DYNAMICS-BASED MICROSTRUCTURAL DESIGN IN MULTICOMPONENT ALLOYS

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Evanston, IL

Morral Symposium
TMS 2005 Annual Meeting, San Francisco
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MTL/SRG

A) Cybersteel 2020: Ultratough Plate Steels (ONR; CAT)
B) HT Carburizing Steels (DOE-OIT; GM, P&W)
C) Superalloys (AF-MEANS, DARPA-AIM; RMCI)
D) Bulk Metallic Glasses (DARPA-SAM)

GOVERNMENT

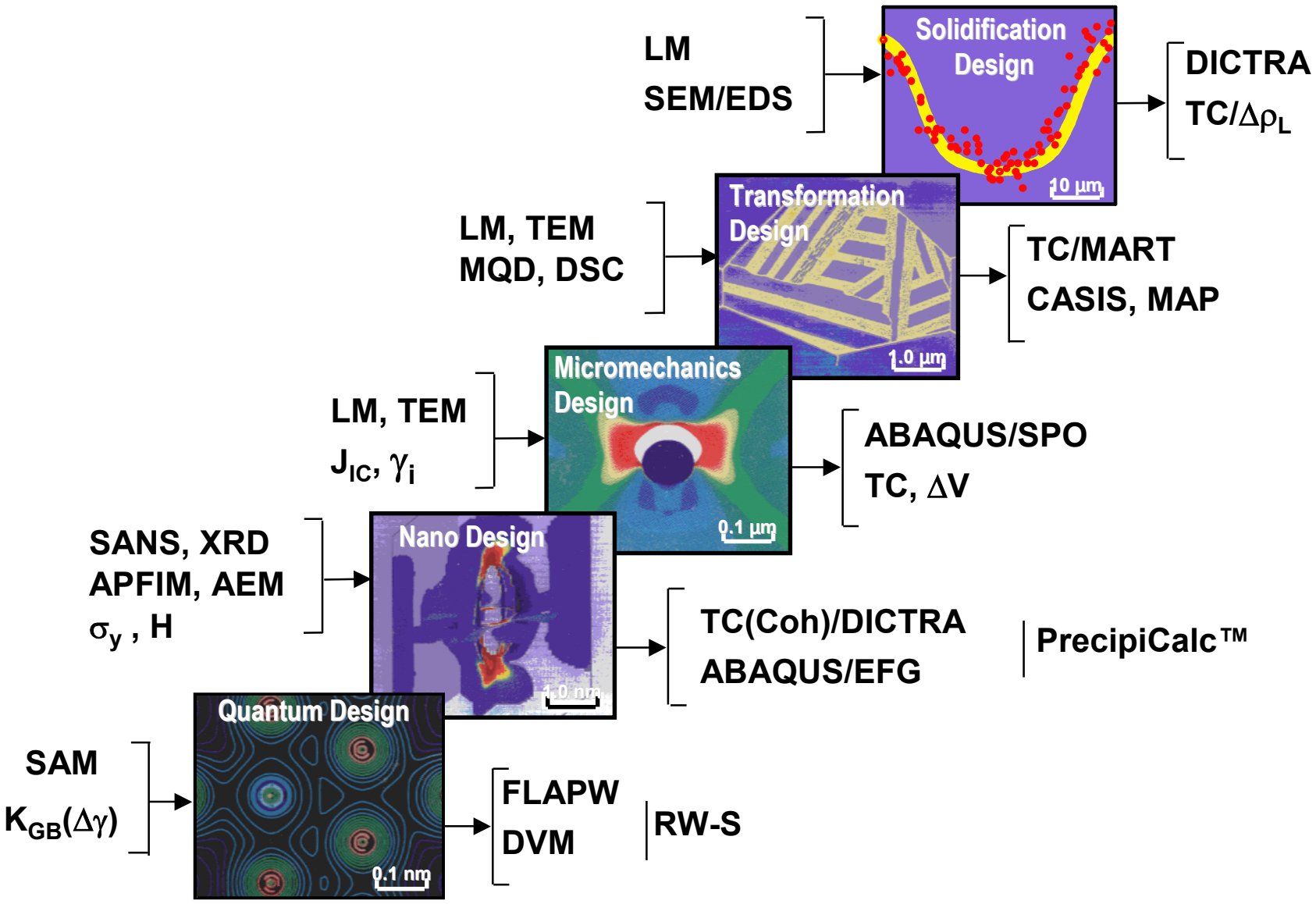
NAWC/AD	A
Lee	
ARL/WMD	B
Montgomery	
AFRL	C,D
Woodward	Miracle
CSM	C
Eberhart	
WISCONSIN-MAD	C,D
Perepezko	
MIT	D
Argon	Parks
IIT	D
Nash	
VIRGINIA	D
Poon	Shiflet

UNIVERSITY

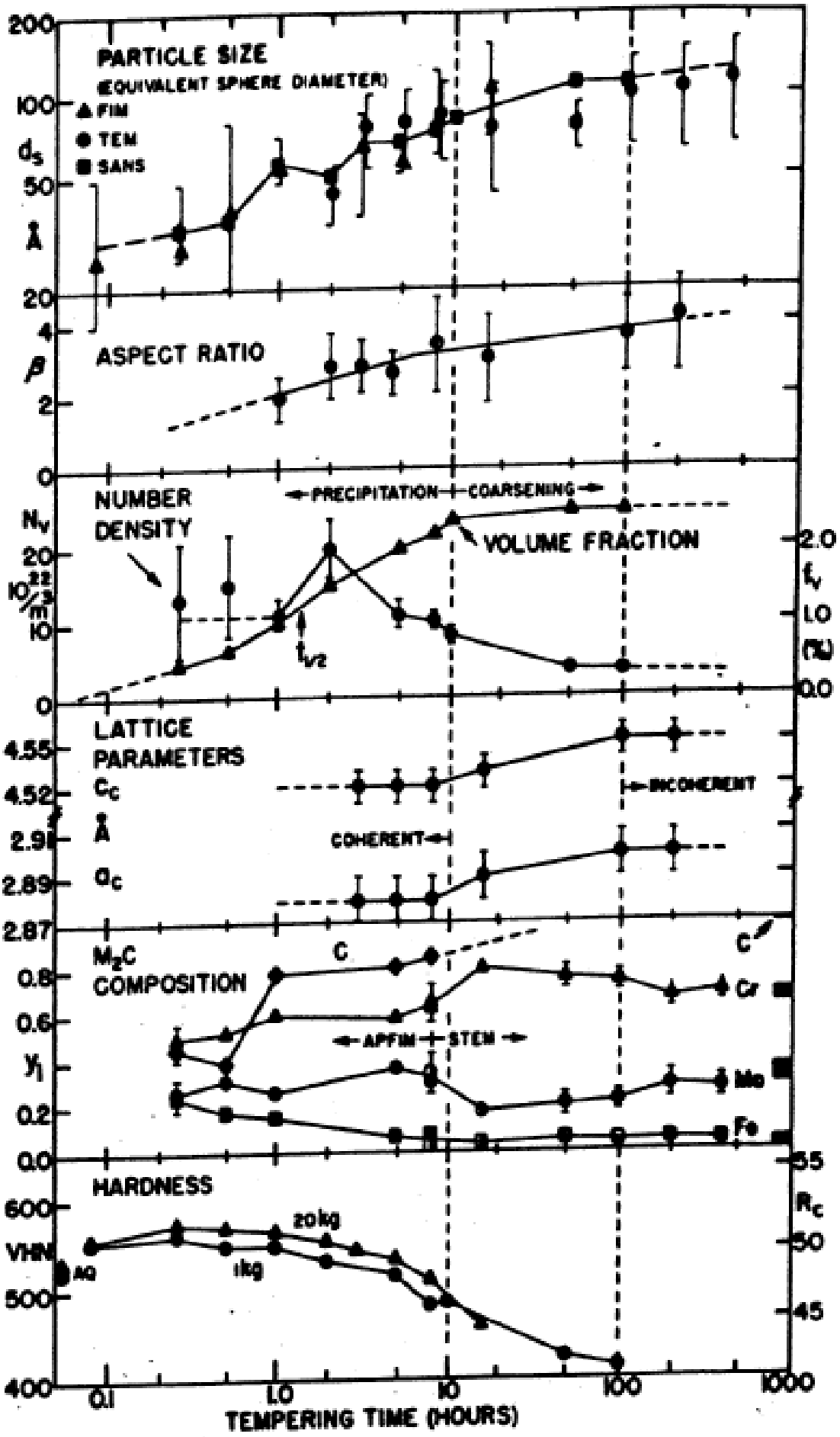
NORTHWESTERN	A,B,C,D
Olson	Freeman
Ankenman	Ghosh
Asta	Ishaim
Brinson	Liu
Dunand	Moran
Fine	Voorhees
High Resolution Microanalysis	
WPI/CHTE	B
Apelian	
PURDUE-CALUMET	B
Abramowitz	
DREXEL	C
Doherty	
KTH (Stockholm)	C
Agren	Sundman
LEHIGH	C
Harlow	
OHIO STATE	C
Fraser	Mills

INDUSTRY

QUESTEK	A,B,C,D
Kuehmann	Qiu Tang
Huang	Rathbun Tufts
Jou	Scharer Wright
CATERPILLAR	A,B
Chen	Johnson
Hsieh	Yang
ALLVAC STEEL	A,B
Lippard	Stevenson
INLAND STEEL	A
Bhattacharya	
GM	B
Mishra	Sachdev
PRATT & WHITNEY	B,C,D
Fowler	Schirra
REFERENCE METALS	C
Carneiro	
HOWMET	D
Wolter	Wright
BOEING	D
Bowden	


LM
SEM/EDS
Solidification Design
10 μm
DICTRA
TC/Δρ_L
LM, TEM
MQD, DSC
Transformation Design
1.0 μm
TC/MART
CASIS, MAP
LM, TEM
J_IC, γ_i
Micromechanics Design
0.1 μm
ABAQUS/SPO
TC, ΔV
SANS, XRD
APFIM, AEM
σ_y , H
Nano Design
1.0 nm
TC(Coh)/DICTRA
ABAQUS/EFG
PrecipiCalc™
SAM
K_GB(Δγ)
Quantum Design
0.1 nm
FLAPW
DVM
RW-S

M_2C Precipitation Strengthening: AF1410



Multicomponent Coarsening Rate Constant

S. Bjorklund, L.F. Donaghey, & M. Hillert (1972)

H.M. Lee, S.M. Allen, & M. Grujicic (1991)

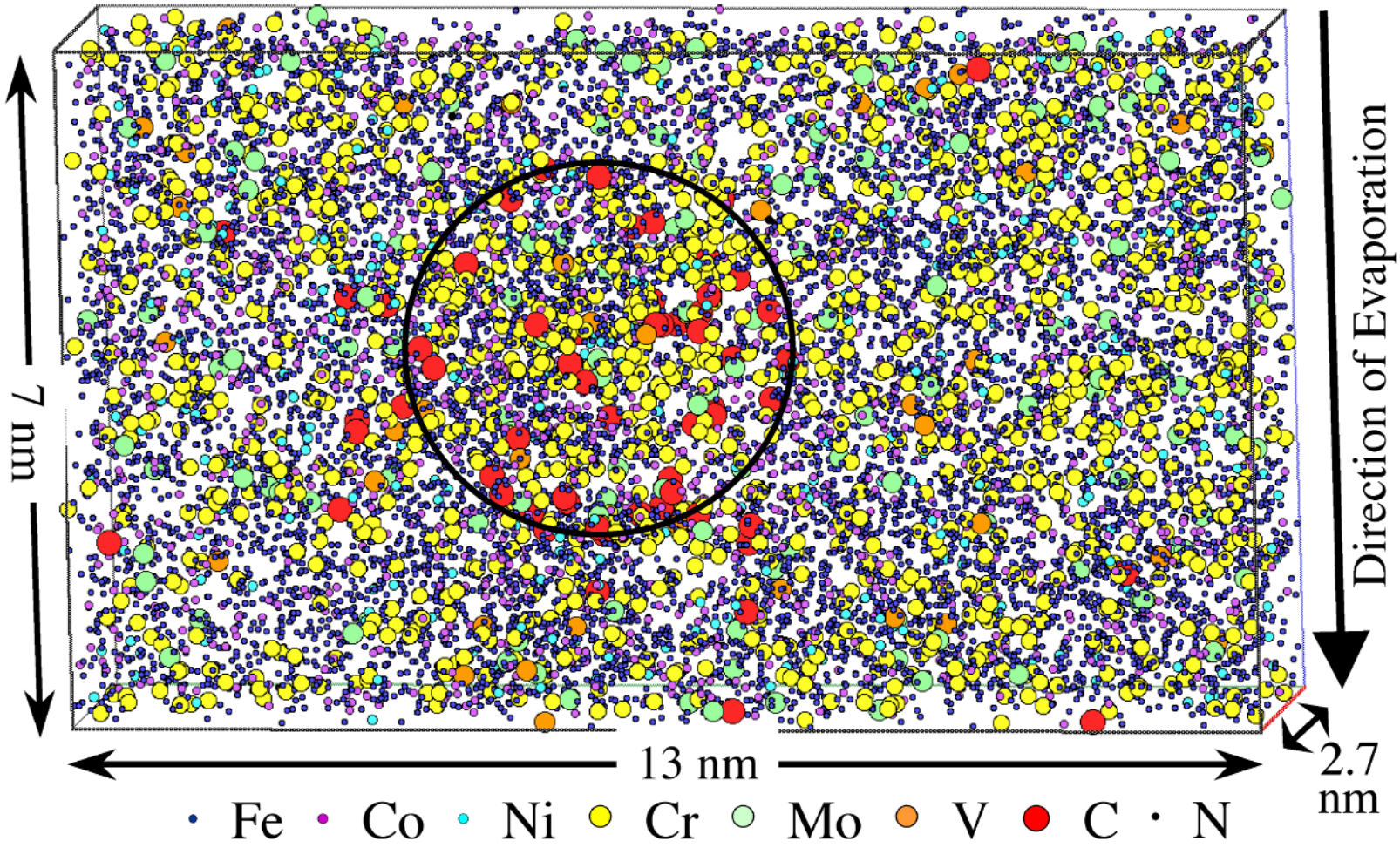
A. Umantsev & G.B. Olson (1993)

C.J. Kuehmann & P.W. Voorhees (1996)

J.E. Morral & G.R. Purdy (1994, 1995)

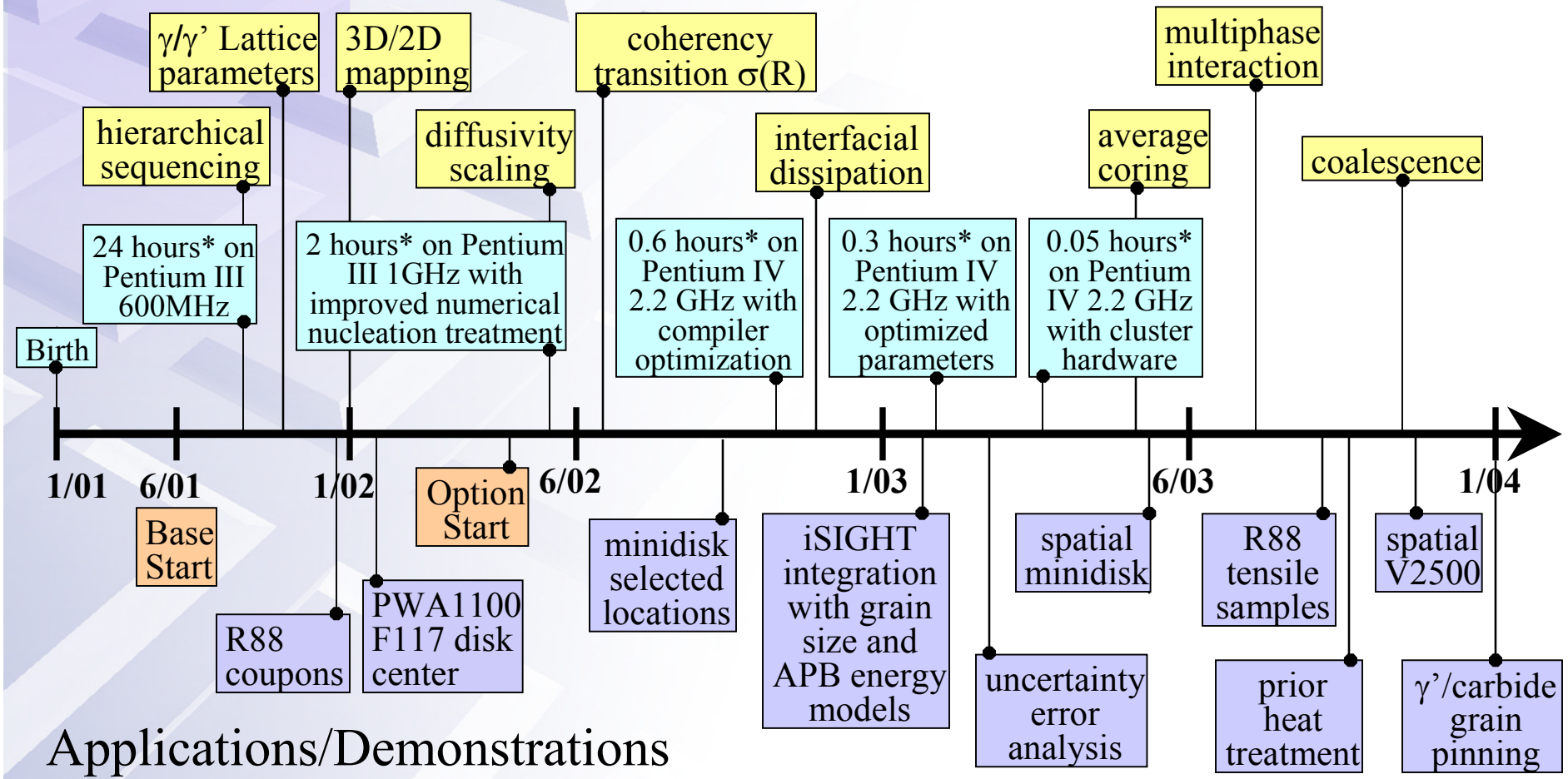
Å Gustafson, L. Höglund, & J. Agren (1998)

NANOTECHNOLOGY NOW



PrecipiCalc™ Timeline

Software/Hardware Improvement



Applications/Demonstrations

* single IN100 PWA1100 simulation

Basic *PrecipiCalc* Equations (2) — Particle Growth

$$\text{Growth}: \frac{dR}{dt} = \frac{\left(1 + R\sqrt{4\pi N_v \langle R \rangle}\right)}{\left(R\Gamma + s(R)\Big/\left(M_0 \exp\frac{-Q}{RT}\right)\right)} \left\{ \Delta G_m - \frac{2\sigma(R)\overline{V}_m^{\beta}}{R} \right\}$$

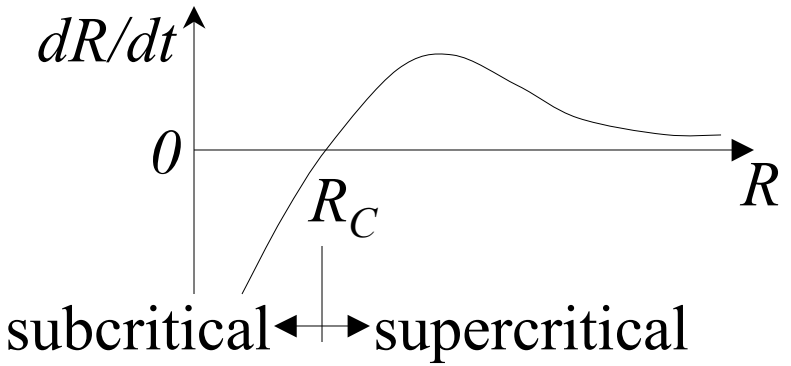
$$\text{where } \Delta G_m = \left[\overline{\Delta C_i}\right]^T \left[\frac{\partial^2 \overline{G}^{\alpha}}{\partial C_i \partial C_j}\right] \left[\Delta C_j^{\infty}\right] + \left[\overline{C}_m^{\beta}\right] \bullet \left(\left[\overline{\mu}_m^{\alpha}\right] - \left[\overline{\mu}_m^{\beta}\right]\right)$$

$$\Gamma = \left[\overline{\Delta C_i}\right]^T \left[\frac{\partial^2 \overline{G}^{\alpha}}{\partial C_i \partial C_j}\right] \left[\overline{D}_{jk}\right]^{-1} \left[\Delta C_k^{e}\right]$$

Thermodynamics

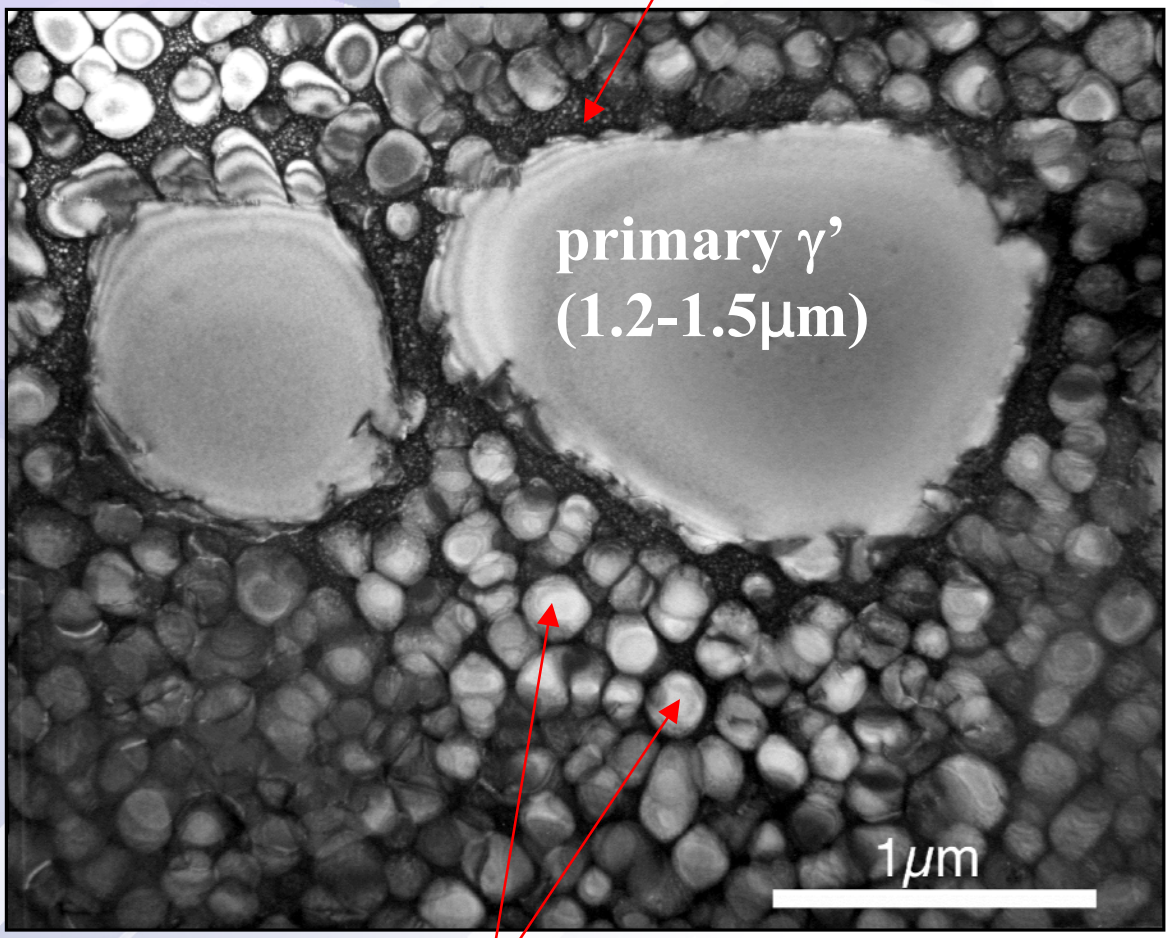
Diffusivity

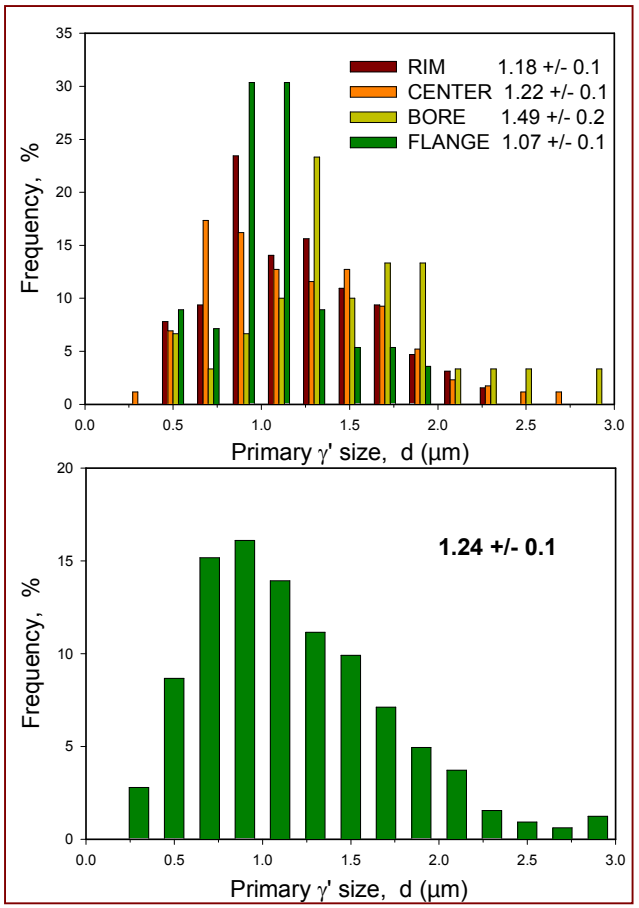
Interfacial Property



γ/γ' Microstructure (1)

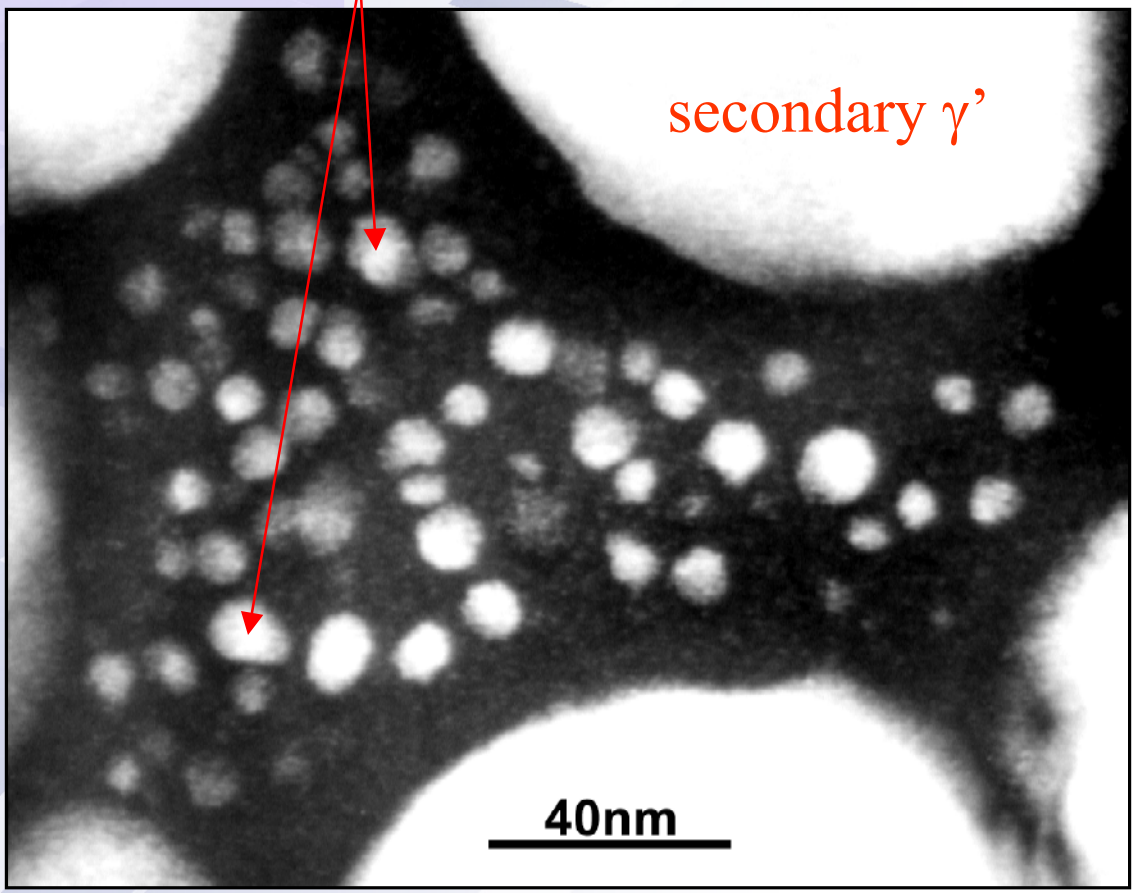
tertiary γ' (10-20nm)

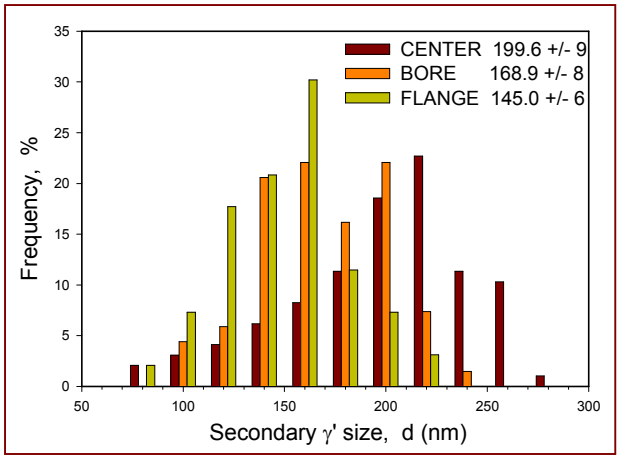


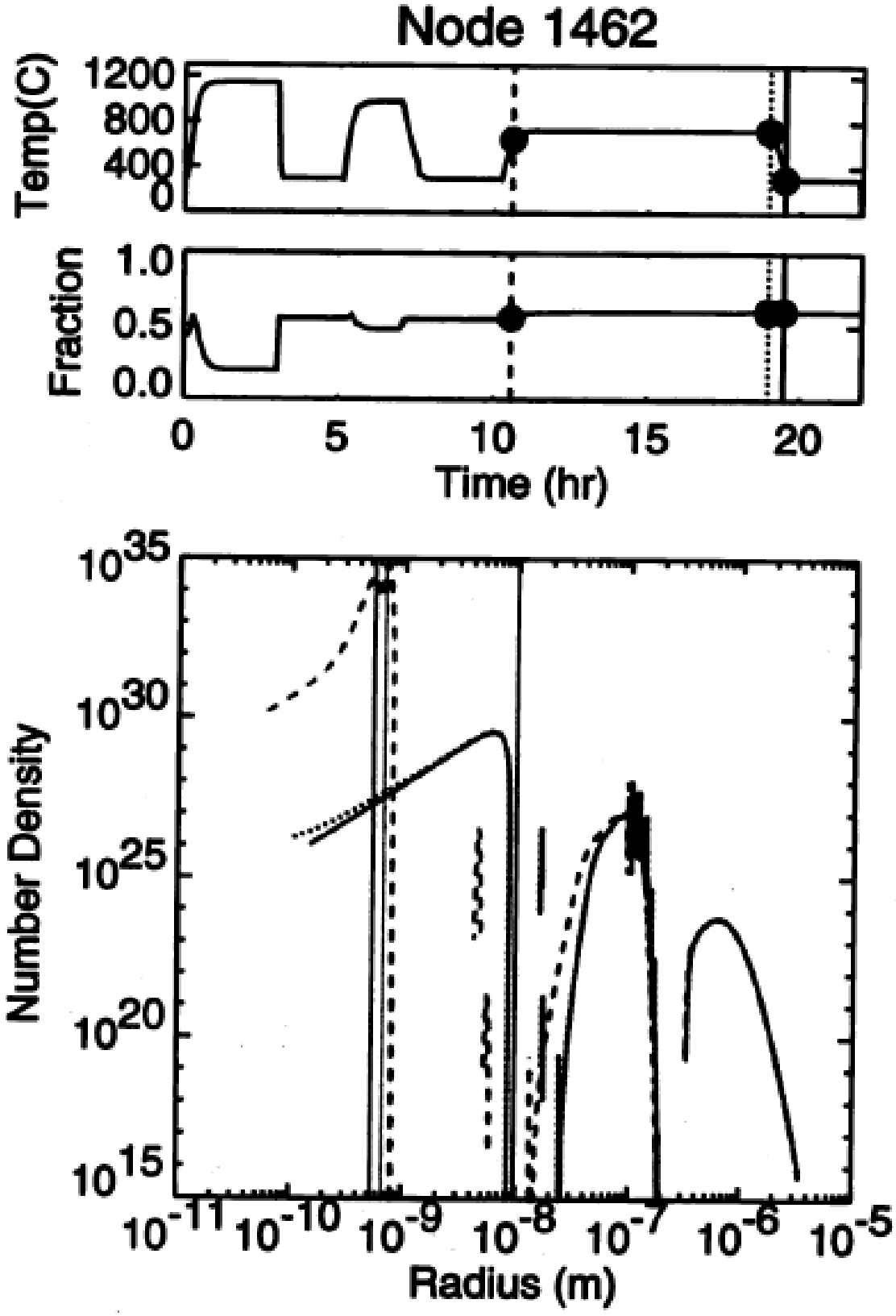


secondary γ' (110-200nm)

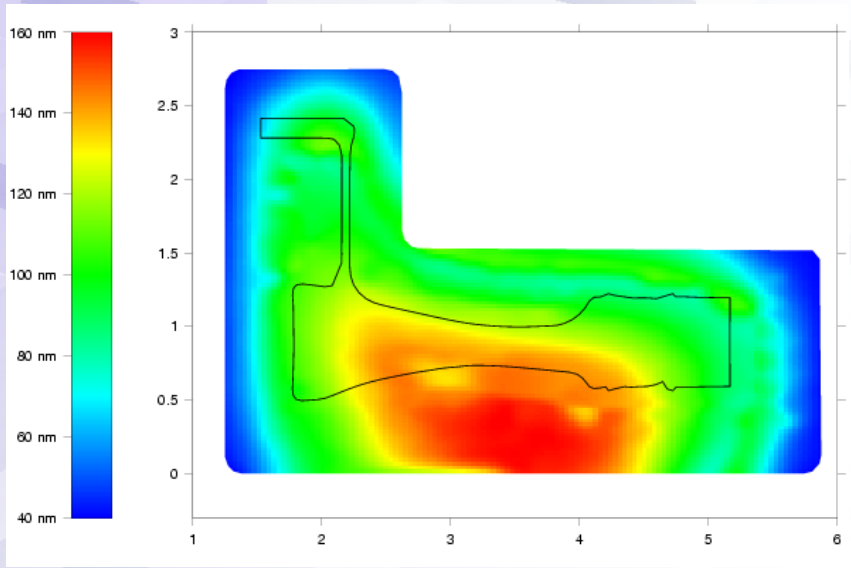
γ/γ' Microstructure (2)

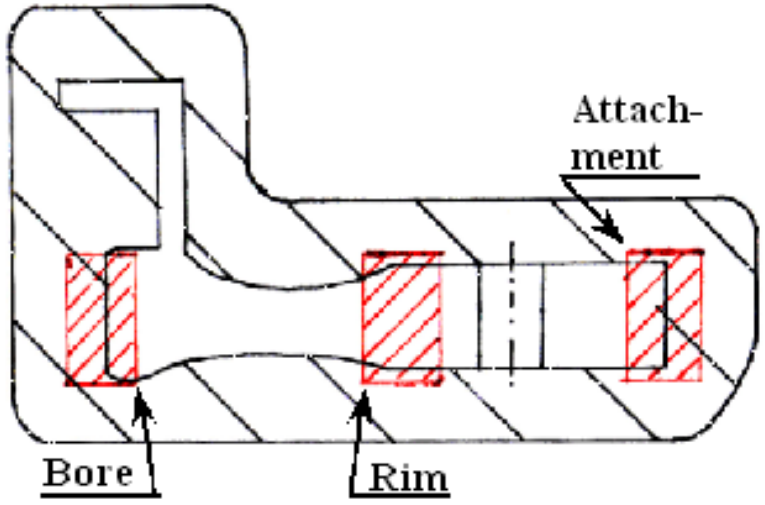





Node 1462
Temp(C)
1200
800
400
0
Fraction
1.0
0.5
0.0
0
5
10
15
20
Time (hr)
Number Density
10^{35}
10^{30}
10^{25}
10^{20}
10^{15}
10^{-11}
10^{-10}
10^{-9}
10^{-8}
10^{-7}
10^{-6}
10^{-5}
Radius (m)

Minidisk Microstructure Prediction with *PrecipiCalc*

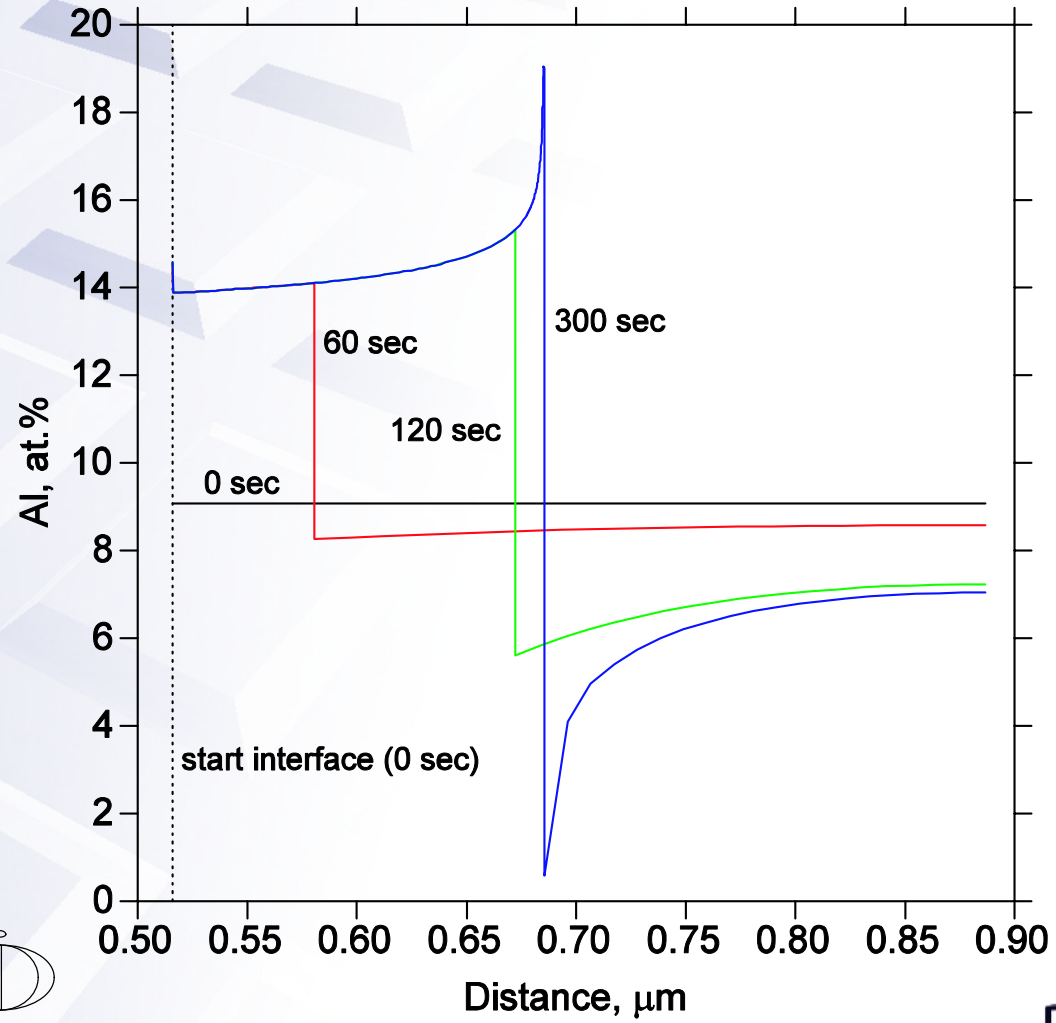




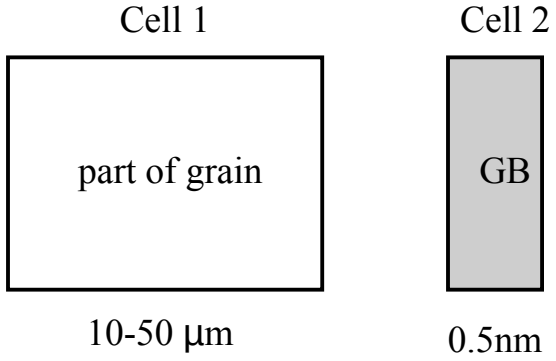
Minidisk Comparison		Bore		Rim		Attachment	
		Exp.	PpC	Exp.	PpC	Exp.	PpC
Primary γ'	Fraction (%)	24 25.2	22.6	23.5 25	23.5	23.1 25.7	23.3
	Size (μm)	1.28	1.29	1.23 1.27	1.32	1.18 1.2	1.31
Secondary γ	Fraction (%)	32.4	35		34		34.6
	Size (nm)	109 129	107.9	132 157	120 135 146	103 114	84.2
Tertiary γ'	Size (nm)	18 20.8	21.5	19.7 21.8	21.4	21.4	20.7

DICTRA Composition Profiles

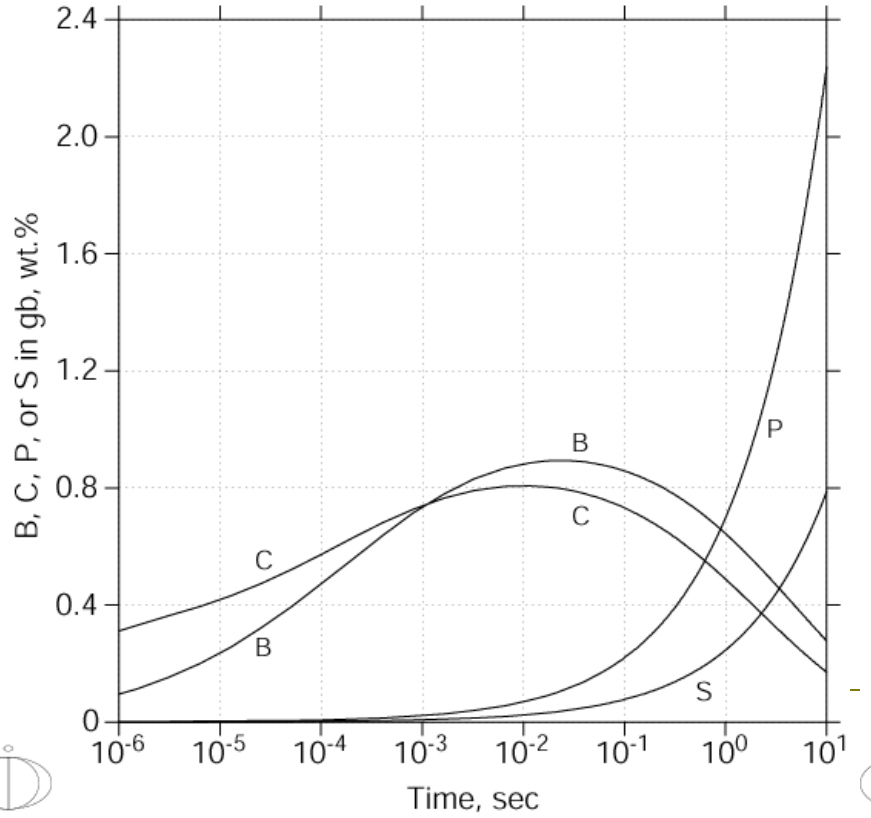
DICTRA Simulation: Al-profiles during γ' growth at node 1462



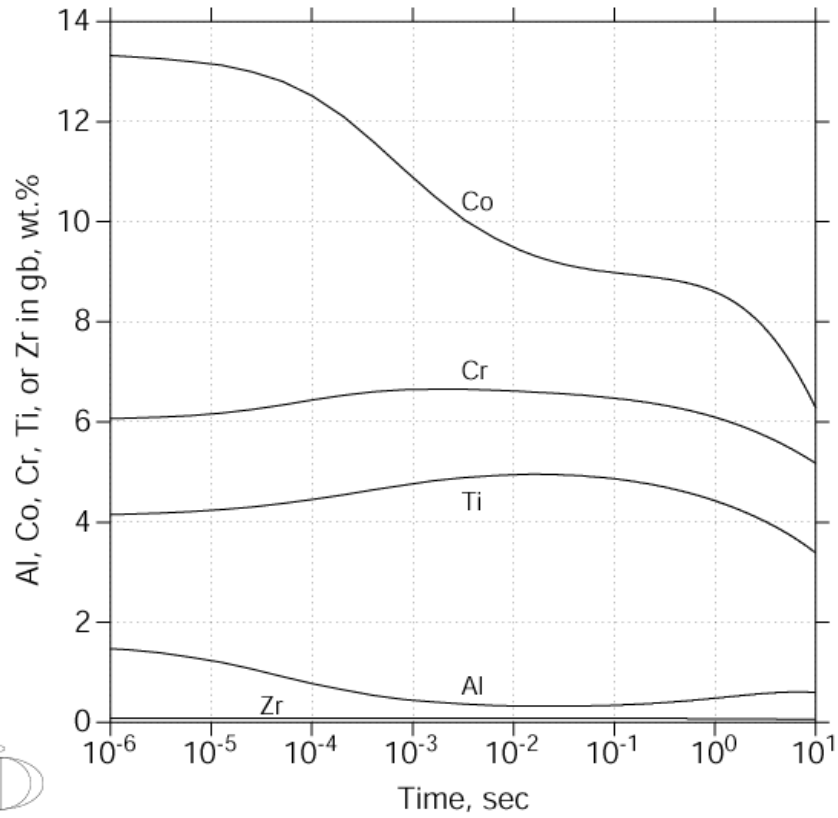
2-Cell Simulation of GB Segregation in DICTRA

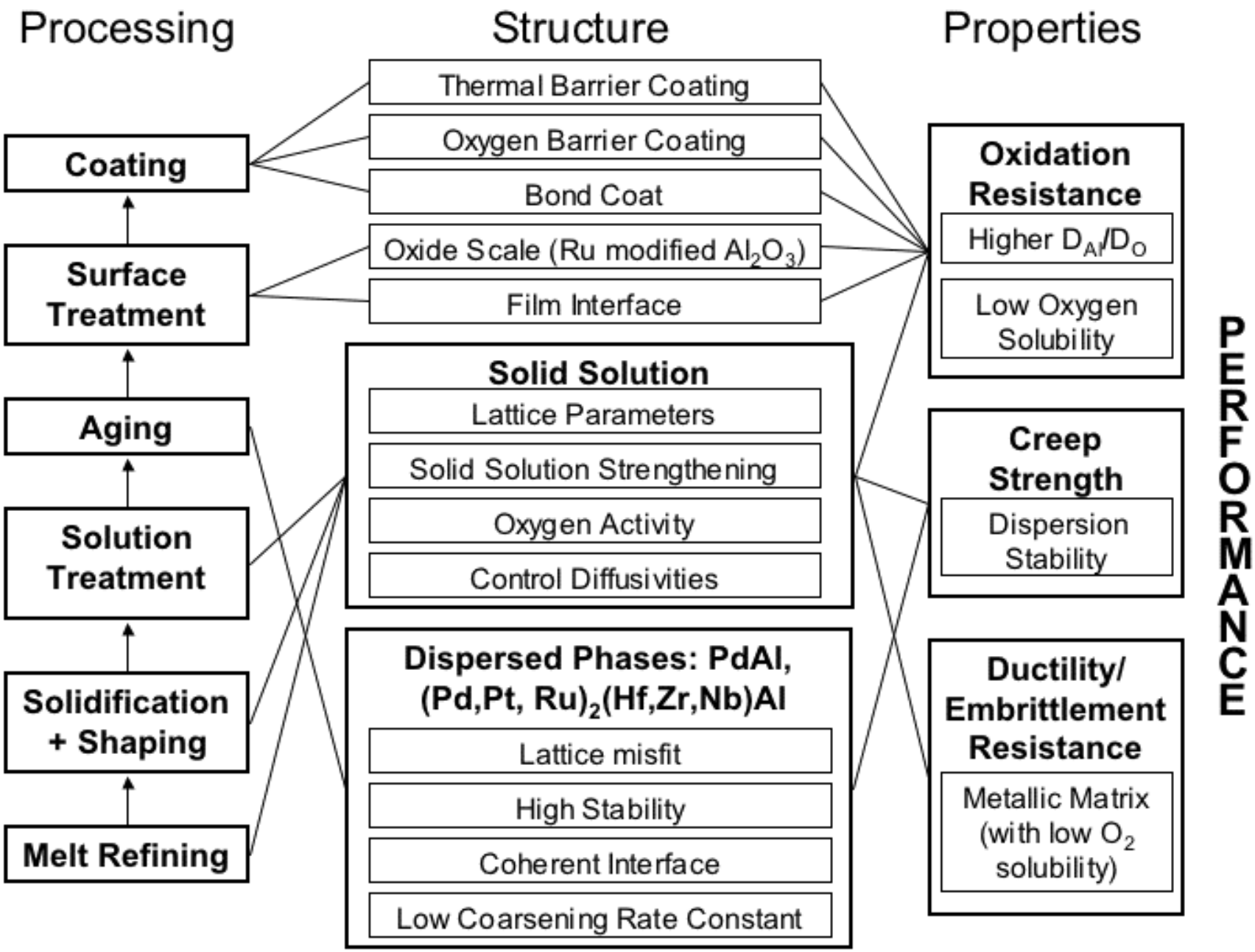


B, C, P, and S inside GB

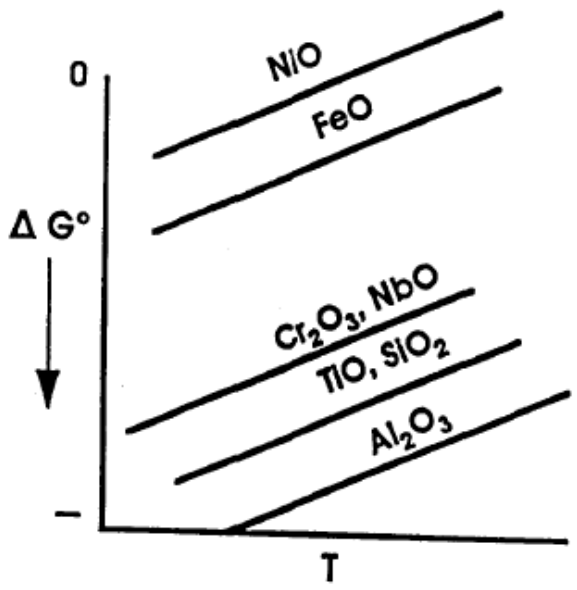


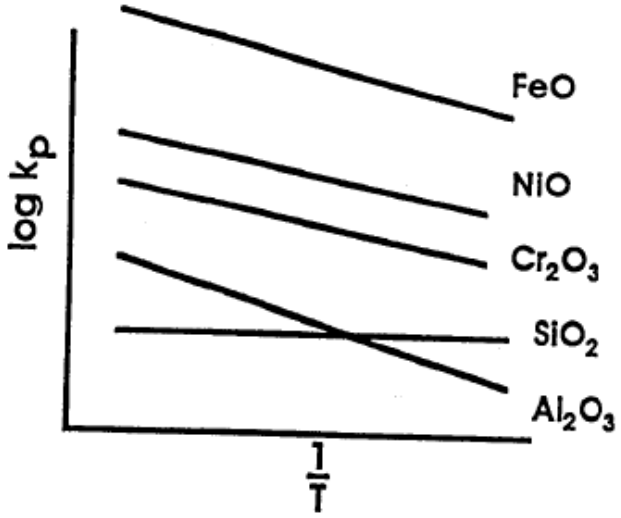
Co, Cr, Ti, Al, Zr inside GB

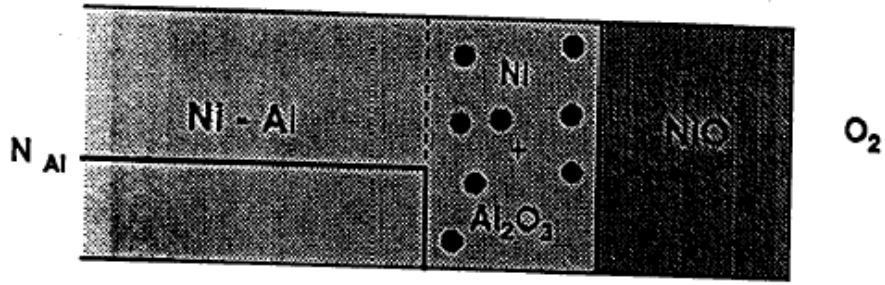



Processing
Structure
Properties
Coating
Surface Treatment
Aging
Solution Treatment
Solidification + Shaping
Melt Refining
Thermal Barrier Coating
Oxygen Barrier Coating
Bond Coat
Oxide Scale (Ru modified Al_2O_3)
Film Interface
Solid Solution
Lattice Parameters
Solid Solution Strengthening
Oxygen Activity
Control Diffusivities
Dispersed Phases: PdAl, $(Pd,Pt,Ru)_2(Hf,Zr,Nb)Al$
Lattice misfit
High Stability
Coherent Interface
Low Coarsening Rate Constant
Oxidation Resistance
Higher D_{Al}/D_O
Low Oxygen Solubility
Creep Strength
Dispersion Stability
Ductility/ Embrittlement Resistance
Metallic Matrix (with low O_2 solubility)
PERFORMANCE

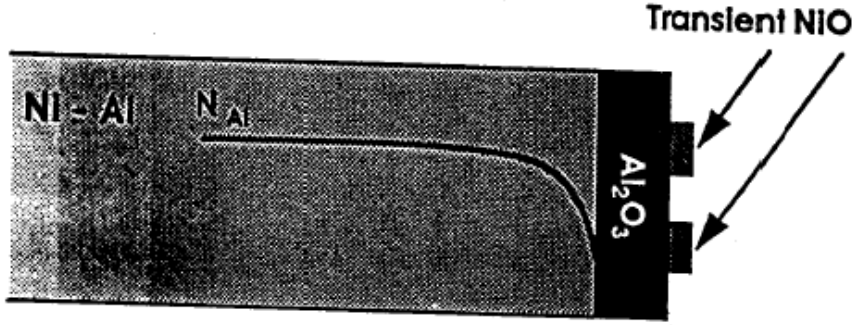
Selective Oxidation





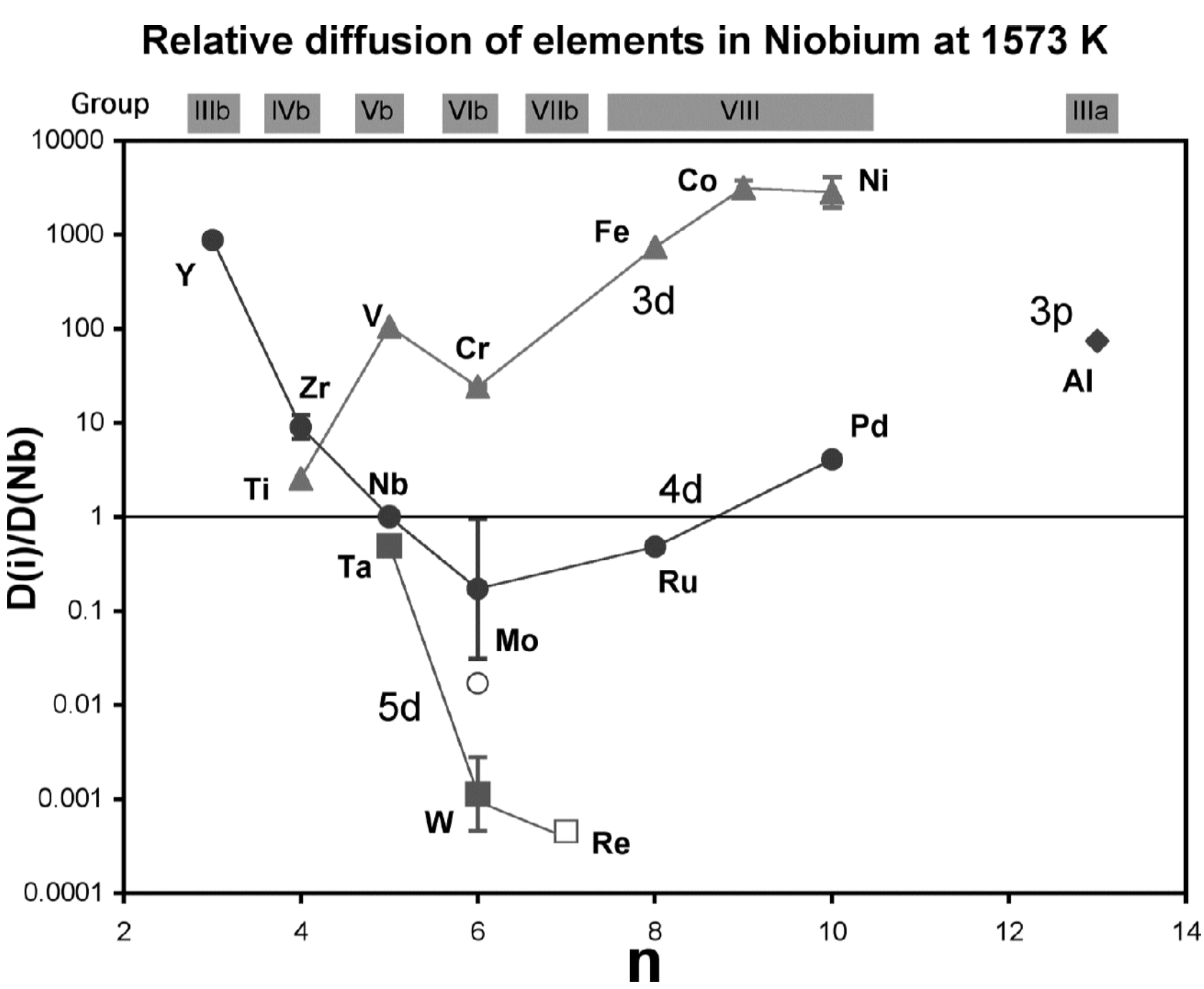


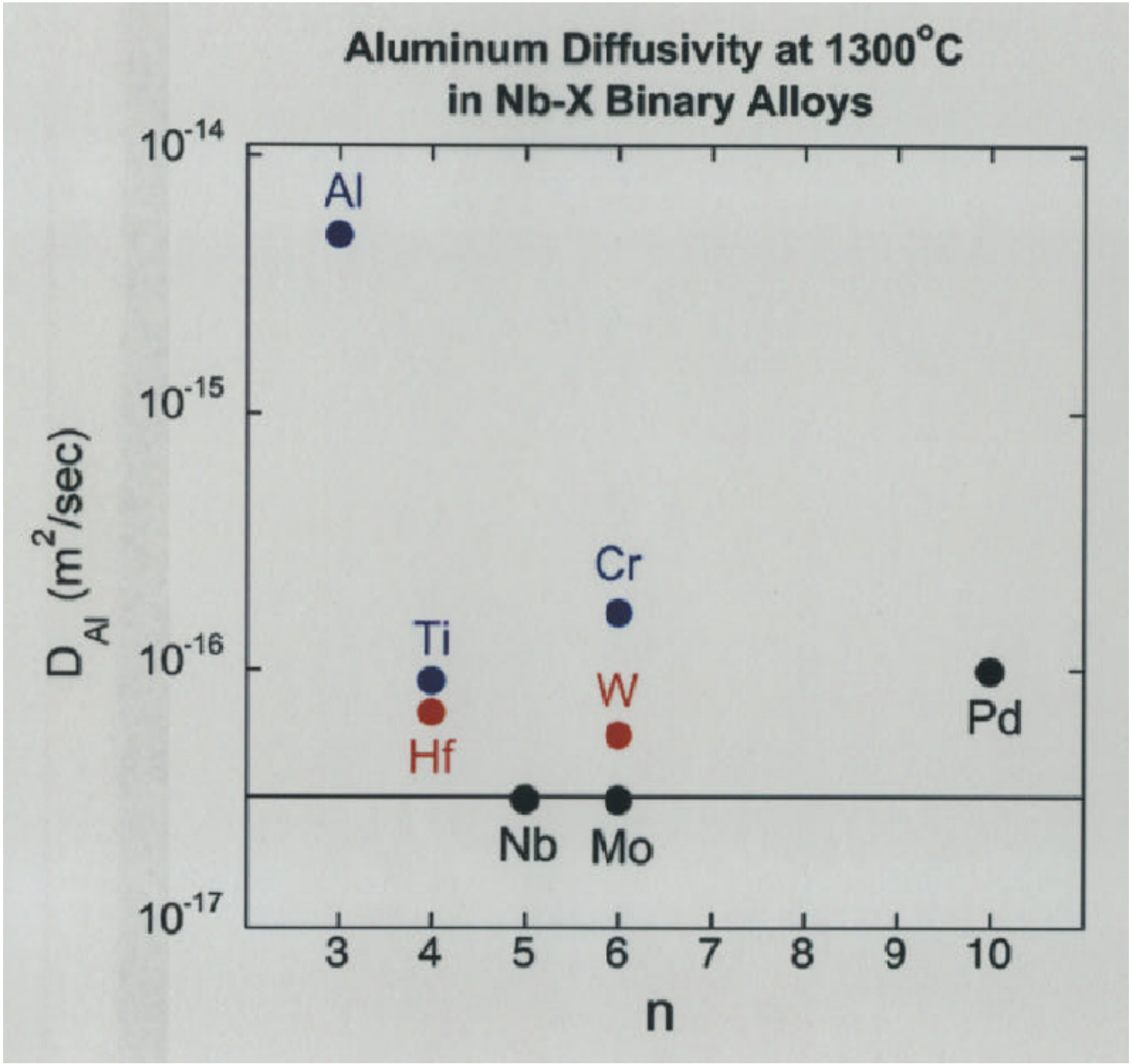
$$N_{Al}^{Crit} = A\left(\frac{N_O^{(S)} D_O}{D_{Al}}\right)^{1/2}$$

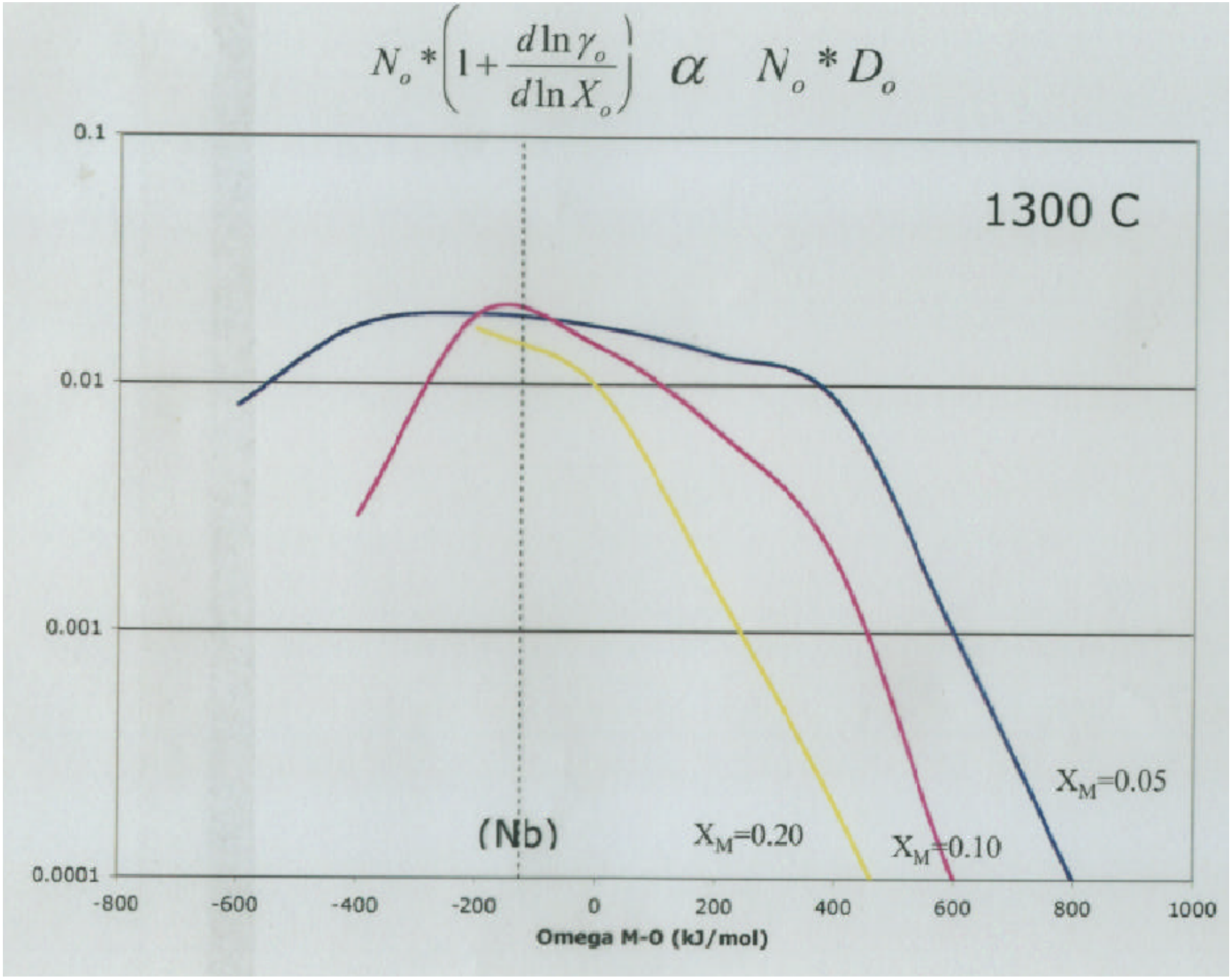


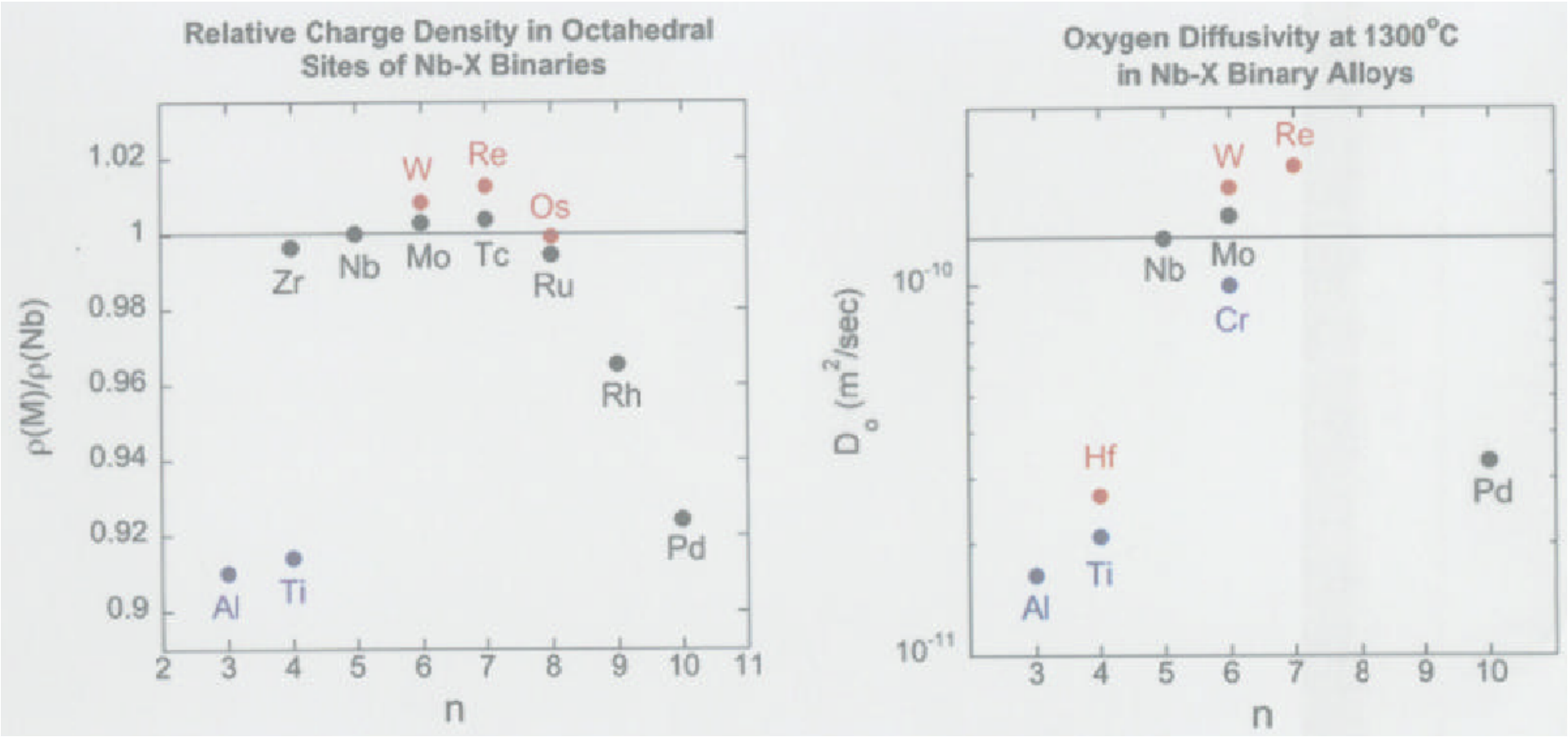
$$N_{Al}^{Growth} = B\left(\frac{k_p}{D_{Al}}\right)^{1/2}$$

$N_{Al}^{Crit} \uparrow$ as $k_p^{\text{Transient oxide}} \uparrow$

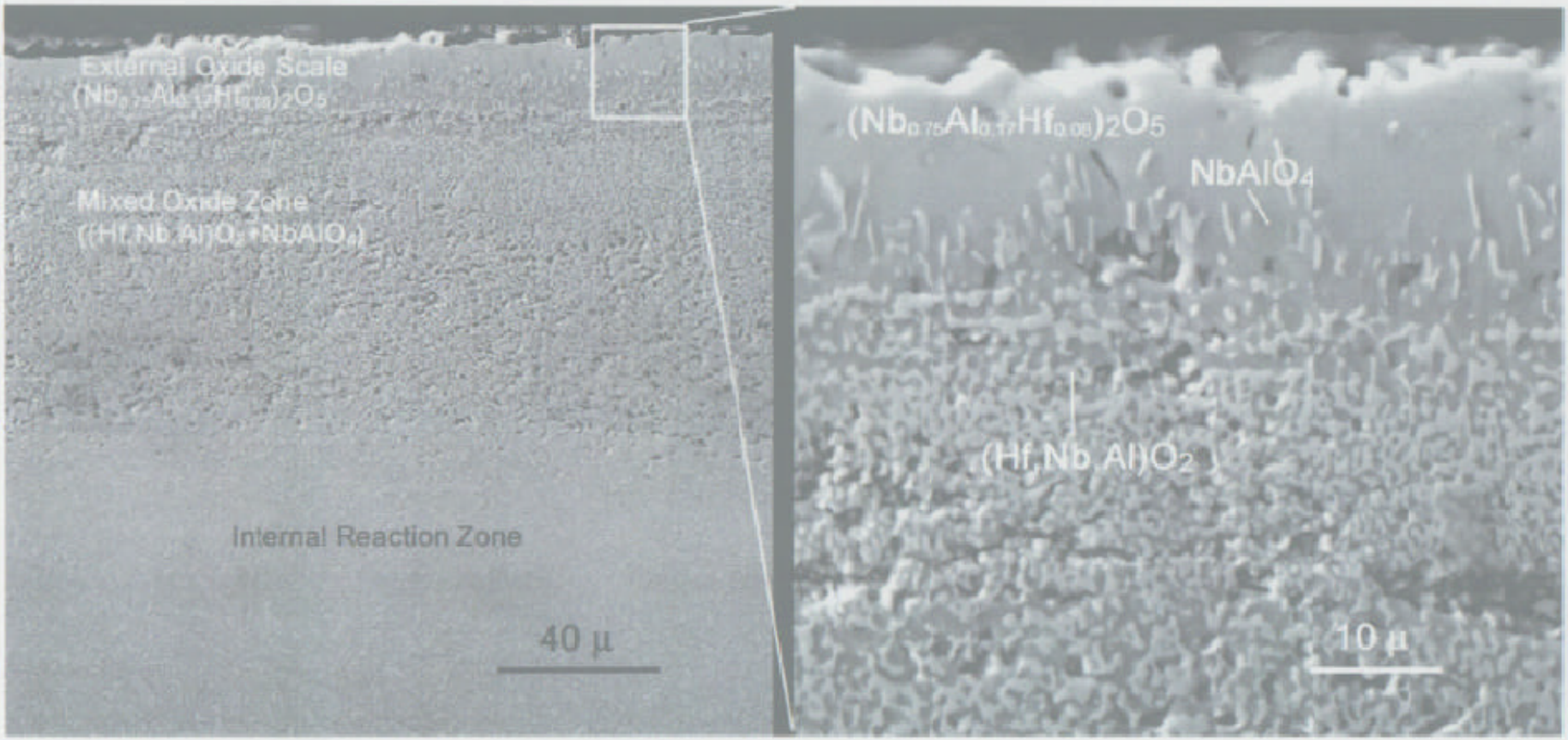

Relative diffusion of elements in Niobium at 1573 K
Group
IIIb
IVb
Vb
VIb
VIIb
VIII
IIIa
10000
1000
100
10
1
0.1
0.01
0.001
0.0001
D(i)/D(Nb)
2
4
6
8
10
12
14
n
Y
Zr
Ti
V
Cr
Fe
Co
Ni
3d
Nb
Mo
Ta
W
Re
5d
Ru
Pd
4d
Al
3p

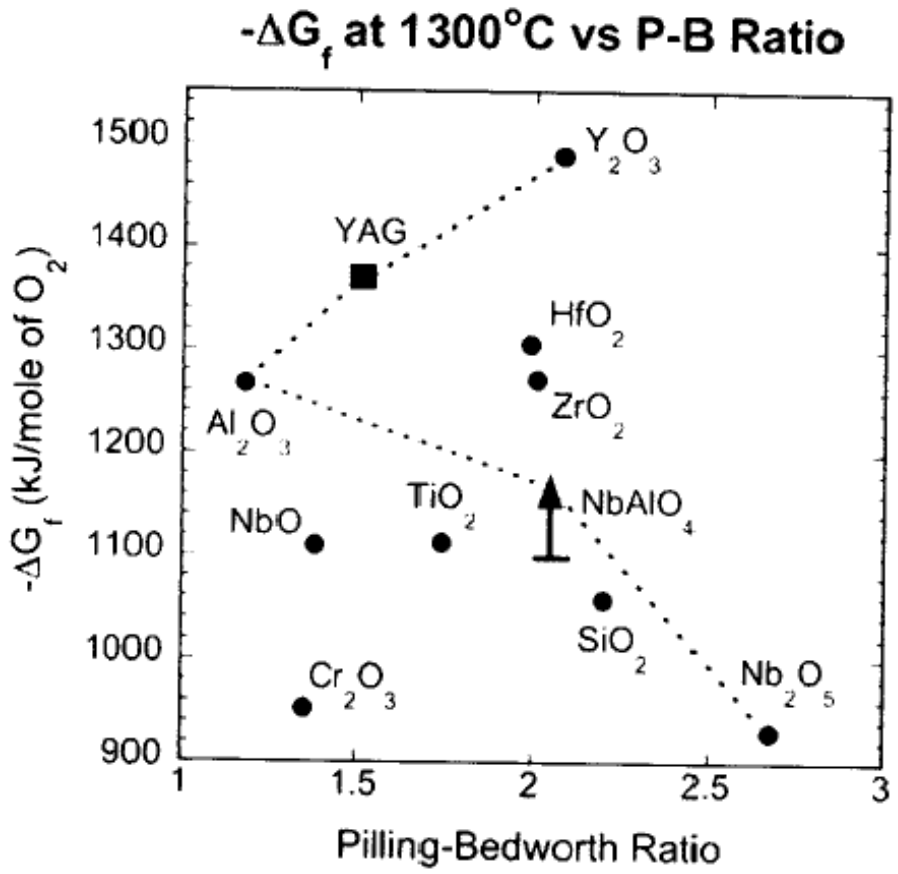

Aluminum Diffusivity at 1300°C
in Nb-X Binary Alloys
D_{Al} (m^2/sec)
10^{-14}
10^{-15}
10^{-16}
10^{-17}
Al
Cr
Ti
W
Hf
Pd
Nb
Mo
3
4
5
6
7
8
9
10
n

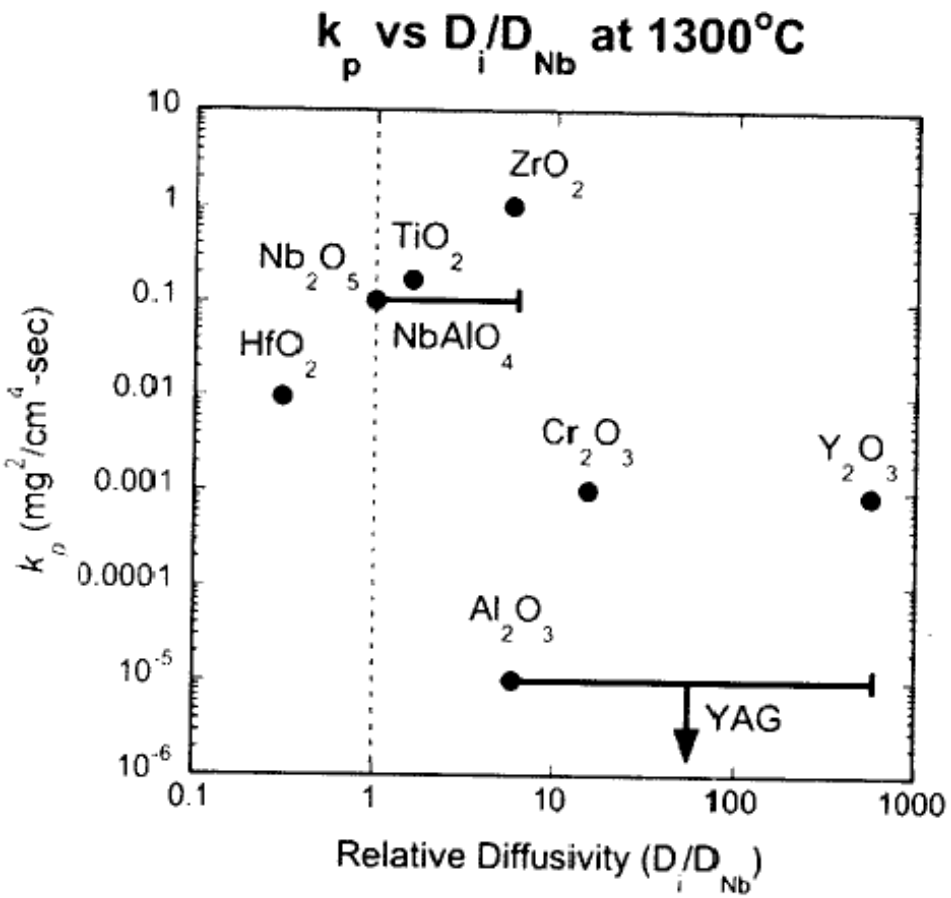

$N_o * \left(1 + \frac{d\ln\gamma_o}{d\ln X_o}\right) \alpha \quad N_o * D_o$
1300 C
0.1
0.01
0.001
0.0001
-800
-600
-400
-200
0
200
400
600
800
1000
Omega M-O (kJ/mol)
(Nb)
X_M=0.05
X_M=0.10
X_M=0.20


Relative Charge Density in Octahedral Sites of Nb-X Binaries
ρ(M)/ρ(Nb)
1.02
1
0.98
0.96
0.94
0.92
0.9
W
Re
Os
Zr
Nb
Mo
Tc
Ru
Rh
Pd
Al
Ti
2 3 4 5 6 7 8 9 10 11
n
Oxygen Diffusivity at 1300°C in Nb-X Binary Alloys
D_o (m²/sec)
10⁻¹⁰
10⁻¹¹
W
Re
Nb
Mo
Cr
Hf
Ti
Al
Pd
3 4 5 6 7 8 9 10
n

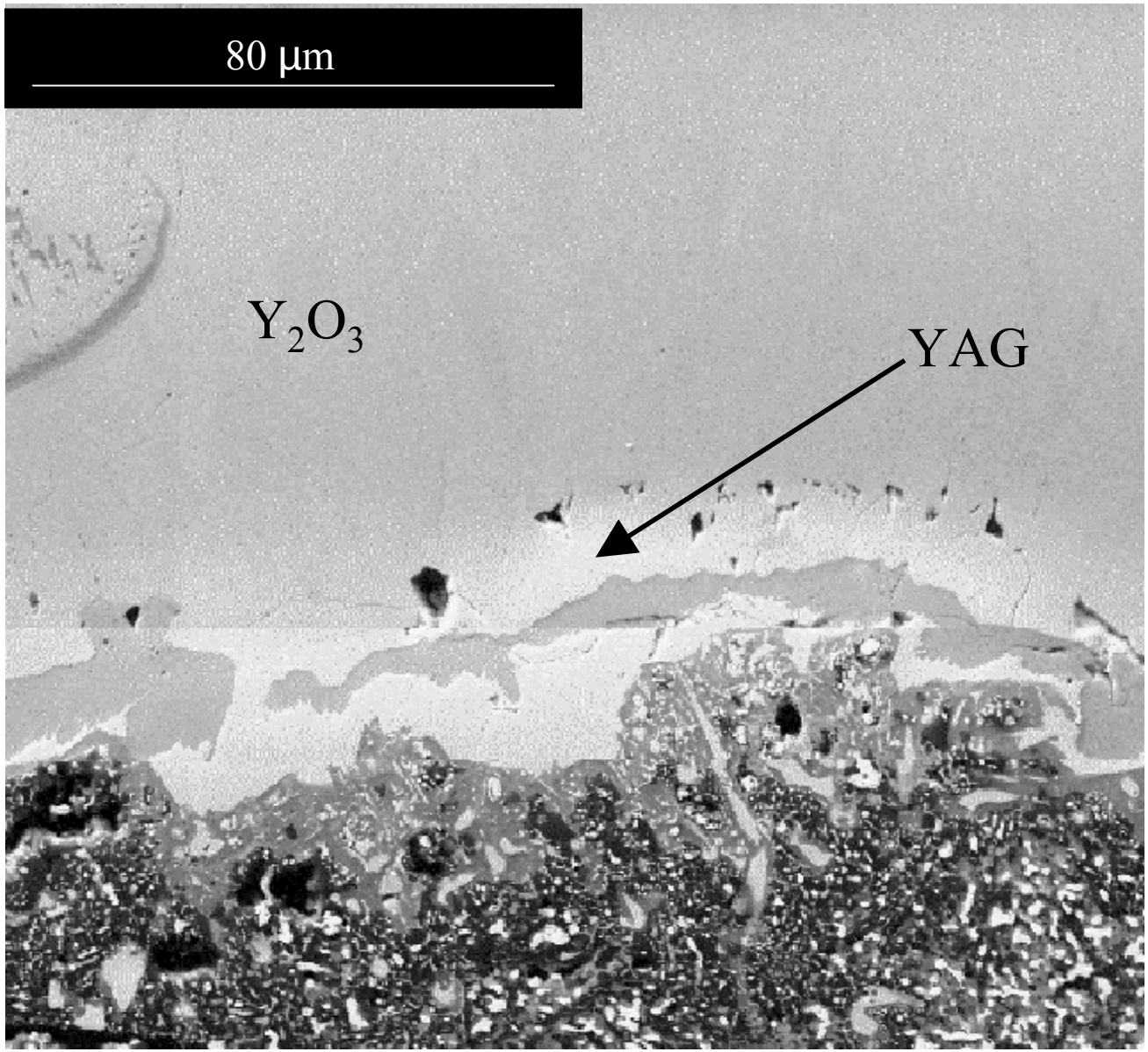
SEM images of 45Nb-34Hf-21Al oxidized in air at 1300°C/5 hrs




-ΔG_f at 1300°C vs P-B Ratio
-ΔG_f (kJ/mole of O_2)
1500
1400
1300
1200
1100
1000
900
1
1.5
2
2.5
3
Pilling-Bedworth Ratio
Y_2O_3
YAG
HfO_2
ZrO_2
Al_2O_3
TiO_2
NbAlO_4
NbO
SiO_2
Cr_2O_3
Nb_2O_5


k_p vs D_i/D_Nb at 1300°C
k_o (mg^2/cm^4-sec)
10
1
0.1
0.01
0.001
0.0001
10^-5
10^-6
0.1
1
10
100
1000
Relative Diffusivity (D_i/D_Nb)
ZrO_2
TiO_2
Nb_2O_5
HfO_2
NbAlO_4
Cr_2O_3
Y_2O_3
Al_2O_3
YAG

Nb(Ti,Cr,Hf)-45PtYAl oxidized 1400°C 5 Hour



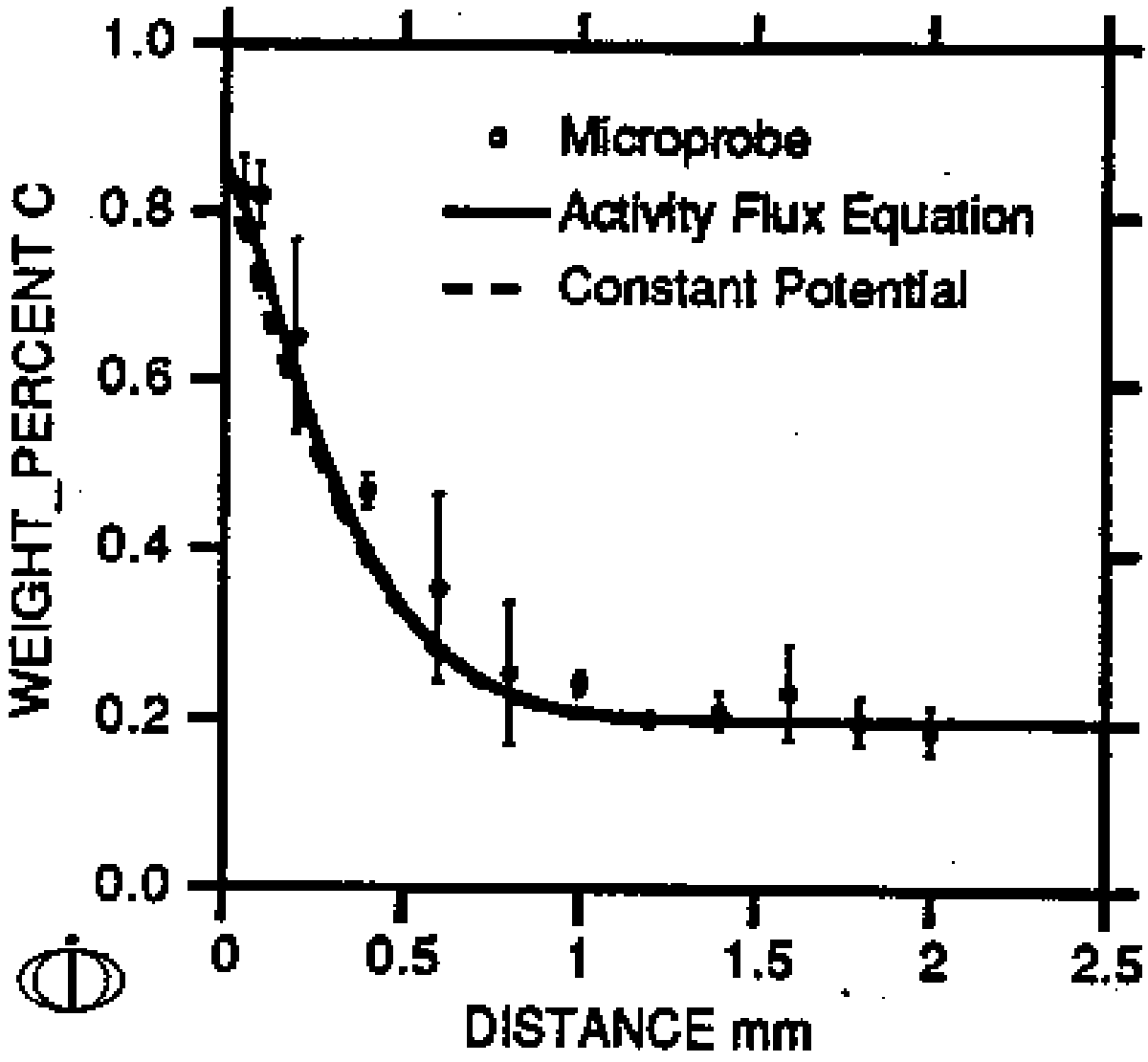


Fig. 3 - DICTRA simulations and microprobe measurements of the carburization of alloy C61.

Current Applications

Gears: NASCAR

-Successfully completed race with narrow gear design

-Moving forward with development

Ring & Pinion: SCORE INTERNATIONAL OFF-ROAD RACING

-Finished entire race with new design

-Production sets being made

Dog Rings and Camshafts: Currently in testing

For more info contact : C. Kuehmann or B. Tufts - QuesTek Innovations LLC - 847-328-5800