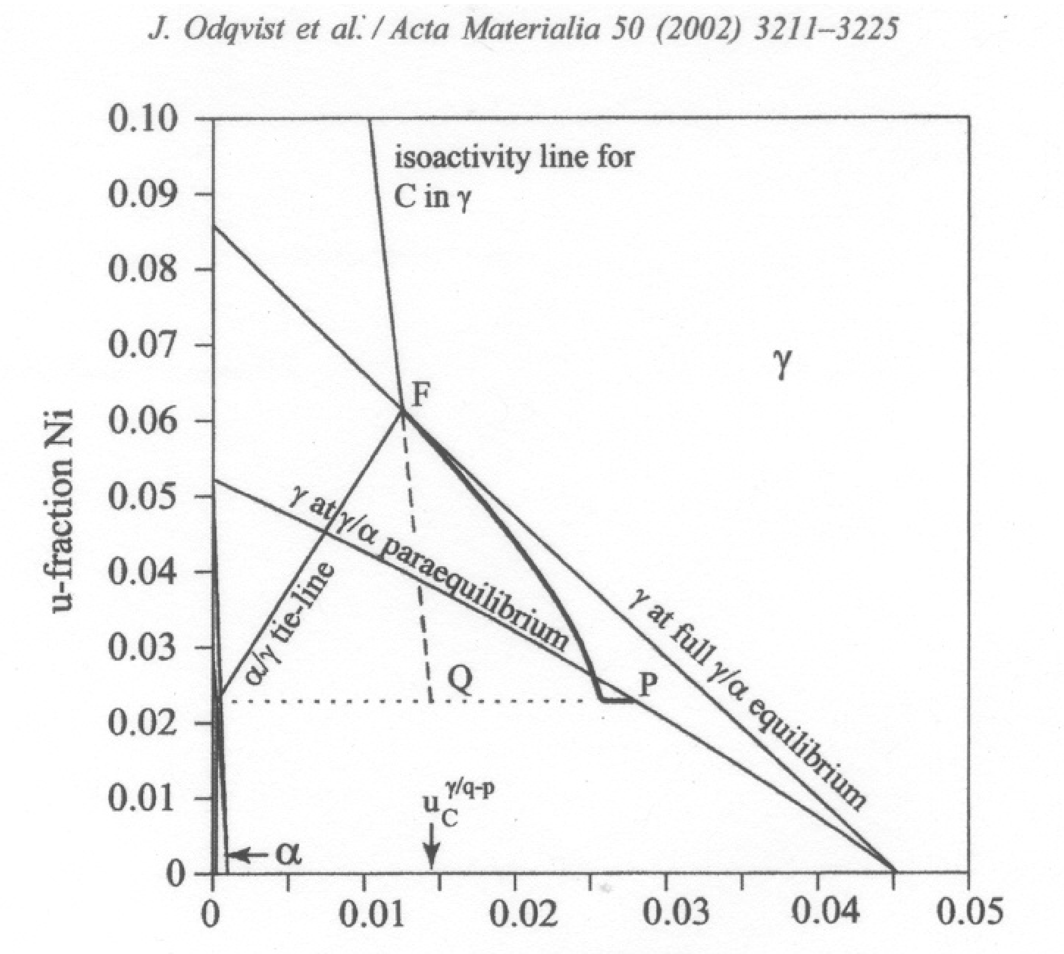
Fe-C-Mo

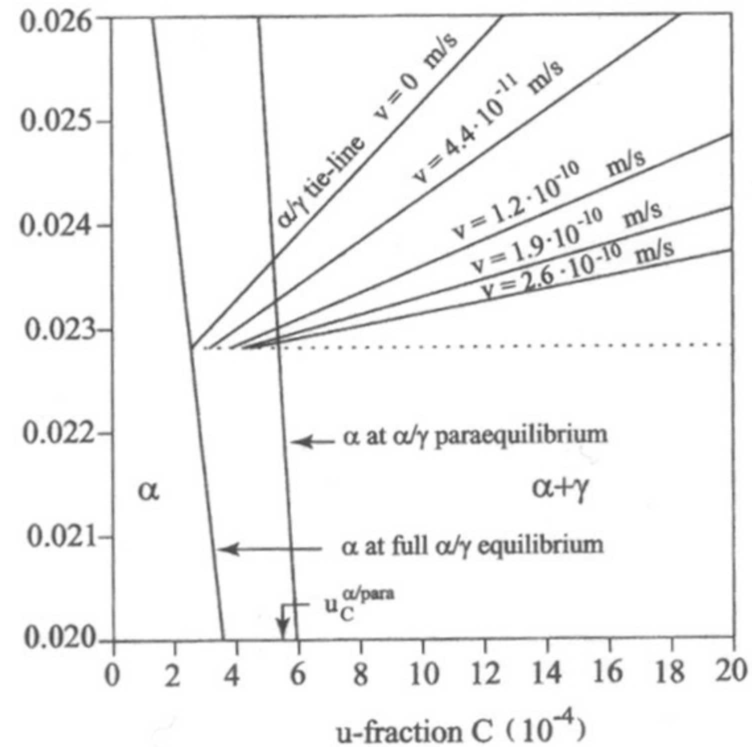


Lui, MMTA, 1997;28A:1625

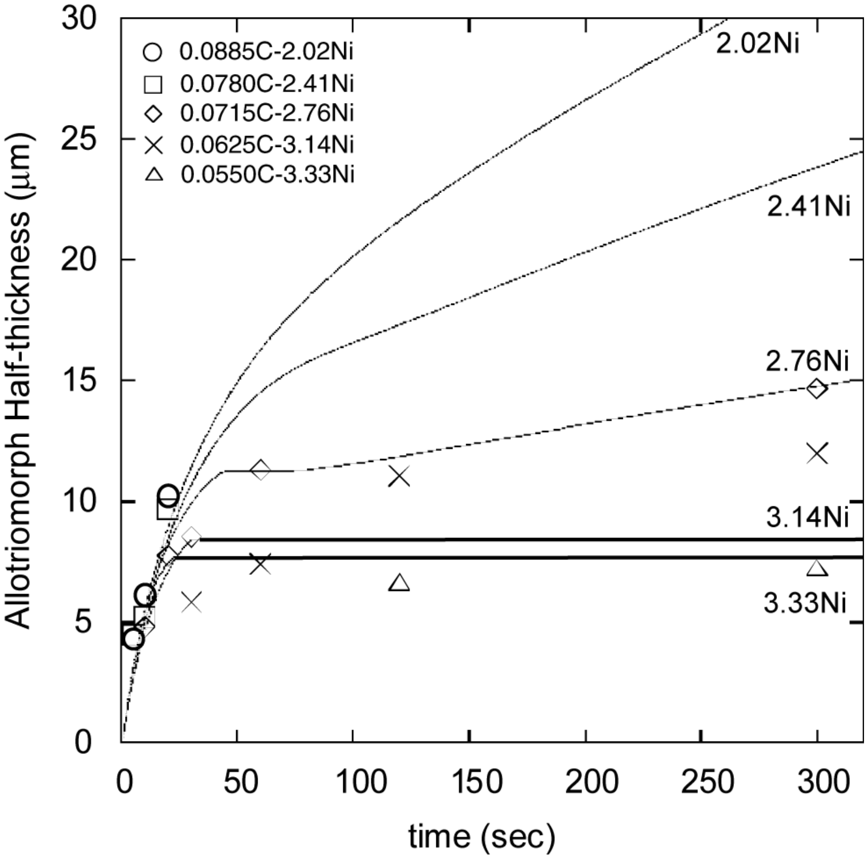

Solution of two force-velocity relations
δGmax/Vm
Pmax
Force
Resistance due to solute drag & intrinsic drag
Thermodynamic driving force
0
Velocity, v
Vmax

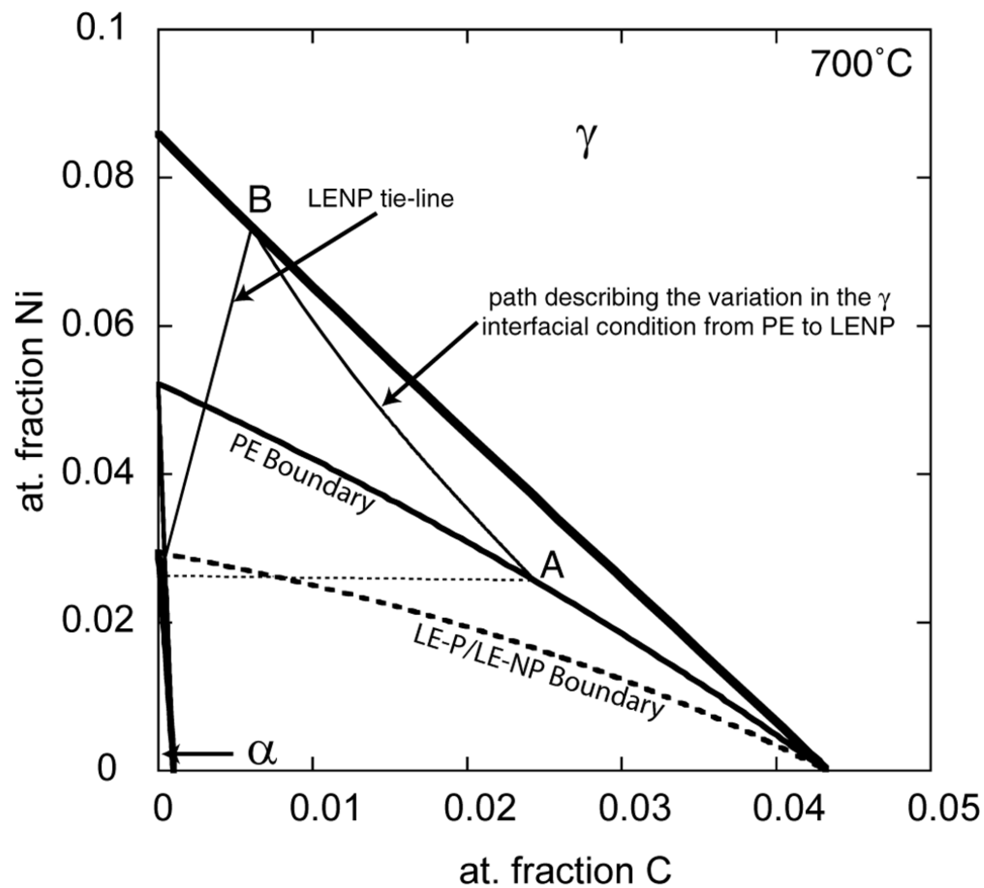

δGmax/Vm
Force
Vmax
Vmax
Vmax
0
Velocity, v



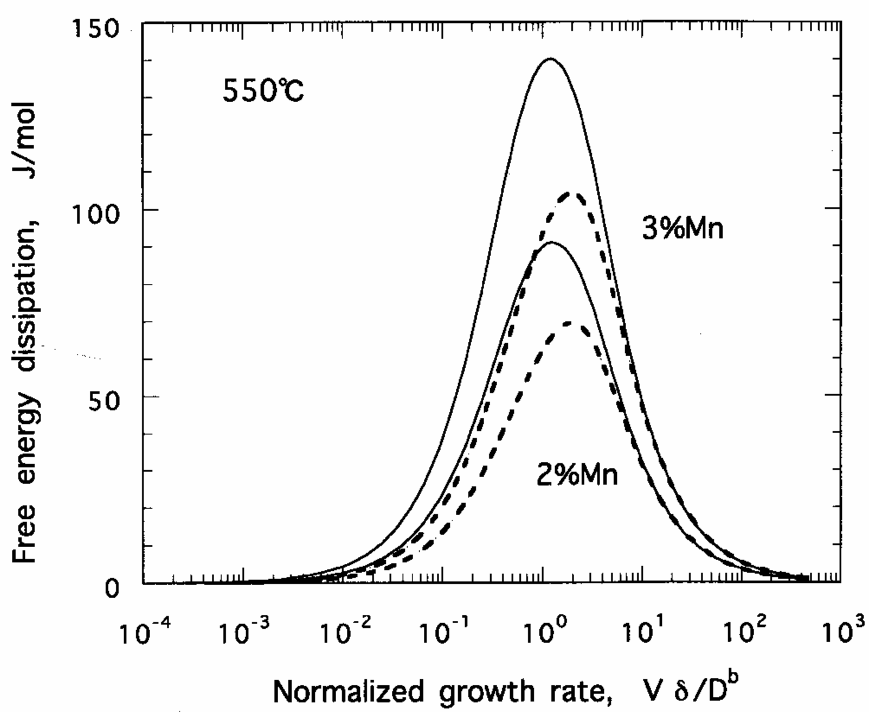


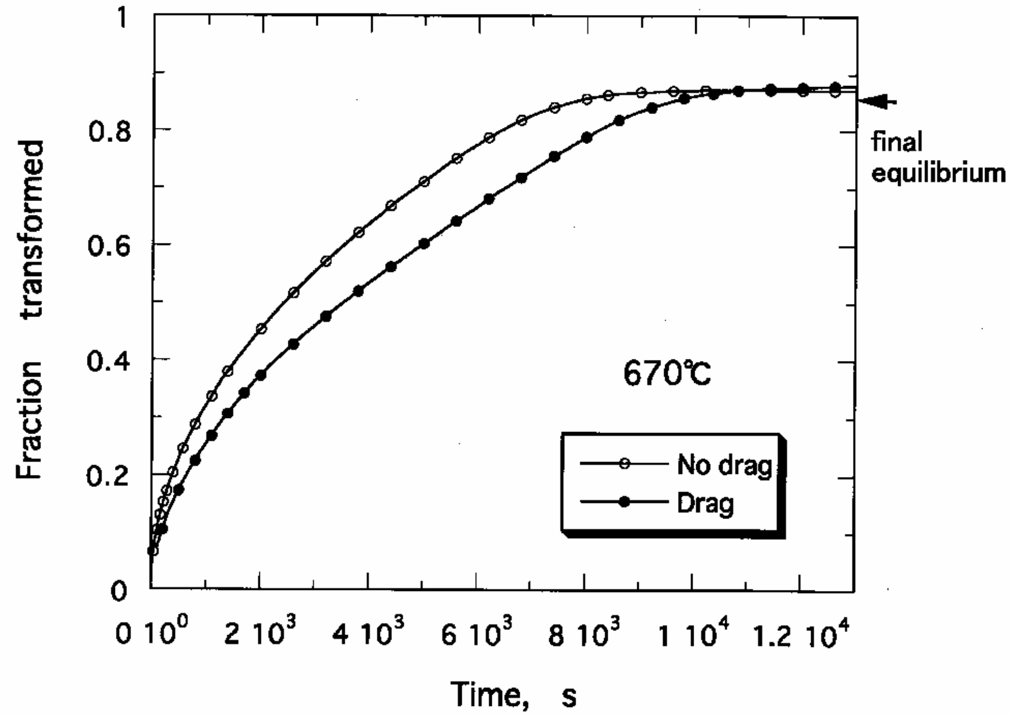
Odqvist et al, Acta Mat. 2002;50:3211





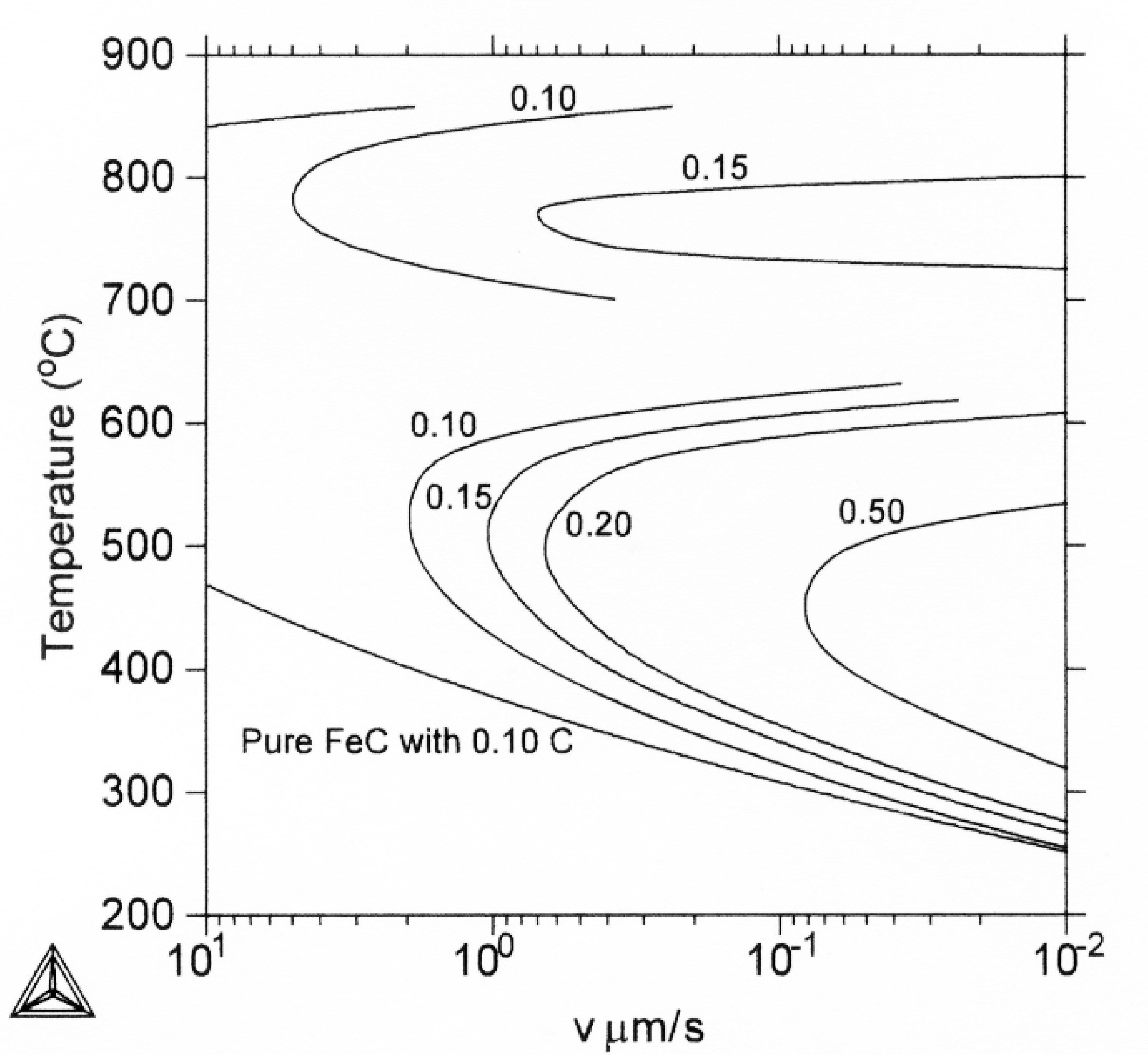
Hutchinson, Fuchsmann, and Brechet, MMTA 2004;39A:1211



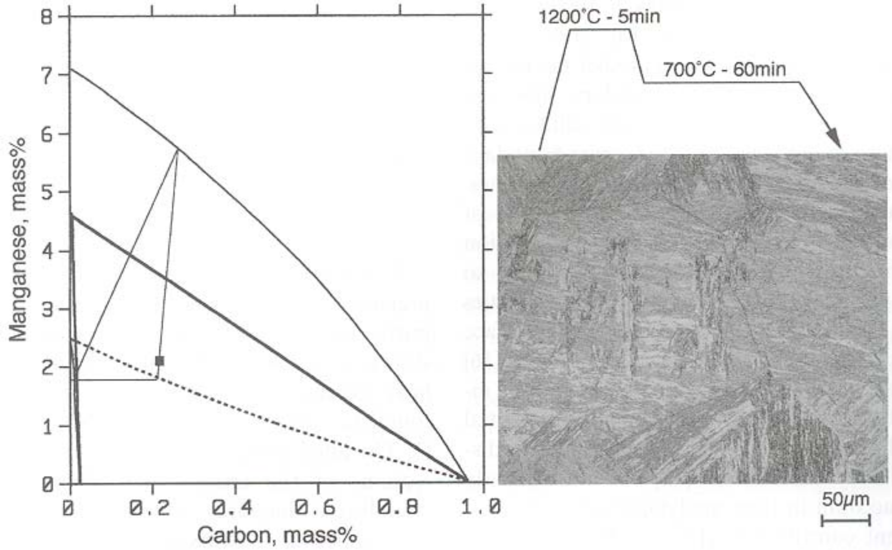


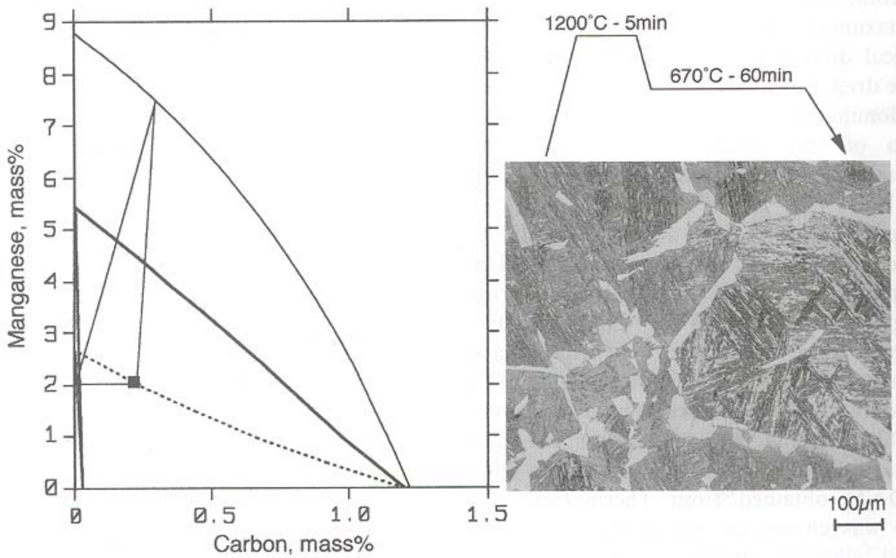
Fe-0.5at%C-2at%Mn at 550^{o}C

Enomoto: Austenite 2003



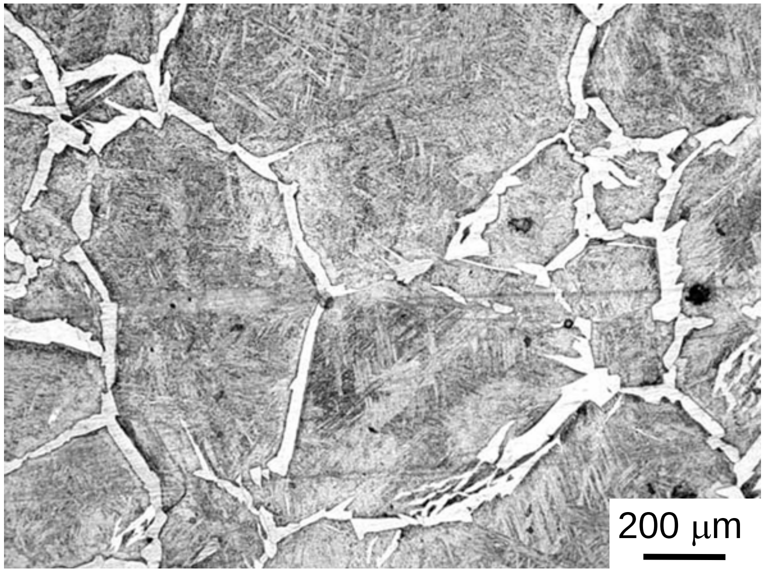
Hillert and Hoglund, Austenite 2003





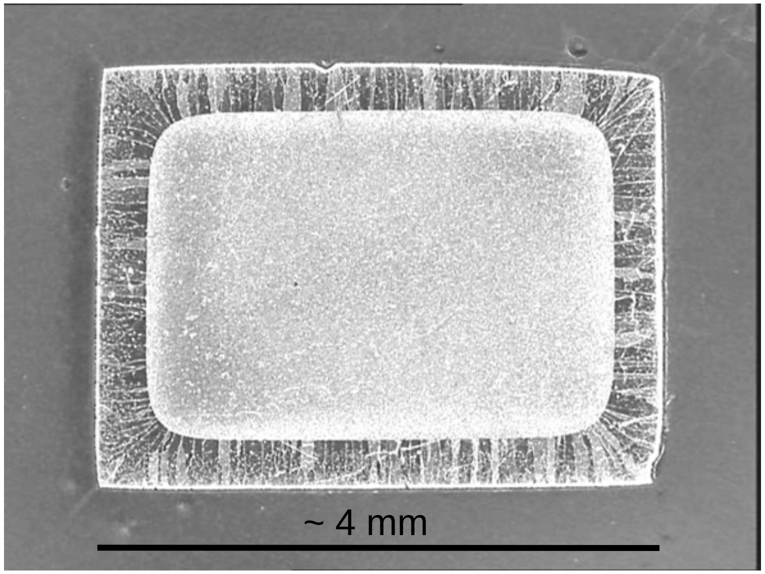
Oi, Lux, Purdy
Acta Mat., 48;2000;2147

traditional

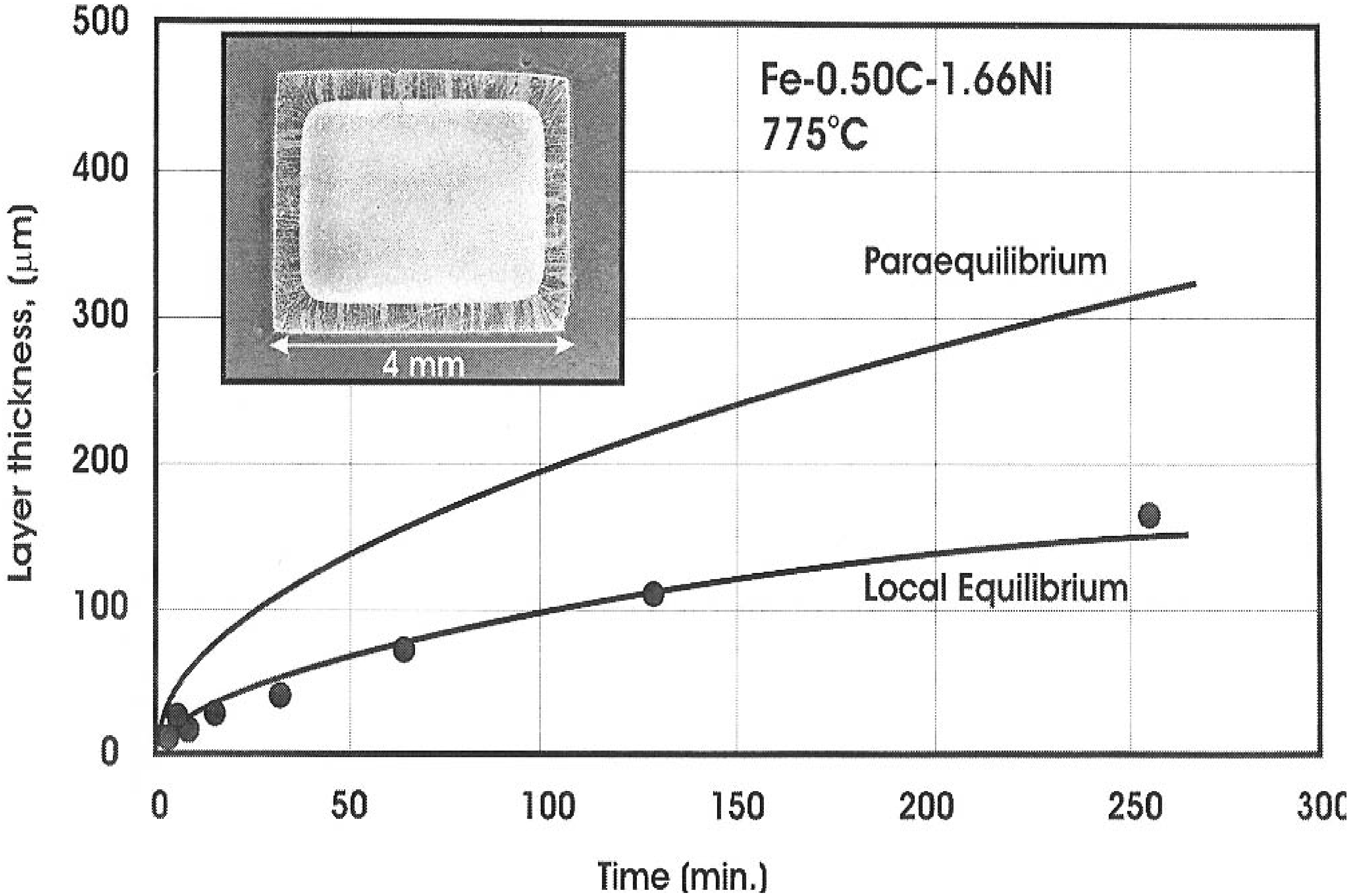


Fe-0.1C-0.1Mo; 800C 1min

decarburization



Fe-0.54C-0.51Mo; 825C 128min

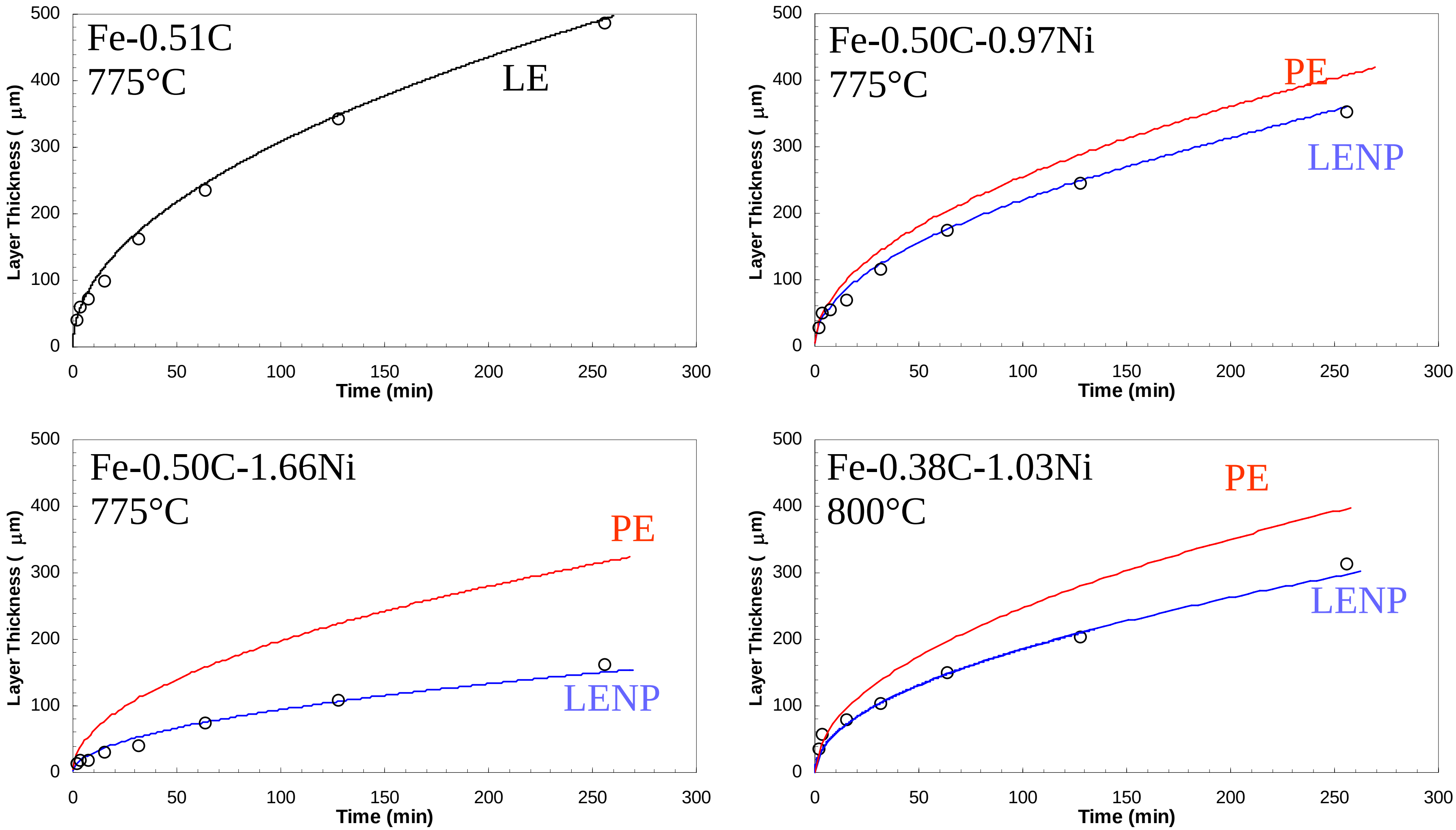


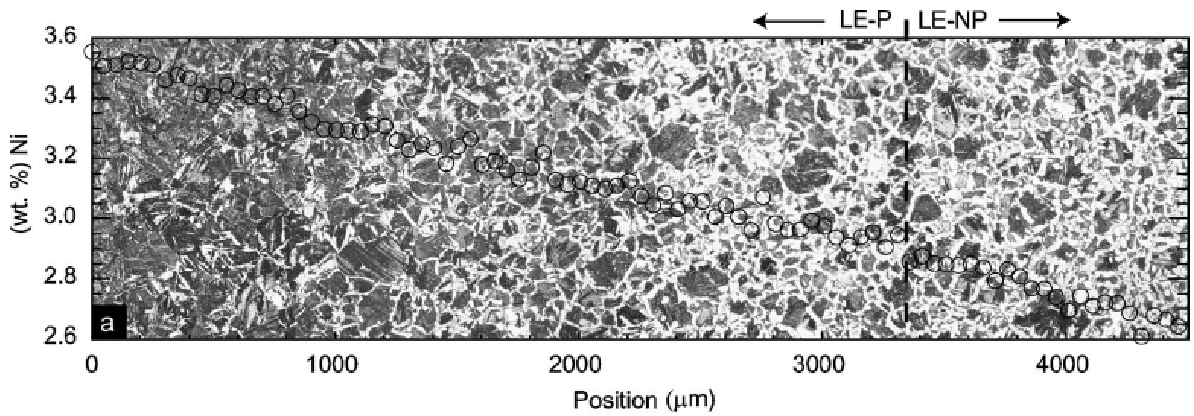
500
400
300
200
100
0
Layer thickness, (μm)
4 mm
Fe-0.50C-1.66Ni
775°C
Paraequilibrium
Local Equilibrium
0
50
100
150
200
250
300
Time (min.)

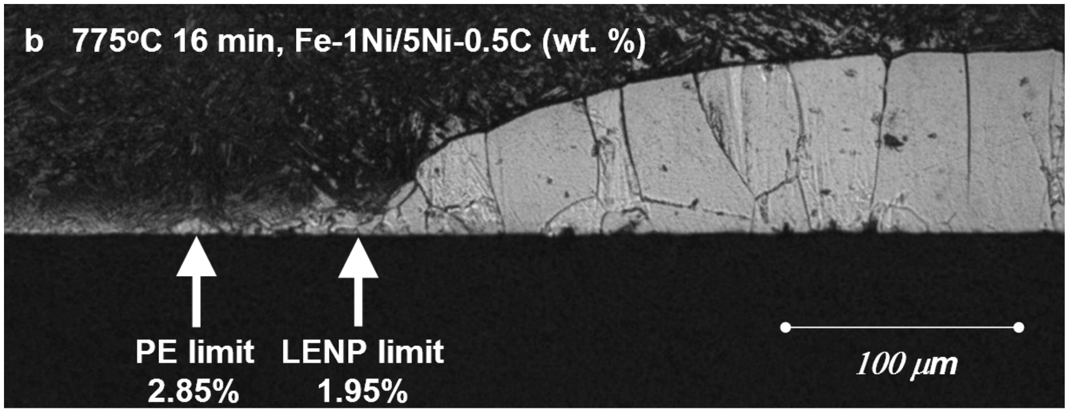
Fe-C-Ni Decarburization Experiments

McMaster University

Phillion, Zurob, Hutchinson, Guo, Malakhov, Nakano and Purdy, *Metall Trans.*, 35A, 1237-1242, 2004.



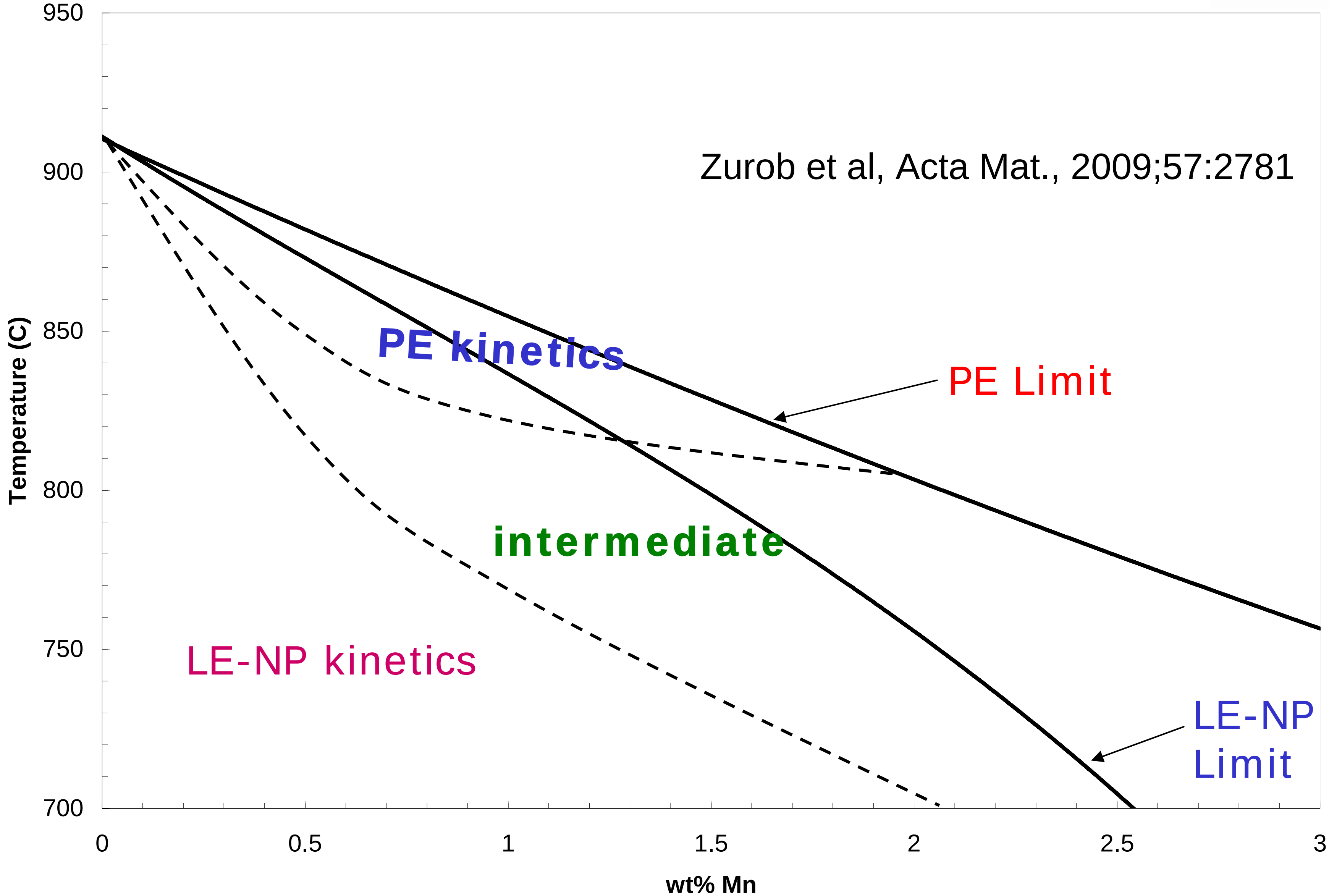




Precipitation, decarburization response to Ni gradients

Fe-C-Mn

McMaster University



Conclusions:

Recent experiments have brought to light a number of new and (perhaps) unexpected aspects of the behaviour of alloying elements at migrating transformation interfaces.

Further experiments are called for, with emphasis on the response of ternary systems (Fe-C-X) to isothermal transformation and decarburization conditions; at the same time, a parallel intensified modelling approach will be required for the deeper understanding of several unanswered (or partially unanswered) questions.

These studies may provide a new window on the nature of driven interfaces, especially in relation to the formation of ferrite from alloyed austenite, but also in relation to the massive transformation, CIGM etc. etc.

Outstanding:

Issues of long standing:

- Role of segregation, co-segregation (C, X), to the interface;
- Physical meaning of "the spike": to be revisited;
- Diffusion across (as opposed to along) the interphase interfaces;
- An improved model for "the bay";
- Application to bainite;
- Relevance of sharp-interface-derived concepts vs diffuse interface and continuum interface models.

Newer Questions:

- PE kinetics at high temperatures (and low temperatures?) in Fe-C-Mn, other systems(?);
- Differences in interface structure: decarburization layer, Widmanstatten, grain boundary allotriomorphs, (as related to kinetic response and segregation potential);

Notes on misuse of the term PE (e.g. CPE for martensite tempering), assumption of PE volume fractions of ferrite after some time (1 hour), *a priori* assumption of either PE or LE-NP in setting up a model, misapplication to intercritical annealing of dual phase, trip, twip etc. steels.

Applications to massive transformation, CIGM, recrystallization, grain growth.