Modeling:
(i) thermal spray rapid solidification
(ii) partially-molten particle impact

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(i) thermal spray rapid solidification

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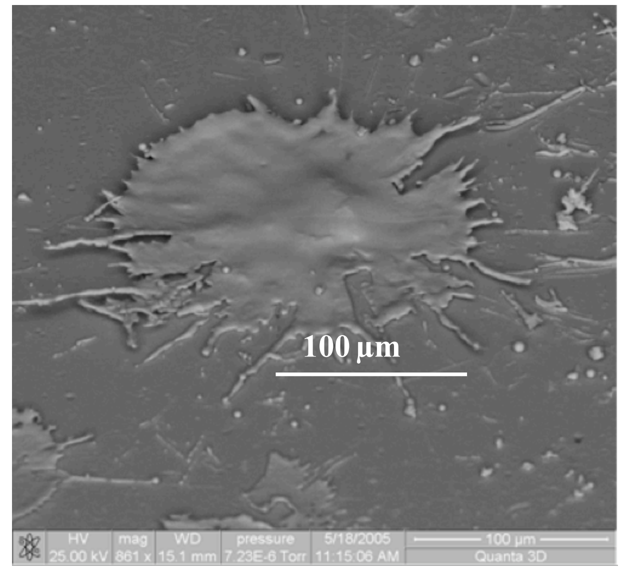
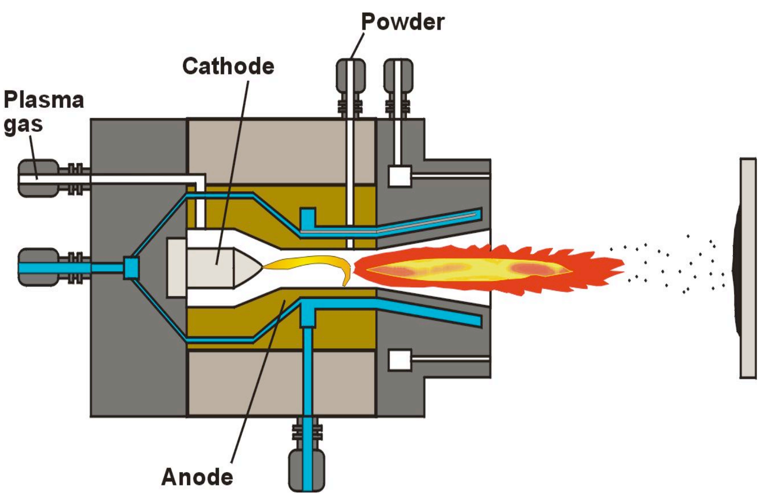
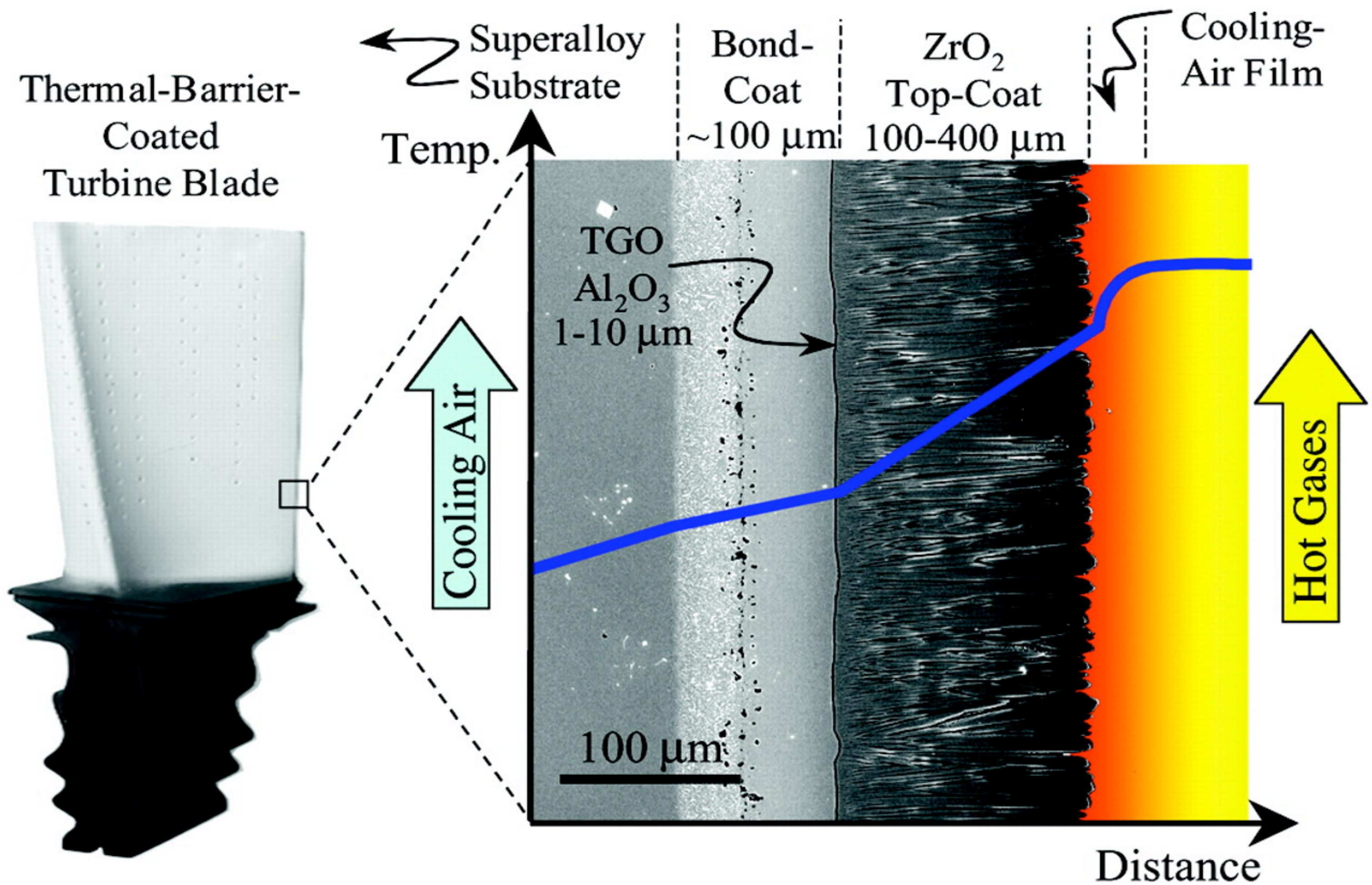
Thermal Spray Coating

- Thermal spraying YSZ (yttria stabilized zirconia)
  - spraying distance: 50 mm
  - velocity: 125 ± 20 m/s
  - particle diameter: 45 - 75 μm
  - splat thickness: 2 μm
  - cooling rate: ~ 10^6 K/s



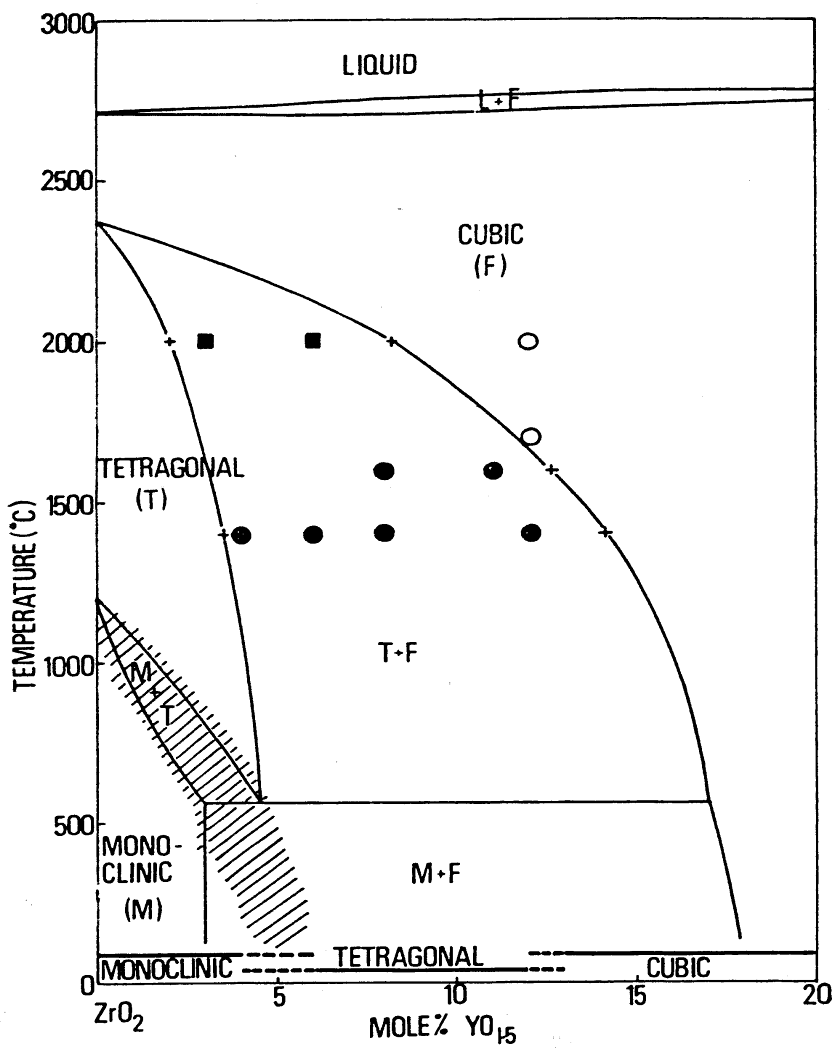


SEM of a TBC cross-section



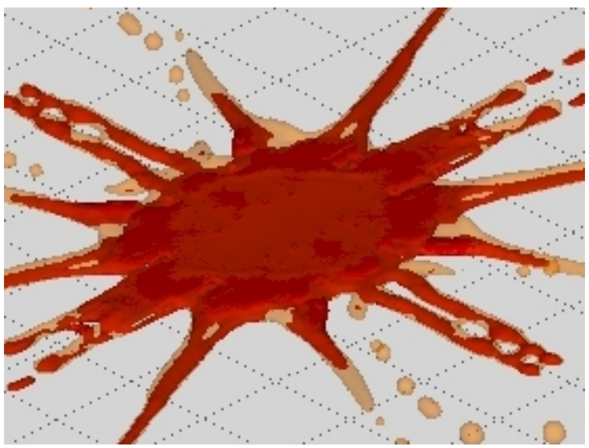
N.P. Padture et al., Science 296, 280, 2002

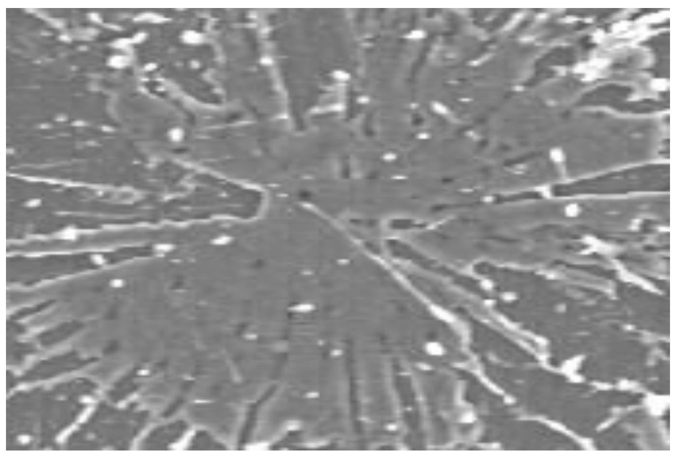
YSZ phase diagram



CACT equilibrium model

- assumes a pure material solidifying at T_m
- good prediction of overall splat shape/ morphology
- no microstructure prediction





Rapid solidification

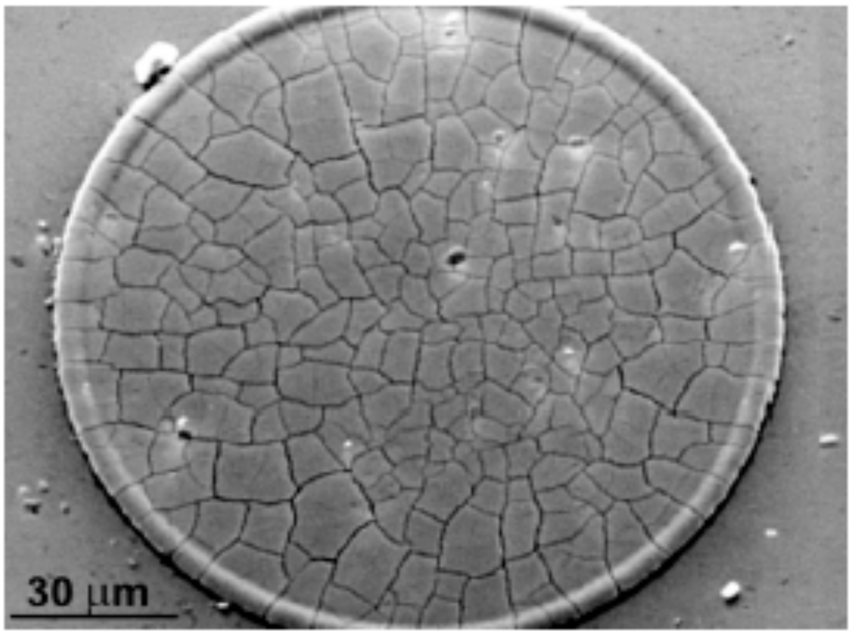
- non-equilibrium or meta/unstable
  - ➪ high interface velocity
  - ➪ undercooling $(T_i < T_m)$
  - ➪ non-uniform distribution of solute
  - ➪ different solid phases

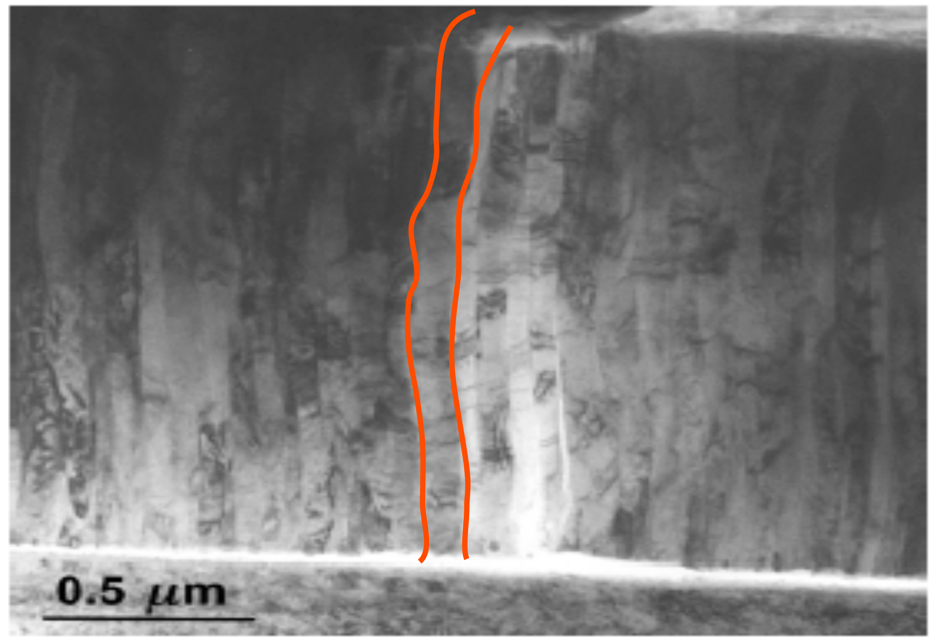
Objective

CACT

- develop a model to predict:
  - microstructure, including: grain size, morphology, transformation, during rapid solidification
  - concentration distribution
  - accurate solidification velocity

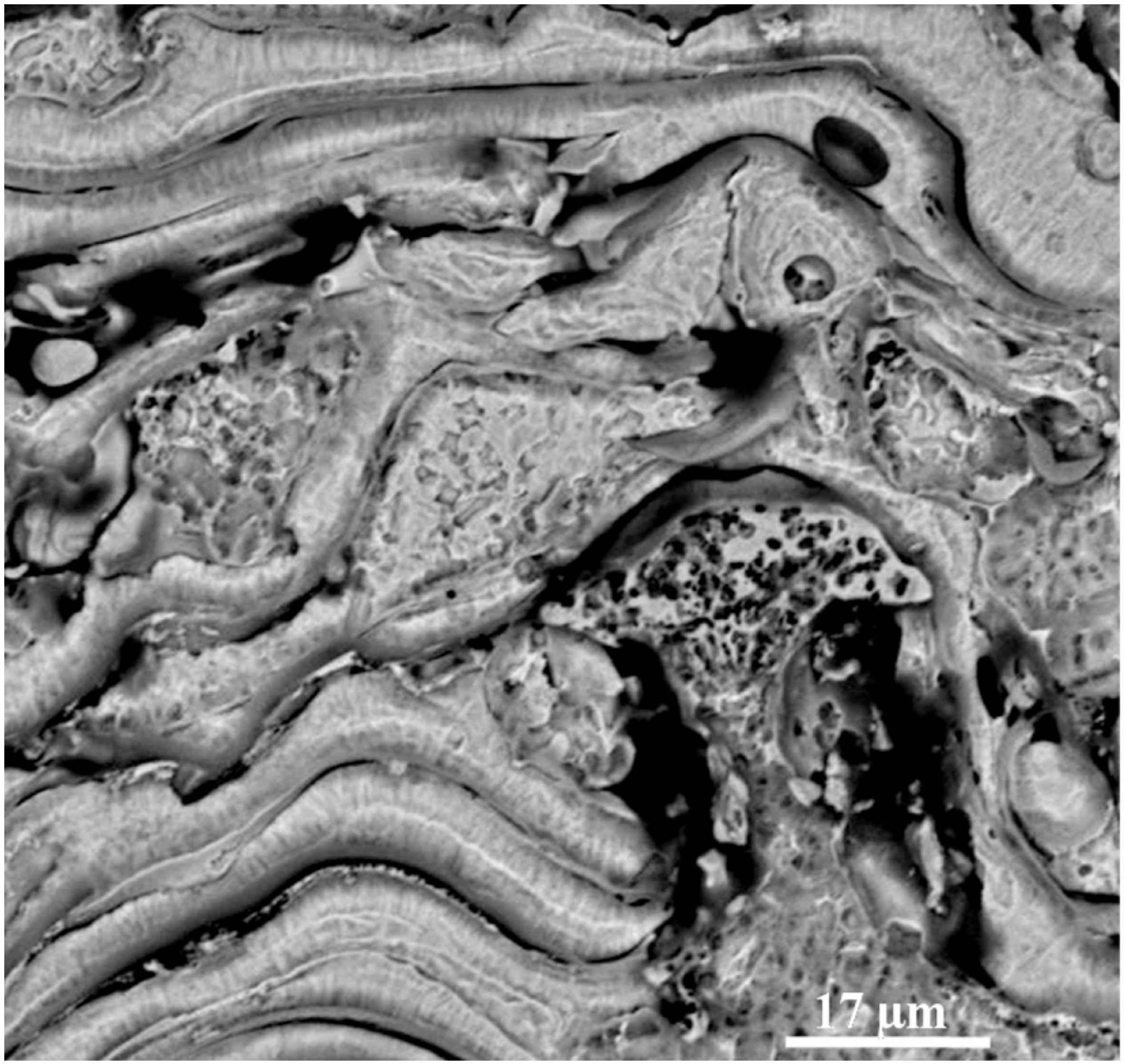
YSZ



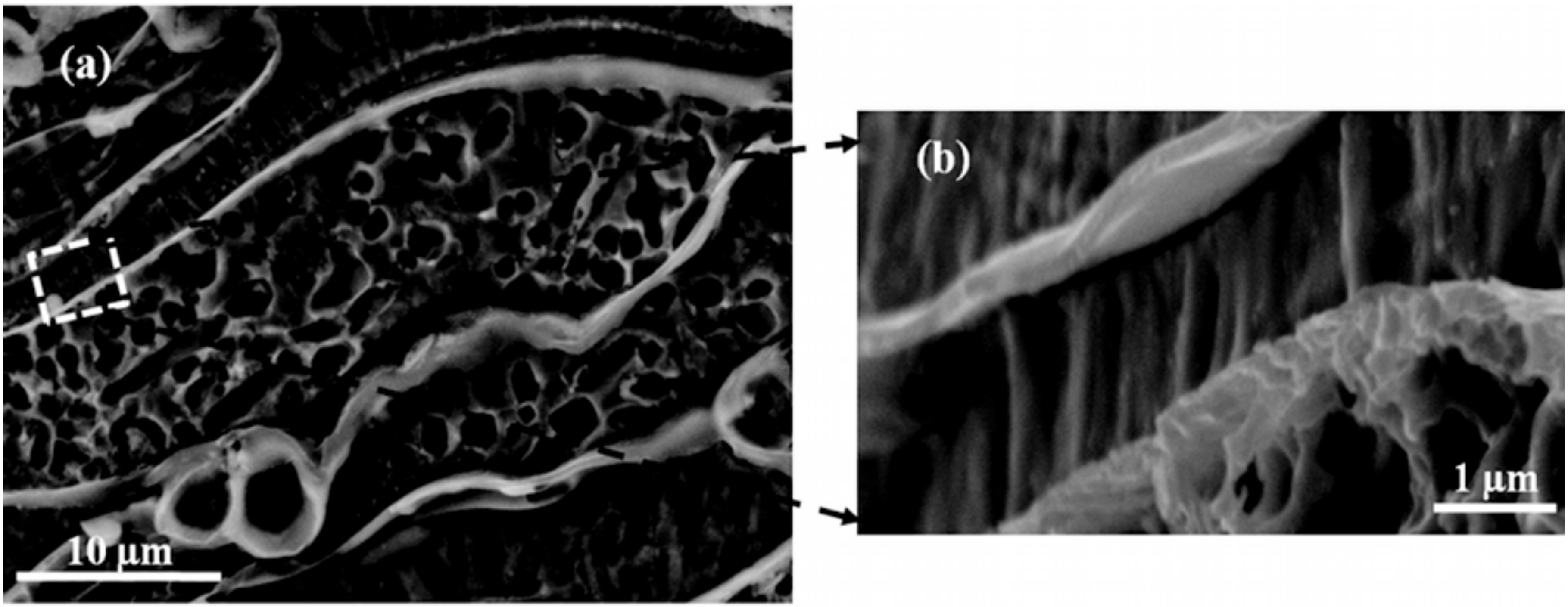


T. Chraska et al, Thin Solid Films 40, 397, 2001

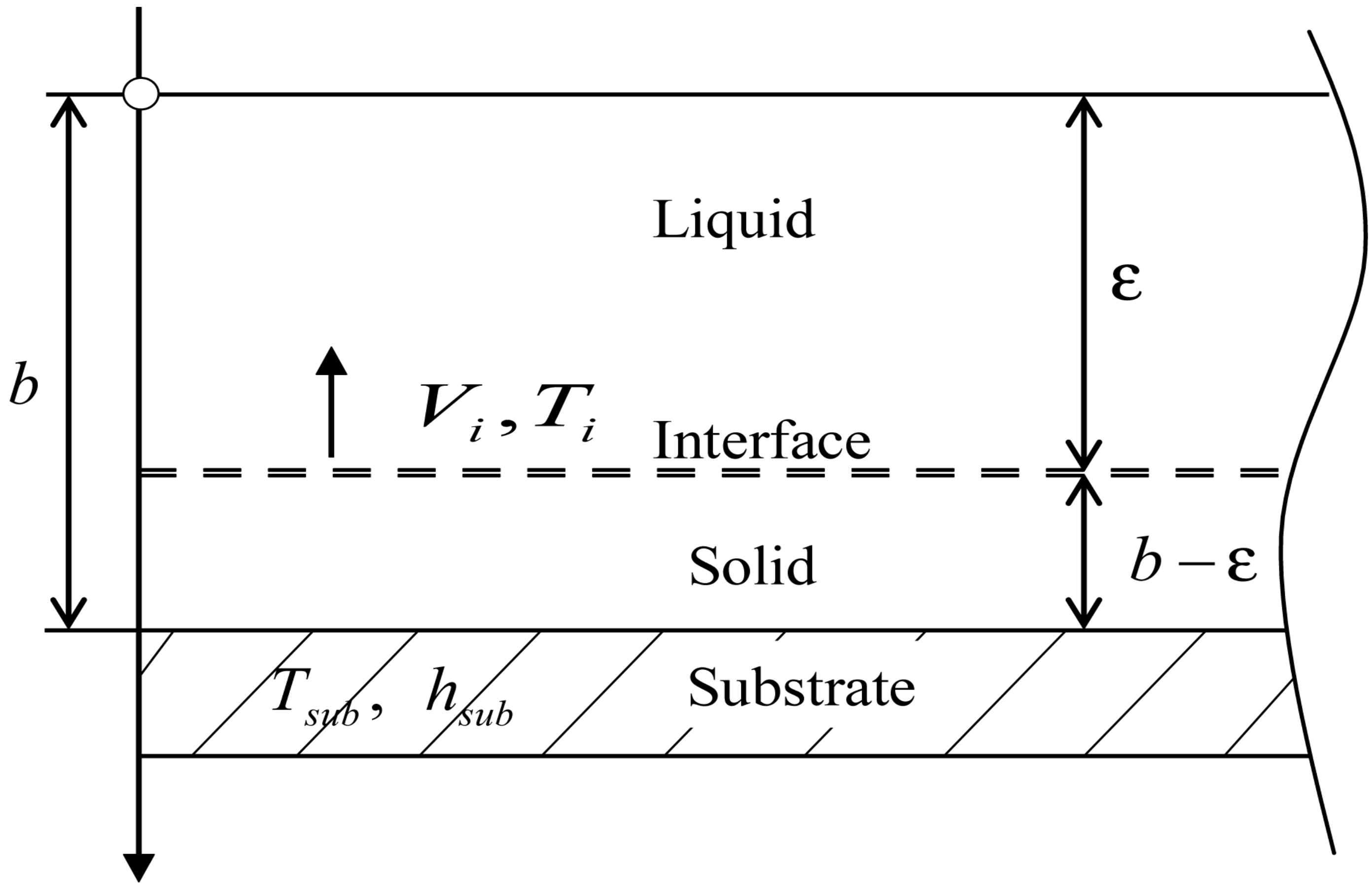
Alloy 625 – Ni-based alloy



Alloy 625



1D Interface Tracking Method



G.-X. Wang et al, Mater. Manuf. Process 19, 259, 2004

T & C eqns + ICs + BCs

$$\frac{\partial T_j}{\partial t} = \alpha_j \nabla^2 T_j$$

$$\frac{\partial C_L}{\partial t} = D_L \nabla^2 C_L$$

$$T(x,0) = T_o$$

$$C(x,0) = C_o$$

$$\frac{\partial T(0,t)}{\partial x} = h\left[T(0,t) - T_\infty\right]$$

$$\frac{\partial C(0,t)}{\partial x} = \frac{\partial C(b,t)}{\partial x} = 0$$

$$\frac{\partial T(b,t)}{\partial x} = 0$$

G.-X. Wang et al, Mater. Manuf. Process 19, 259, 2004

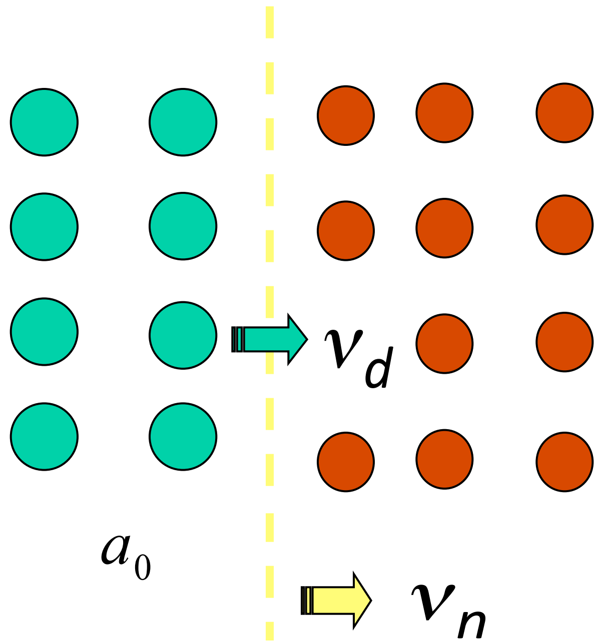
interface conditions

- energy conservation : $\rho_L V_i L = K_s \left.\frac{\partial T_S}{\partial x}\right|_i - K_L \left.\frac{\partial T_L}{\partial x}\right|_i$
- mass conservation : $(C_L - C_S)V_i = -D_L \left.\frac{\partial C_L}{\partial x}\right|_i$
- from phase diagram : $C_S = k_f C_L$
- undercooling : $T_i = T_m + m \cdot C_L - V_i / \mu$

parabolic model

- everything so far is traditional
  - why? – because the diffusion equations are based on:
  - Fourier's Law: $J = -k\nabla T$
  - Fick's Law: $J_c = -D\nabla C$
- but these assume an infinite "diffusive speed"
  - i.e. a sudden change in T or C is instantaneously felt everywhere in a domain

finite diffusive speed v_d



non-equilibrium diffusion:

$v_d = D / a_0$: diffusive speed

a_0 : inter-atomic spacing

v_n : solid/liquid interface velocity

leads to a "relaxation time" $\tau_D = D / v_d^2$

v_d vs v_n ?

$v_n = 0$	global equilibrium: *T=const*, *C=const*
$v_n << v_d$	local equilibrium: steady states
$v_n < v_d$	diffusional local equilibrium: parabolic equations (non-equilibrium partition coefficient *k* at the interface)
$v_n \sim v_d$	diffusional non-equilibrium: hyperbolic equations
$v_n > v_d$	$C_S = C_L = C_0$ (partitionless)

S.L. Sobolev, Phys. Rev. E 55, 6845, 1997

- Cattaneo devised modified laws in 1948:

  - Fourier's Law: $\tau \frac{\partial J}{dt} + J = -k\nabla T$

  - Fick's Law: $\tau_D \frac{\partial J_C}{\partial t} + J_c = -D\nabla C$

hyperbolic model

$$\frac{\partial T}{\partial t} + \tau \frac{\partial^2 T}{\partial t^2} = \alpha \nabla^2 T$$

$$\frac{\partial C_L}{\partial t} + \tau_D \frac{\partial^2 C_L}{\partial t^2} = D \nabla^2 C_L$$

$$T(x,0) = T_o$$

$$C(x,0) = C_o$$

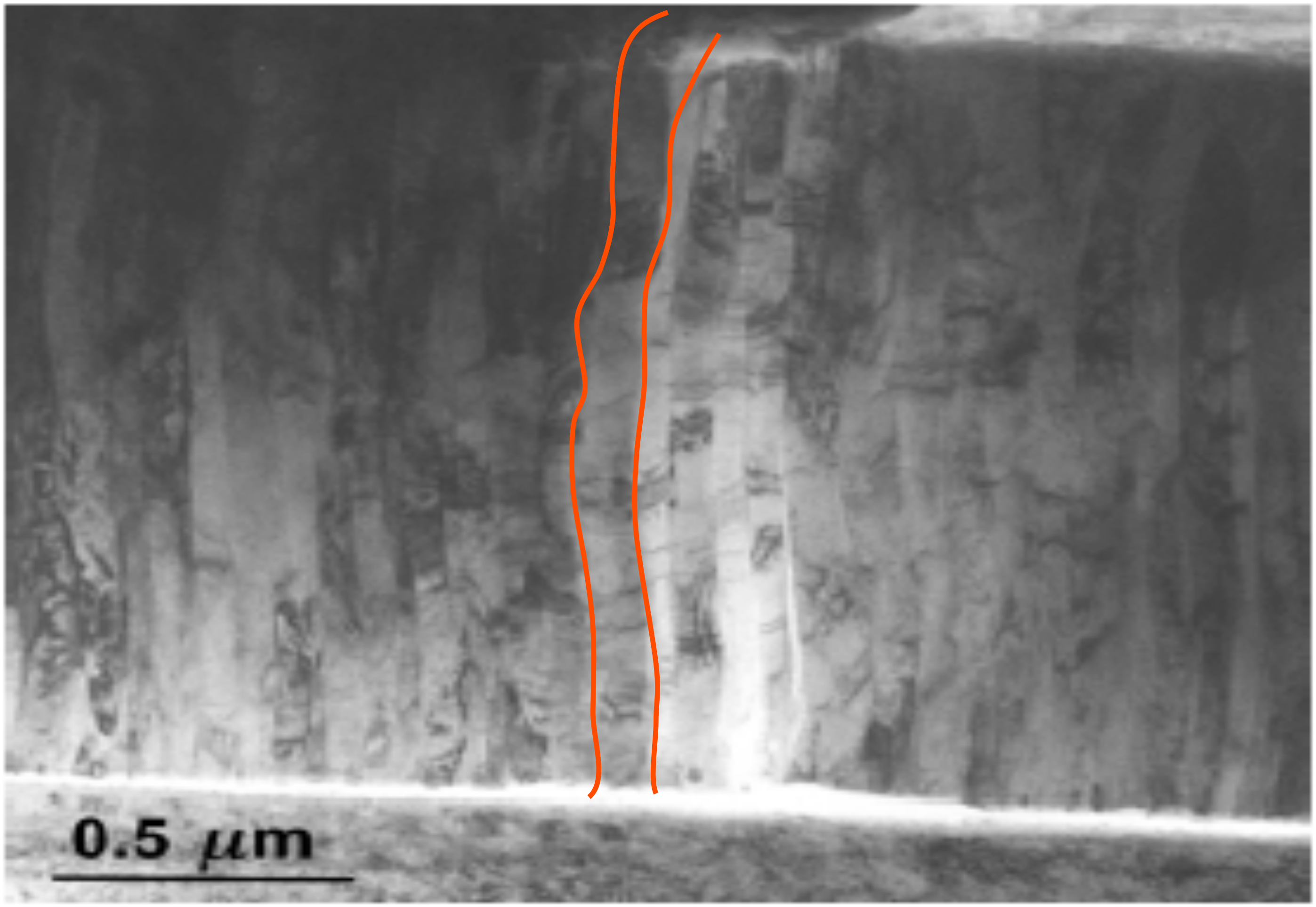
$$\frac{\partial T(0,t)}{\partial x} = h\left[T(0,t) - T_\infty\right]$$

$$\frac{\partial C(0,t)}{\partial x} = \frac{\partial C(b,t)}{\partial x} = 0$$

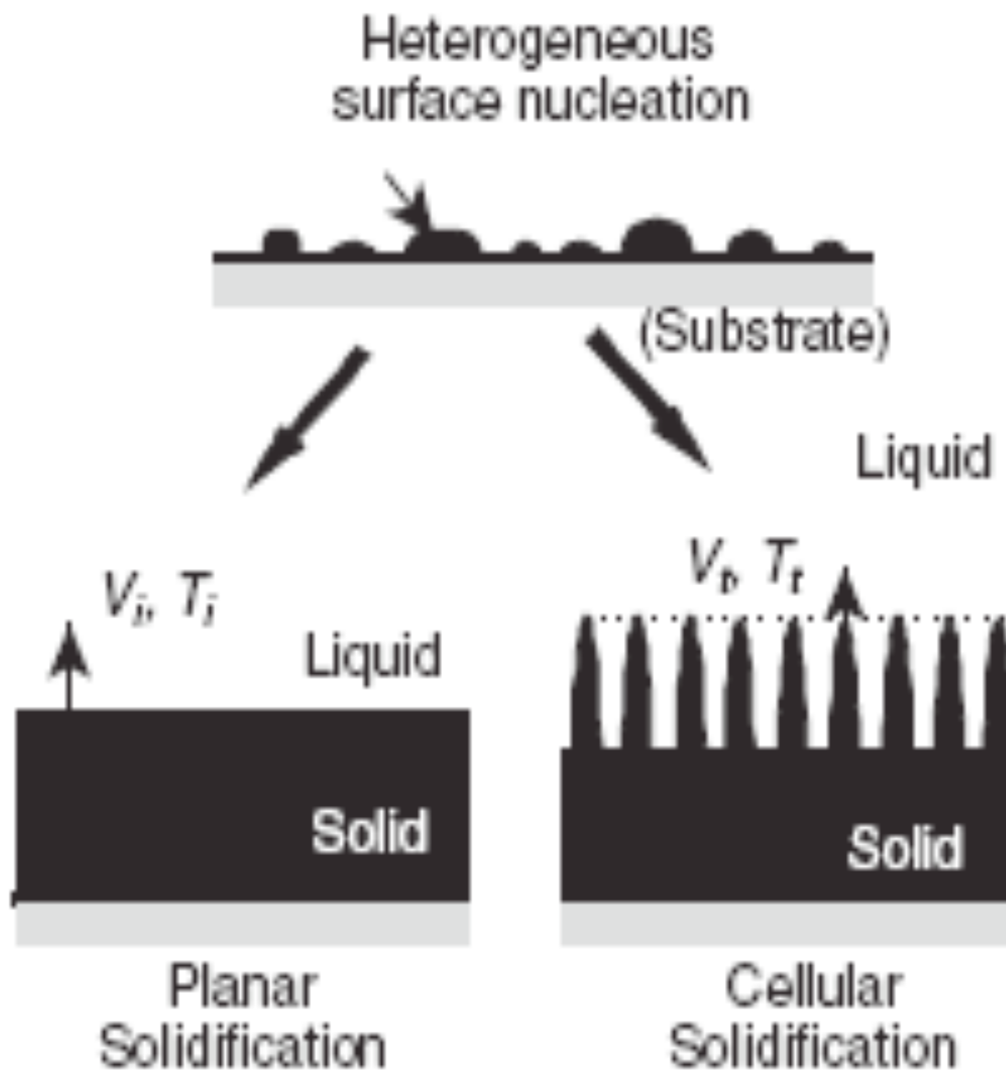
$$\frac{\partial T(b,t)}{\partial x} = 0$$

hyperbolic interface BCs

- energy conservation : $(\tau \frac{\partial}{\partial t} + 1)\rho_L V_i L = K_s \frac{\partial T_S}{\partial x}\Big|_i - K_L \frac{\partial T_L}{\partial x}\Big|_i$
- mass conservation : $\left(C_L - C_S\right)V_i + \tau_D \frac{\partial}{\partial t}((C_L - C_s)V_i) = -D_L \frac{\partial C_L}{\partial x}\Big|_i$
- from phase diagram : $C_S = k_f C_L$
- undercooling : $T_i = T_m + m \cdot C_L - V_i / \mu$

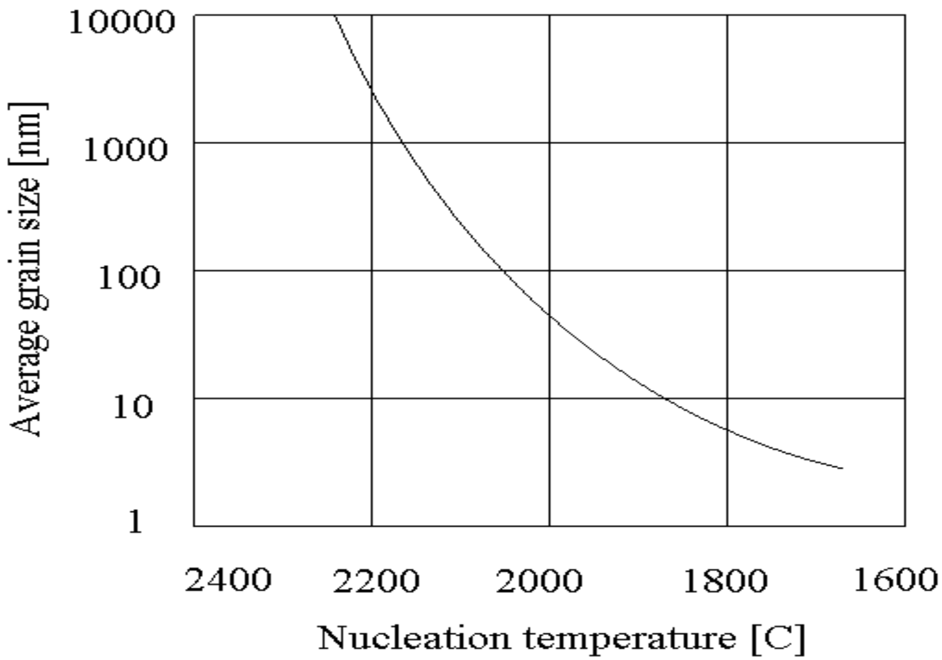

0.5 μm

planar vs cellular interface morphology



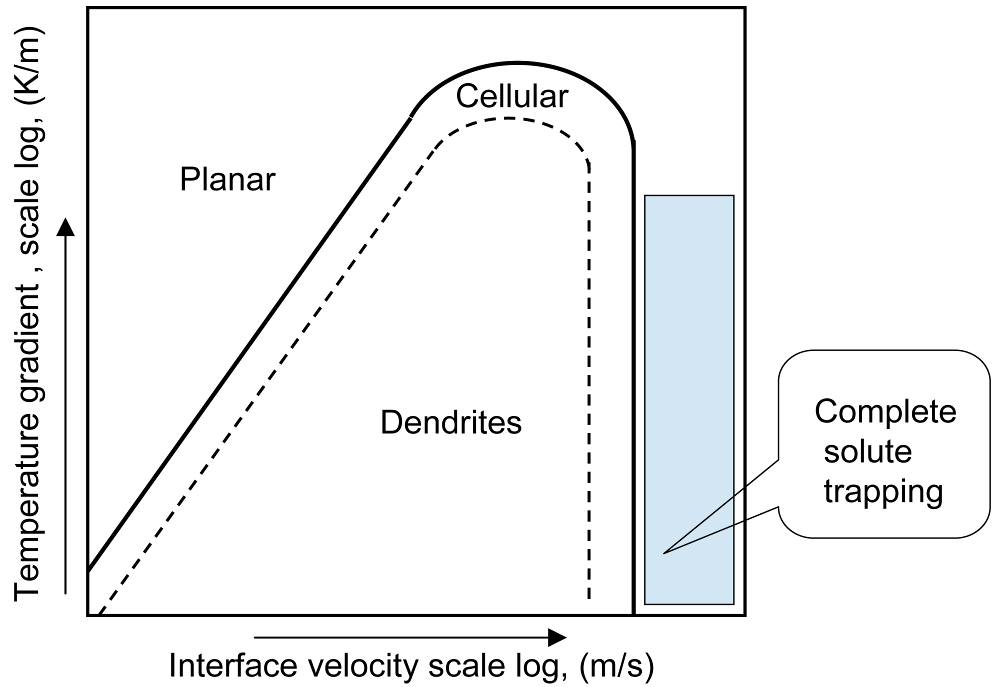
two indications of grain size

- 1) if planar, then grain size is determined by the initial nucleation density, which is a function of initial undercooling (nucleation temperature)



T. Chraska et al, Thin Solid Films 40, 397, 2001

- 2) if cellular, the grain tips are curved; curvature can be determined via stability theory; and curvature determines grain size (KGT model)

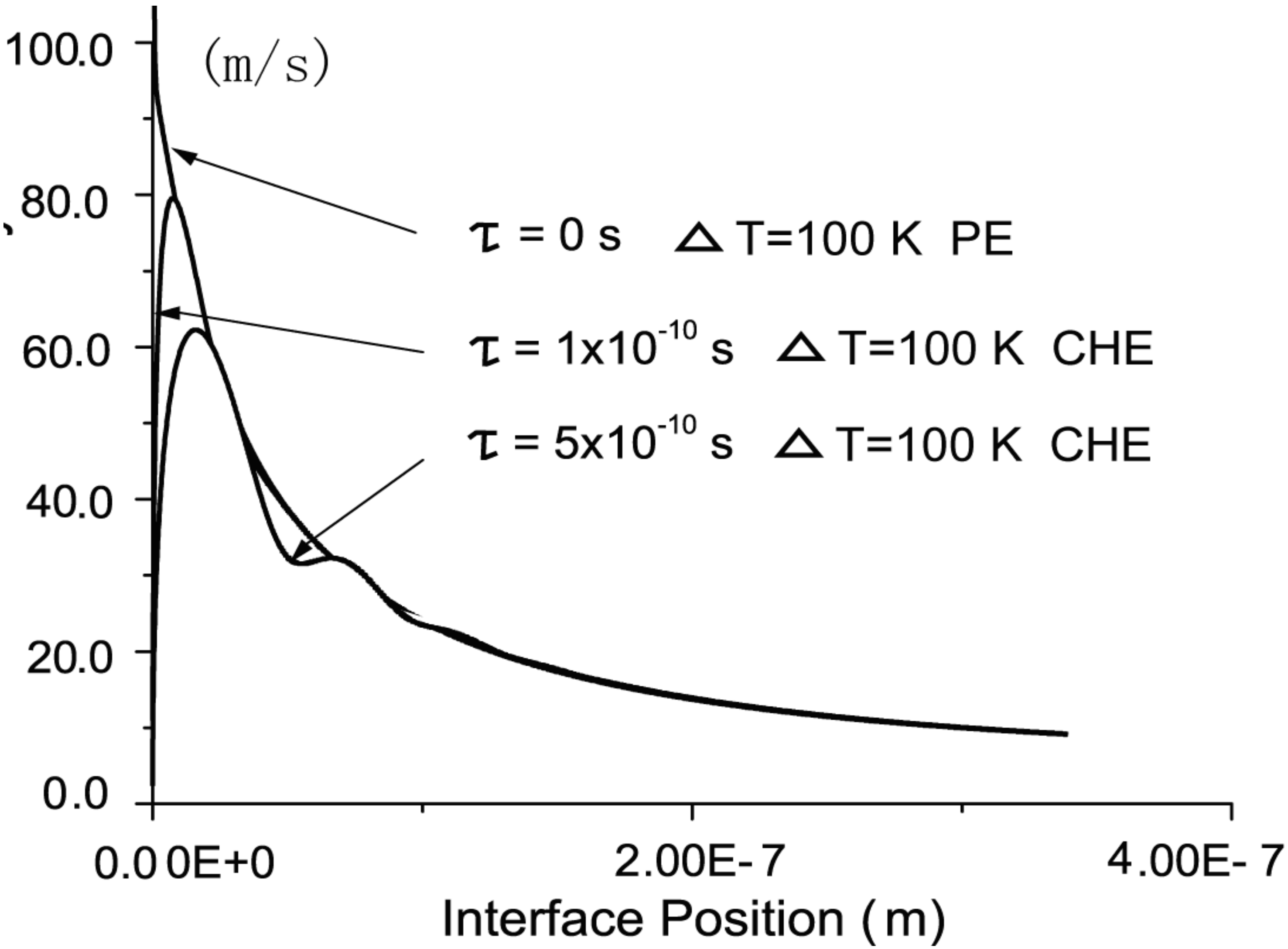


Results

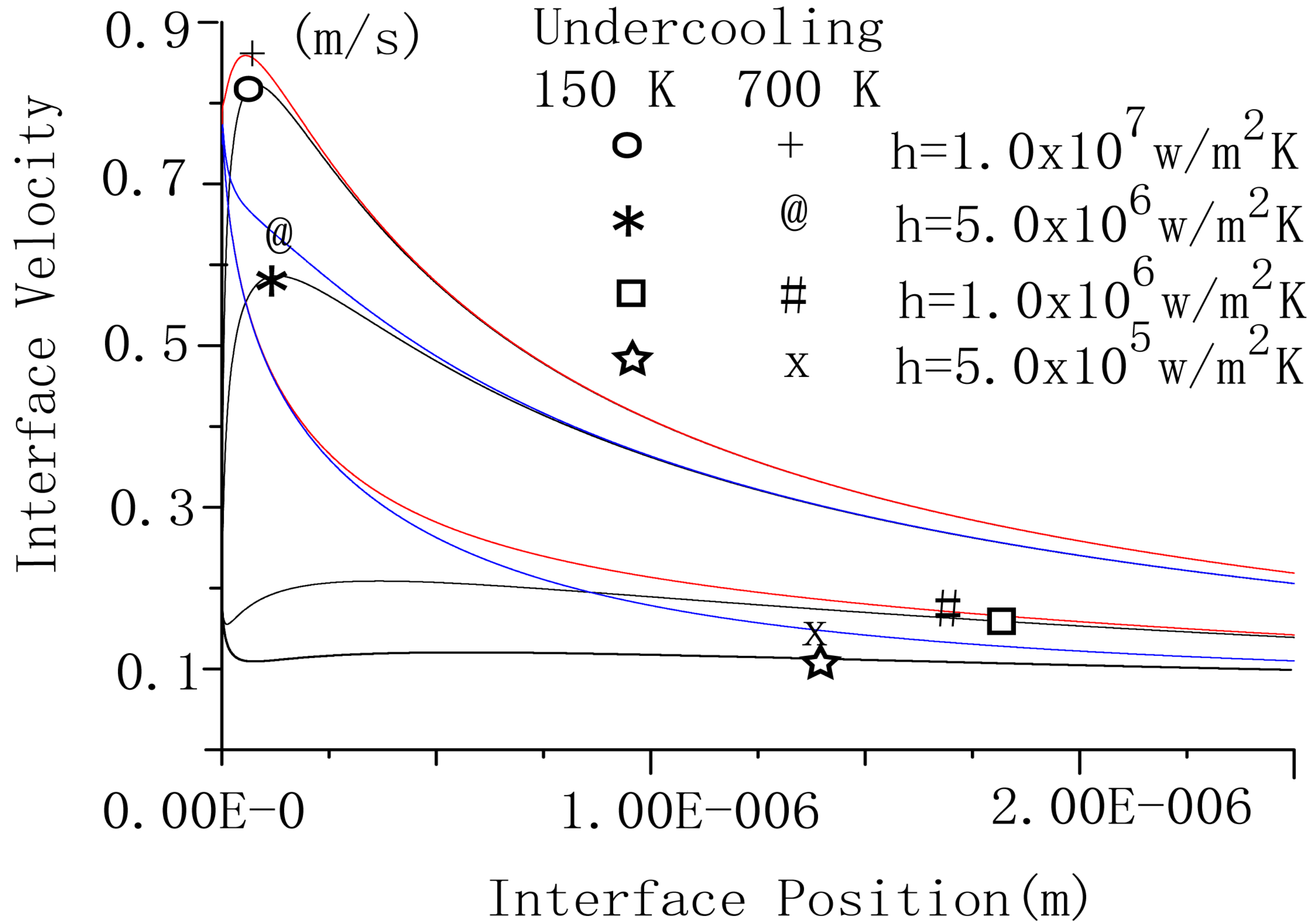
- solved the hyperbolic T and C equations using the same relaxation time
- solution method: MacCormack's predictor-corrector scheme

- pure Al – temperature only
- YSZ – 8 wt% yttria
- Alloy 625 – Ni - 21 wt% Cr alloy

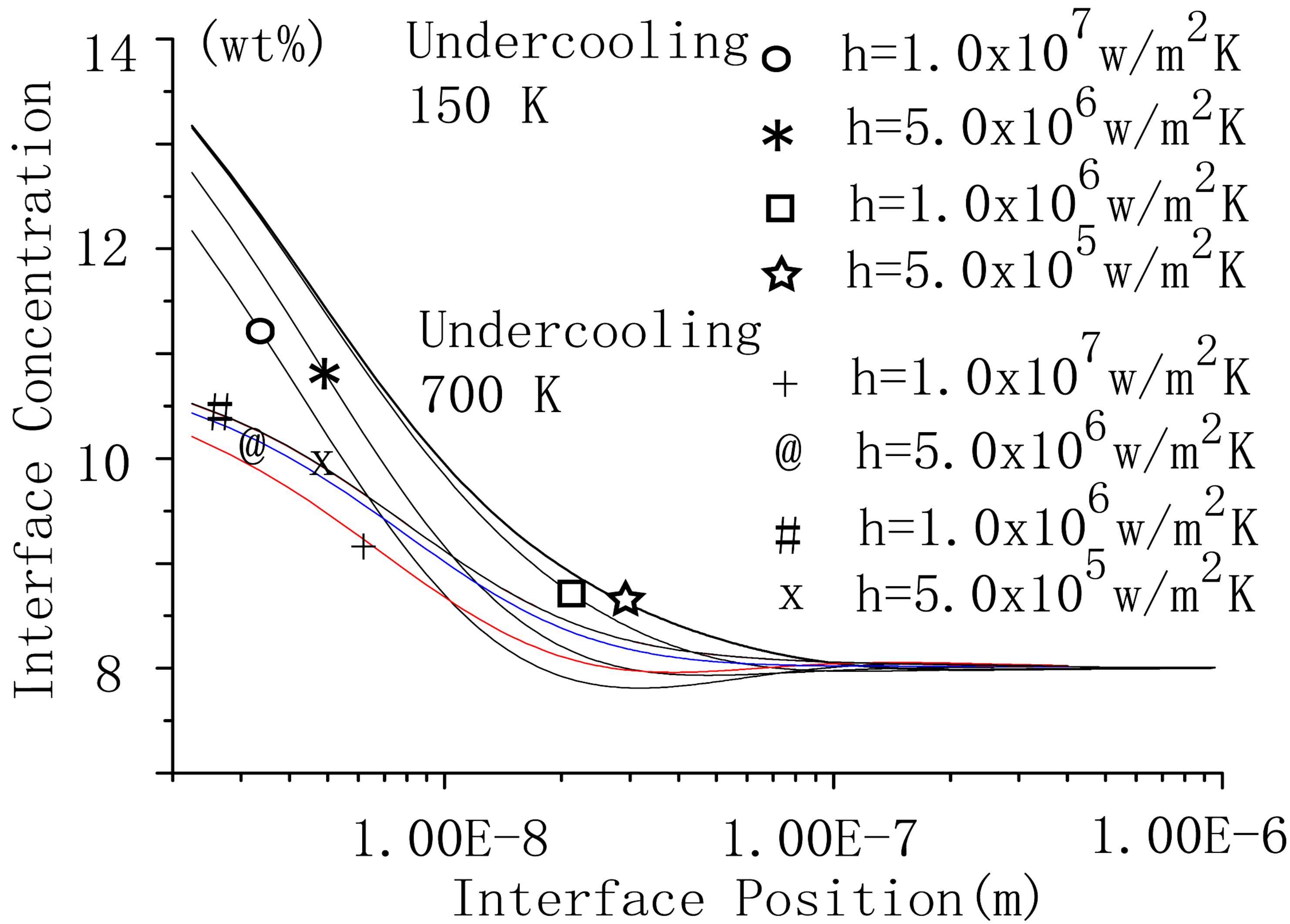
Al – temperature only



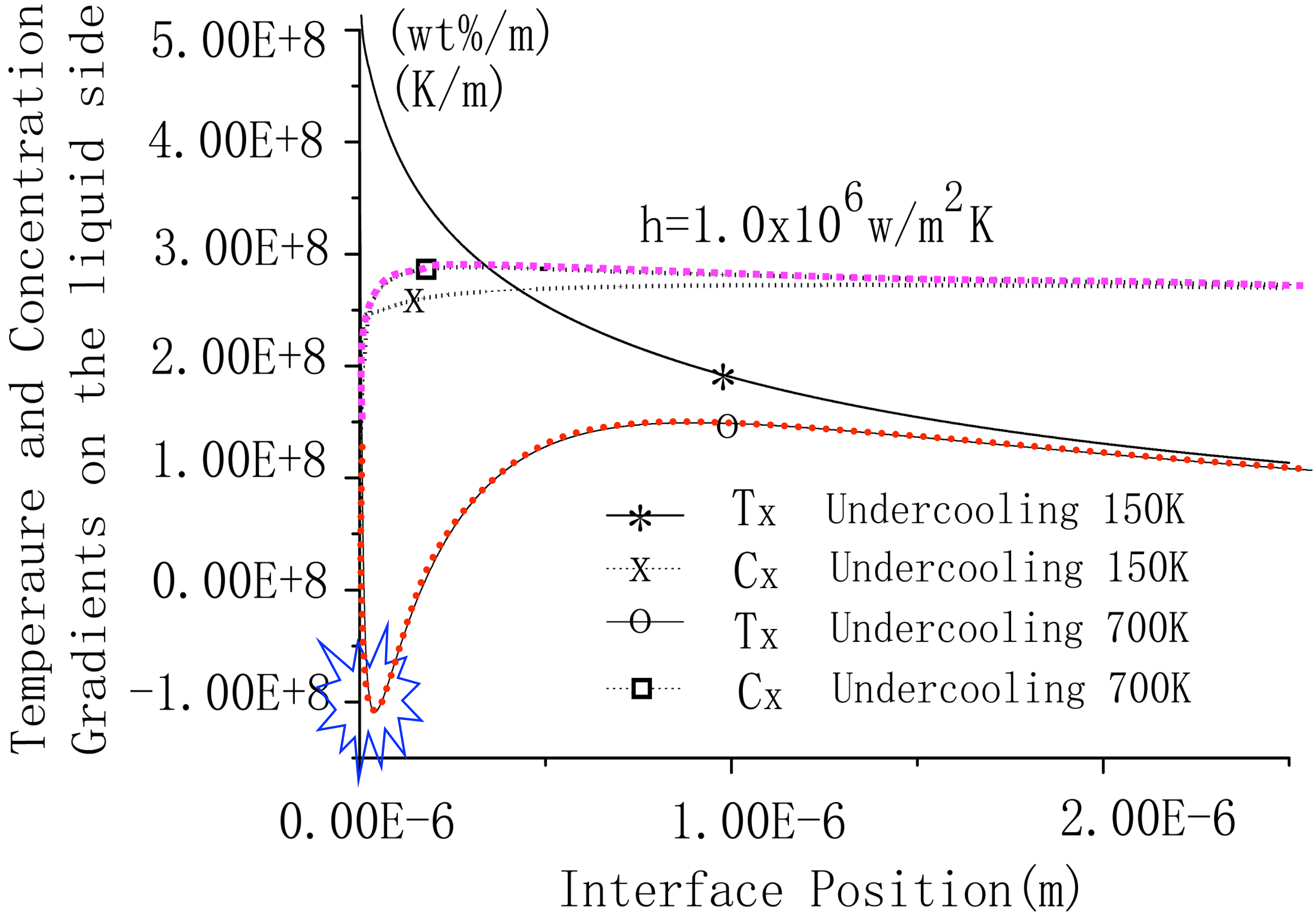
YSZ interface velocity



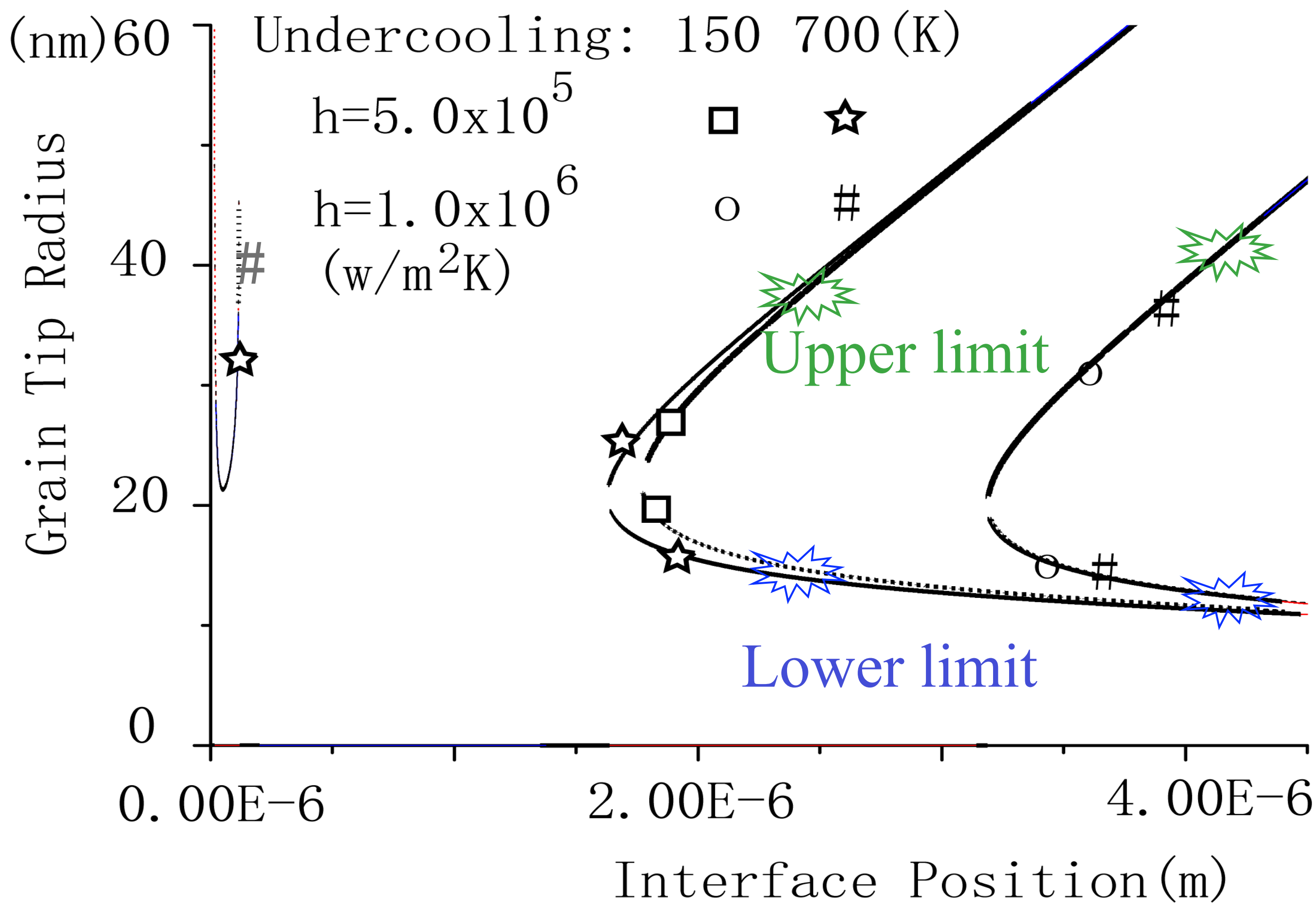
YSZ solid-side concentration



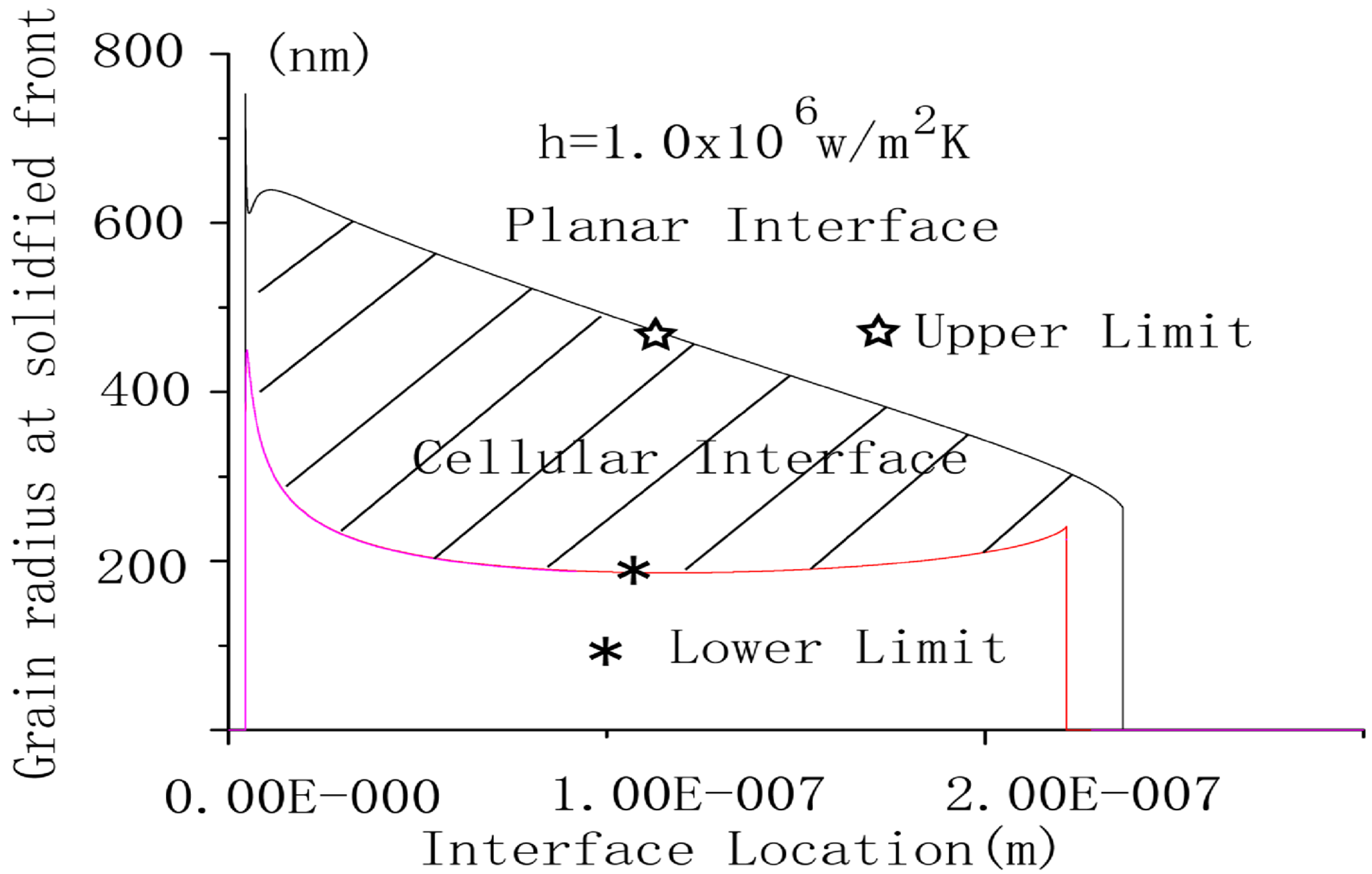
YSZ liquid side gradients



YSZ grain radius



grain radius for Alloy 625



(ii) partially molten particle impact

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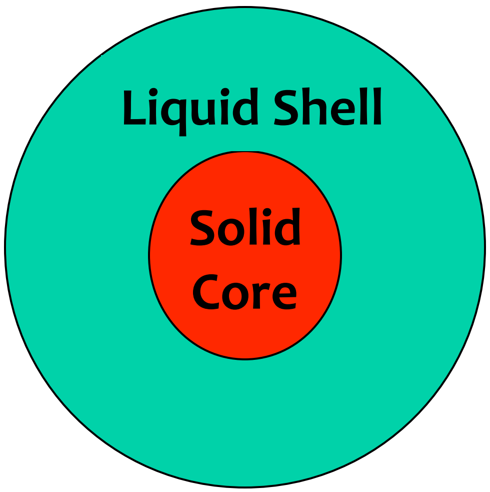
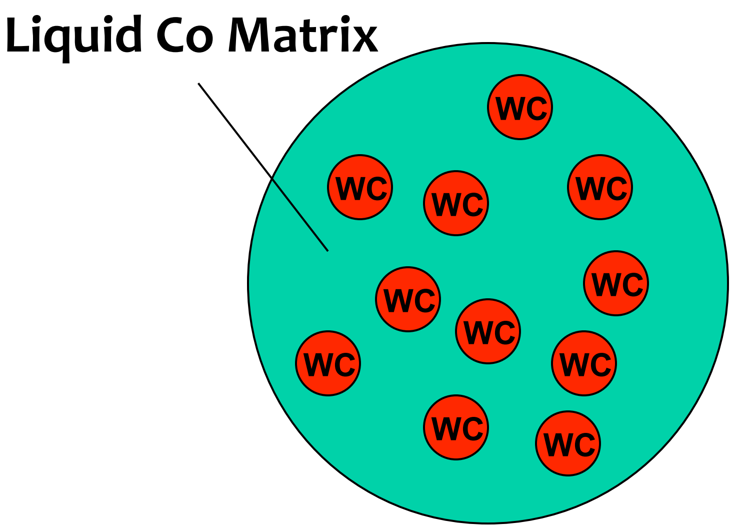
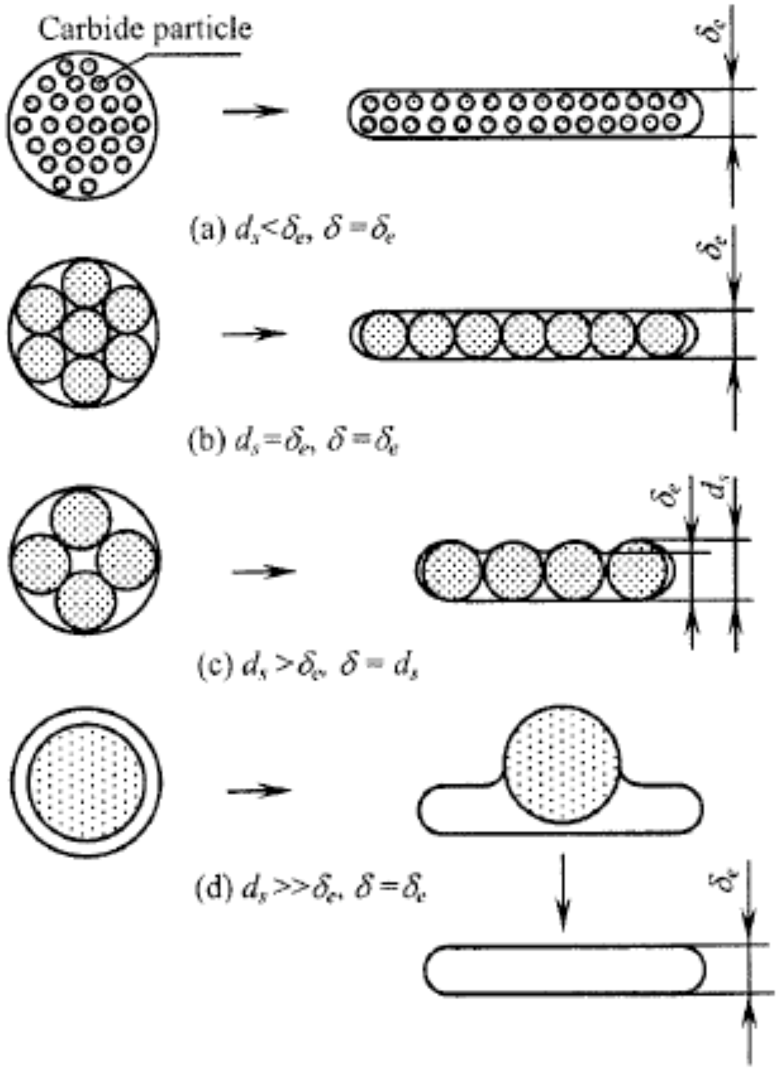
Semi-Molten Droplets?

- Insufficient heating of oxidation-sensitive materials (e.g. MCrAlY)

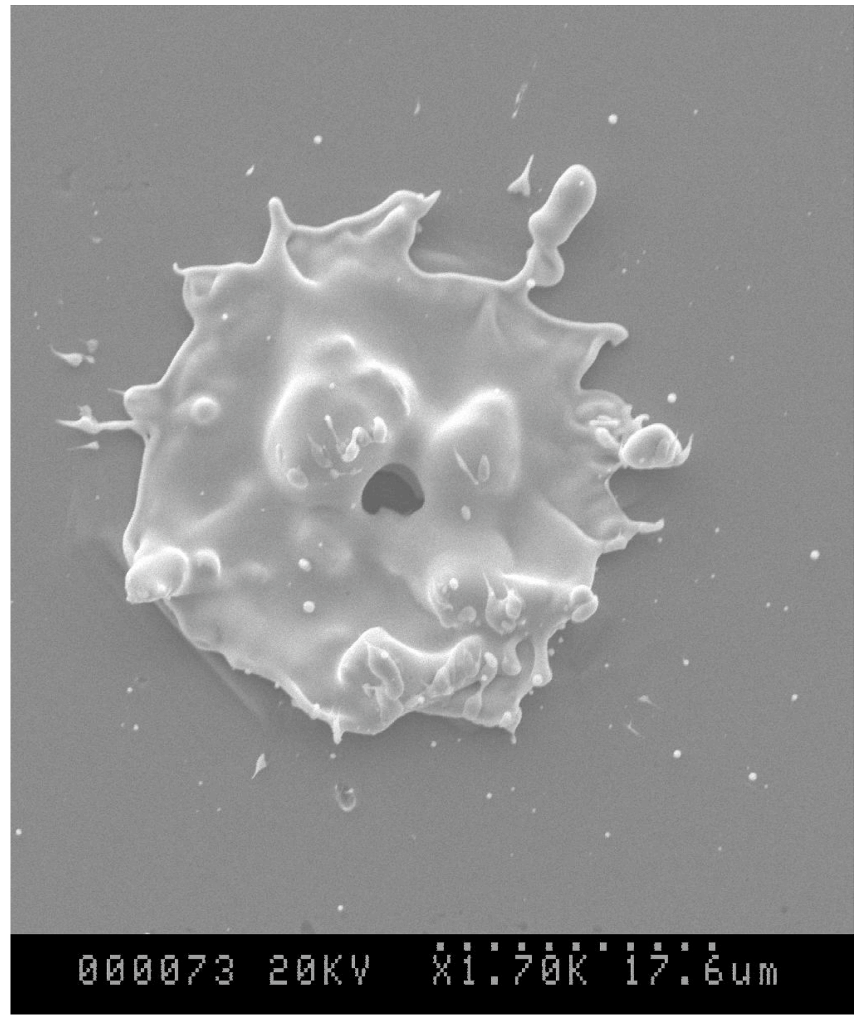


- Composite coatings (e.g. WC-Co – carbides in a cobalt matrix)



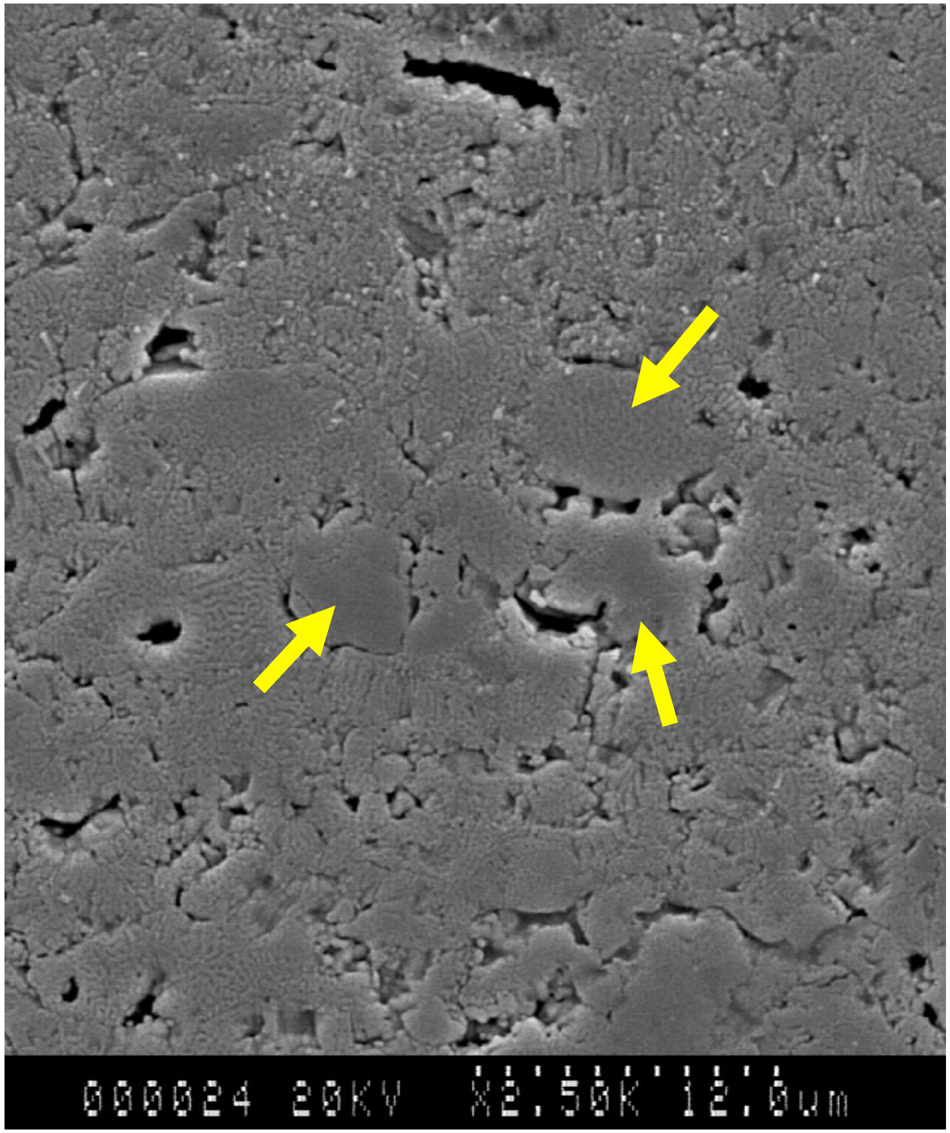


a, *b* Case I; *c* Case II; *d* Case III

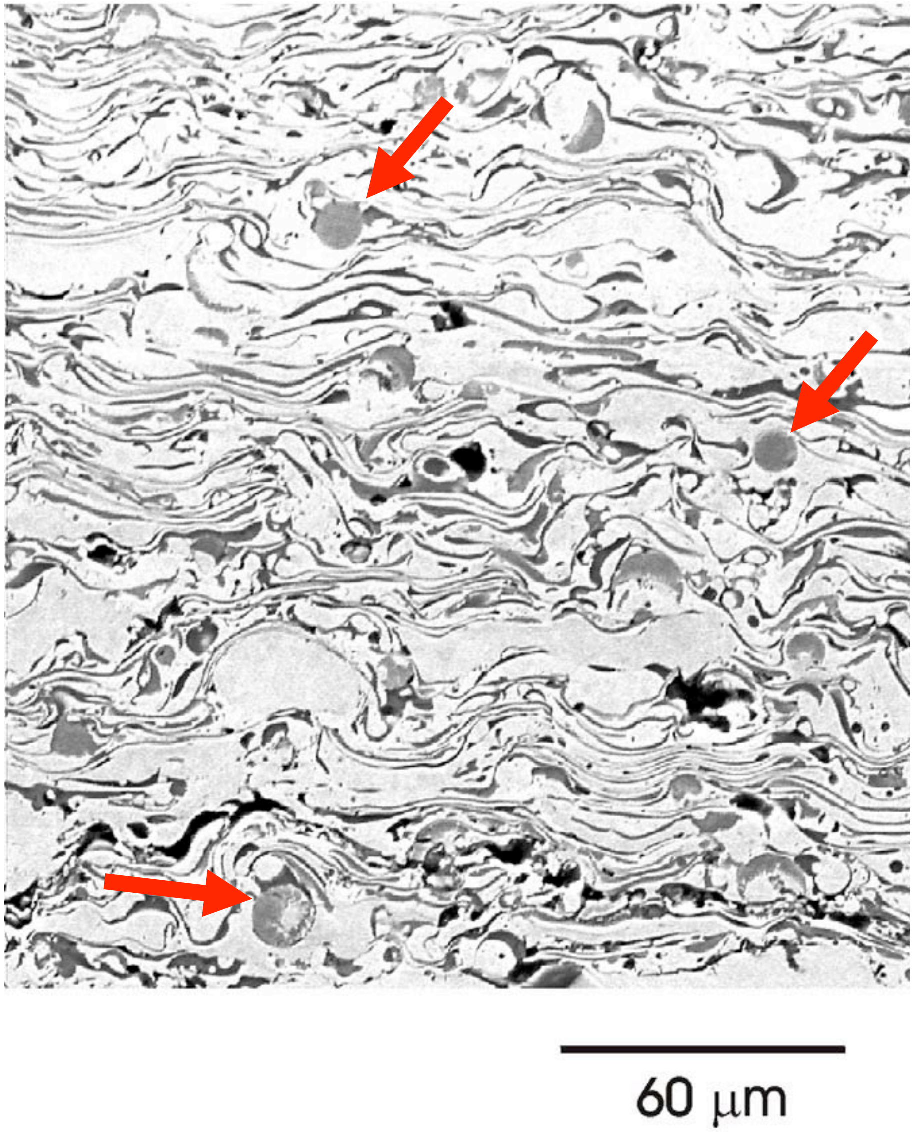


C.J. Li et al., Materials Science and Technology, 2004

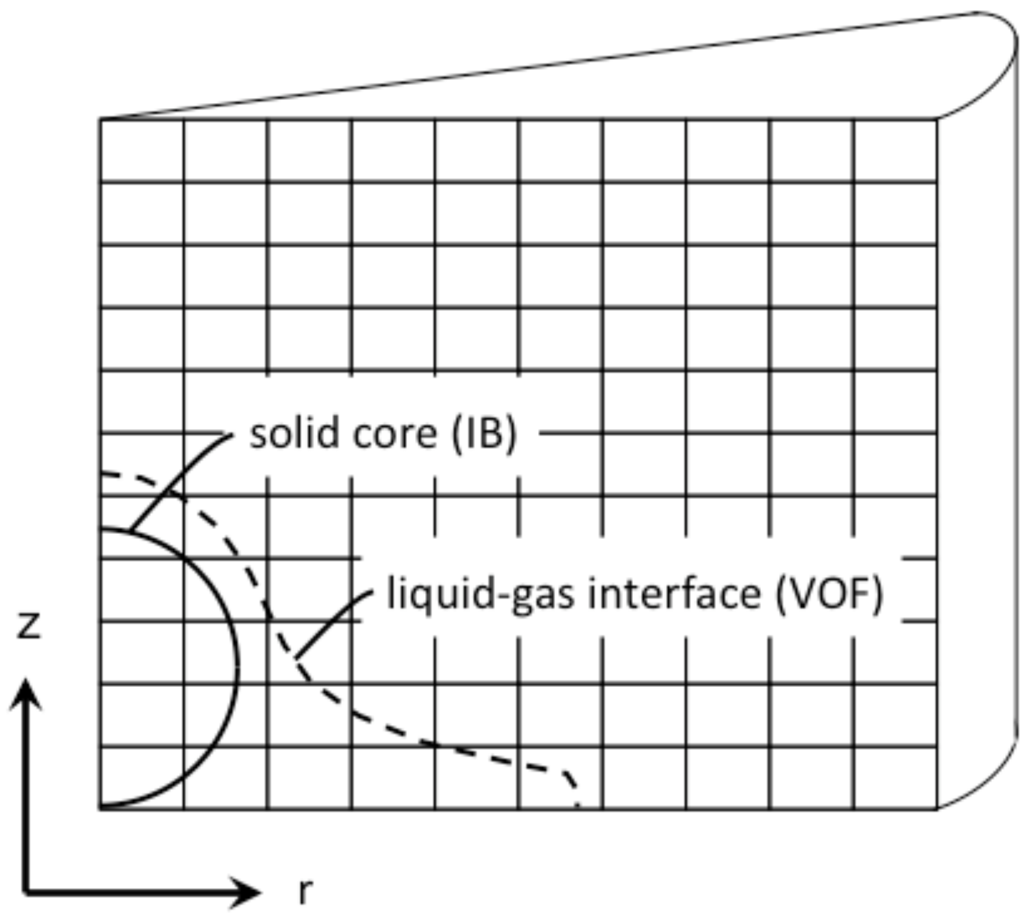
YSZ cross-section



Ni cross-section



model



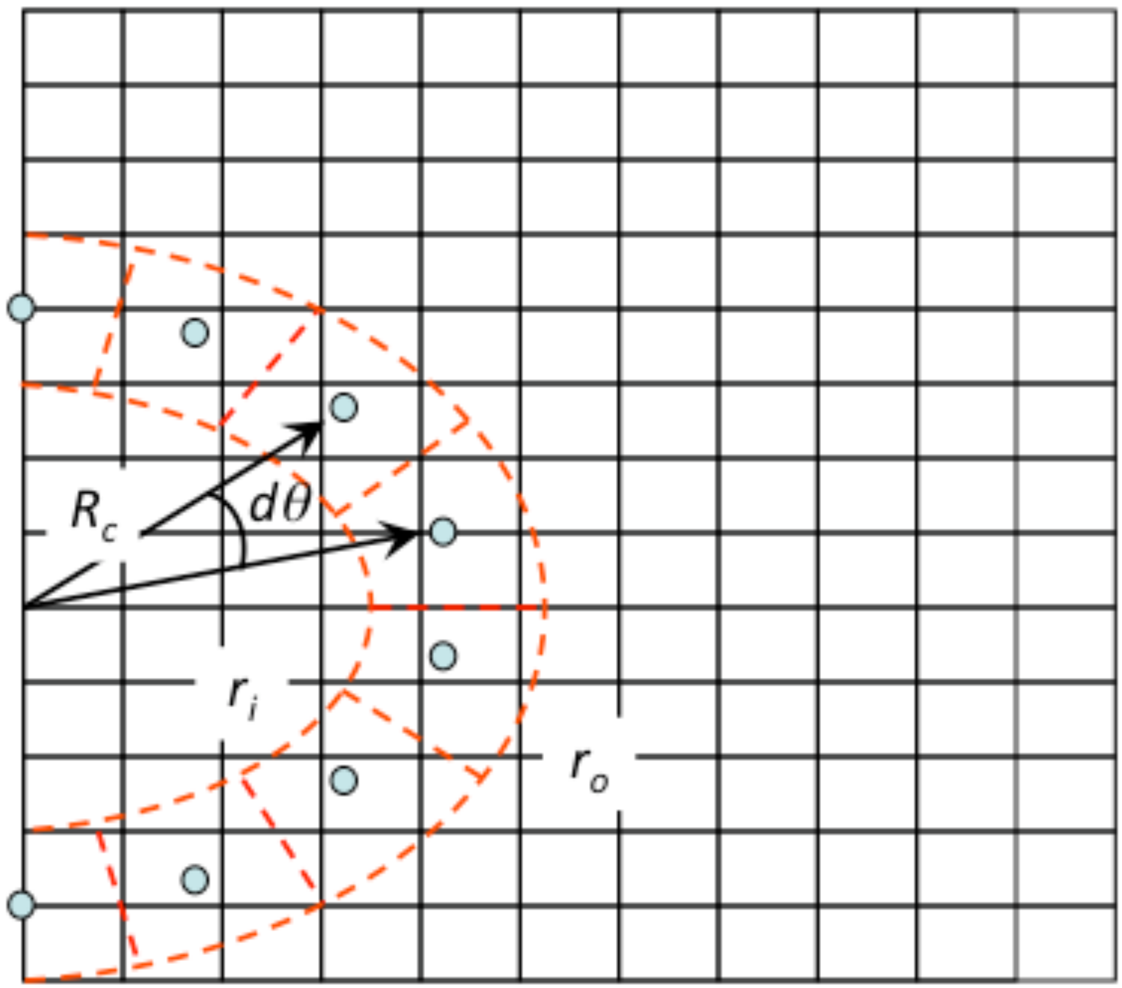
model

$$\frac{(\rho\vec{u}\,')-(\rho\vec{u}^{\,n})}{\Delta t} = \underbrace{-\nabla\cdot(\rho\hat{u}\vec{u})^{n} + \nabla\cdot\boldsymbol{\tau}^{n} - \nabla p\big|_{c}^{n}}_{rhs^{n}}$$

$$\frac{(\rho\vec{u}\,'')-(\rho\vec{u}\,')}{\Delta t} = \vec{f}_{IB} + \vec{F}_{ST} + \nabla p^{n}$$

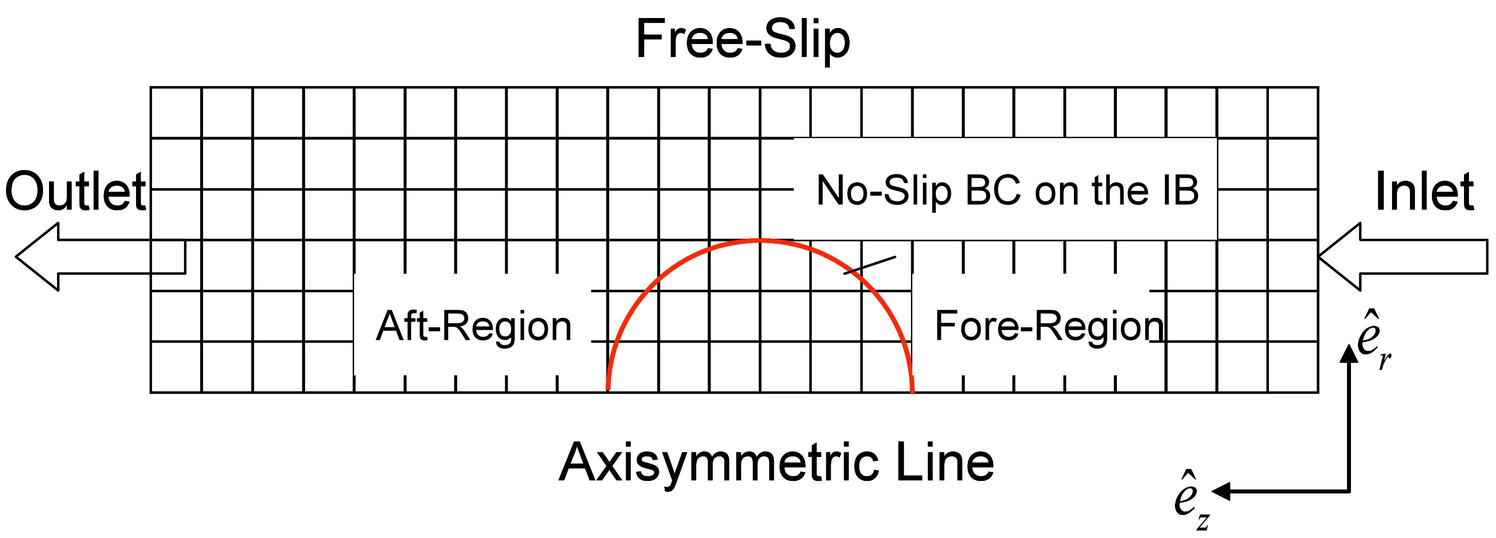
$$\nabla\cdot\left(\frac{\nabla p^{n+1}}{\rho}\right) = -\frac{\nabla\cdot(\vec{u}\,'')}{\Delta t}$$

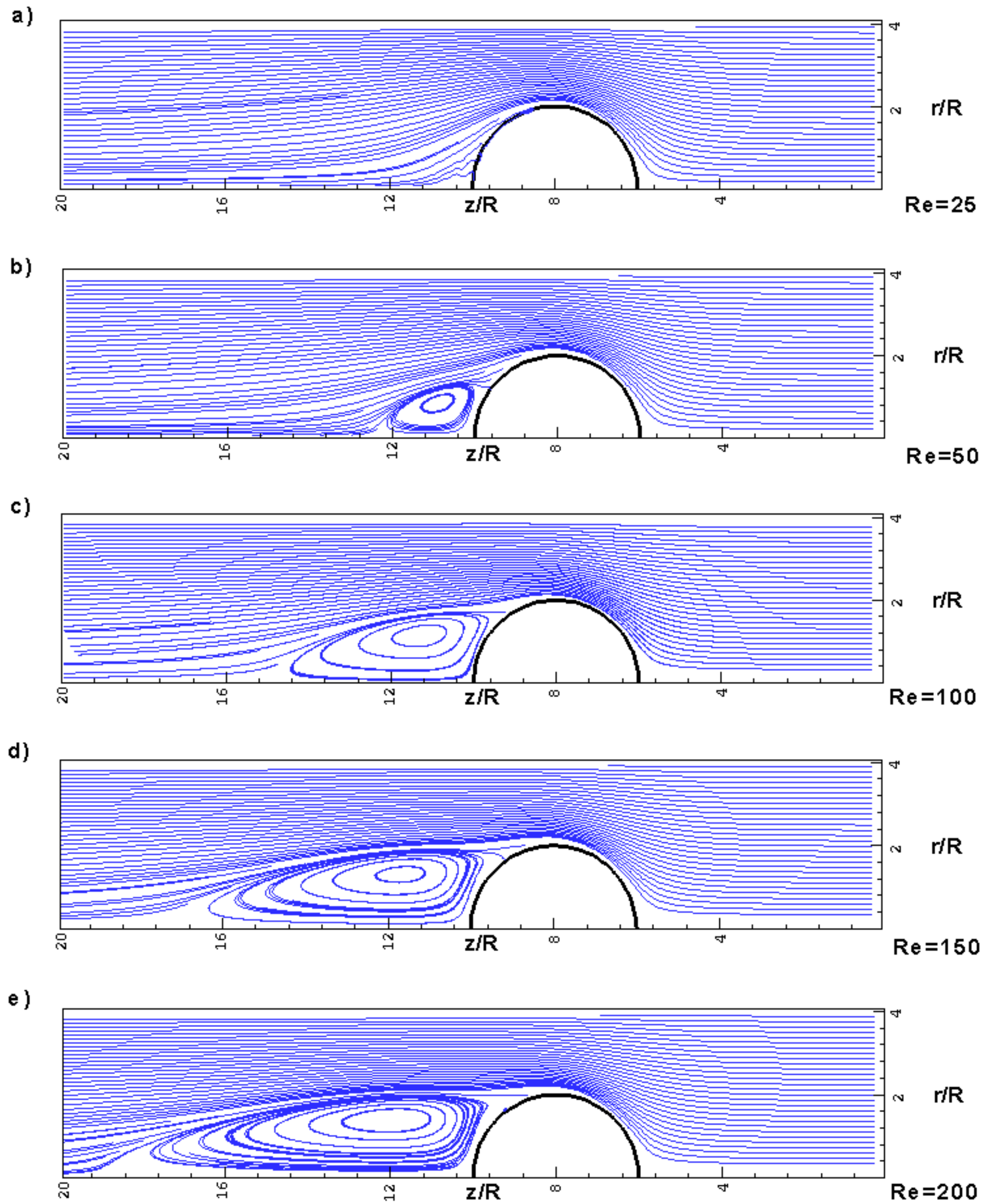
IB method of Uhlmann

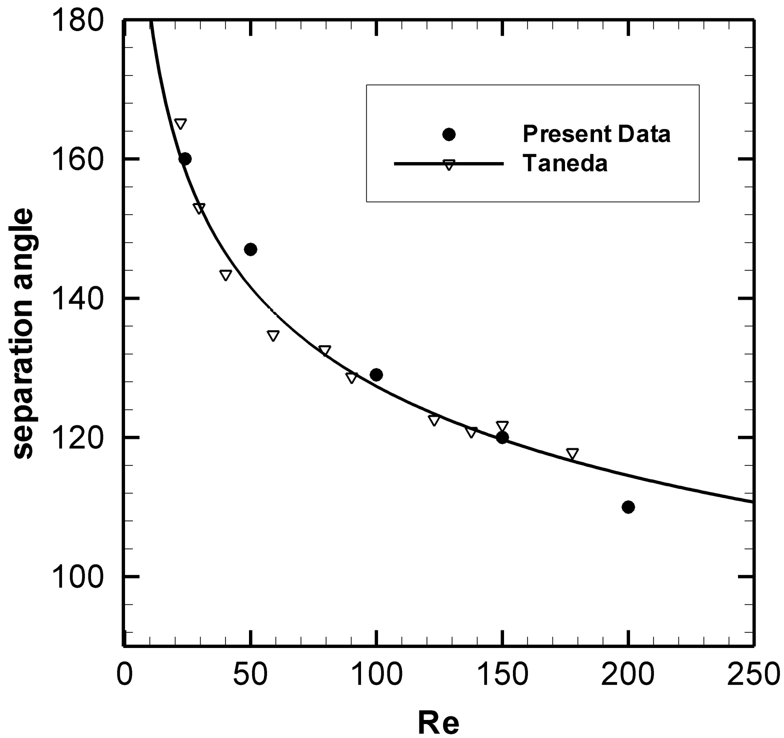


Validation

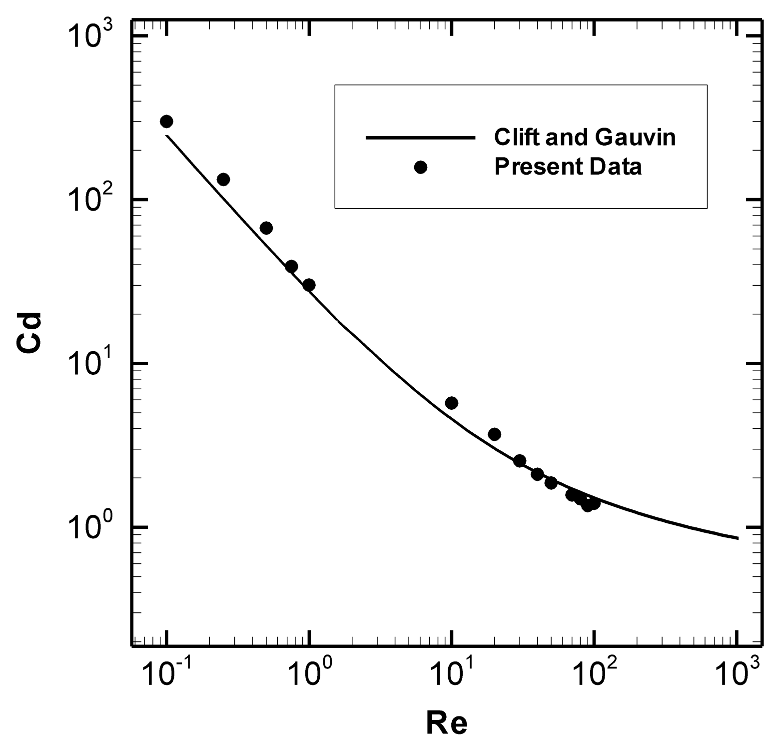
axisymmetric flow past a solid sphere, at various Re




a)
r/R
z/R
Re=25
b)
r/R
z/R
Re=50
c)
r/R
z/R
Re=100
d)
r/R
z/R
Re=150
e)
r/R
z/R
Re=200
20
16
12
8
4
2



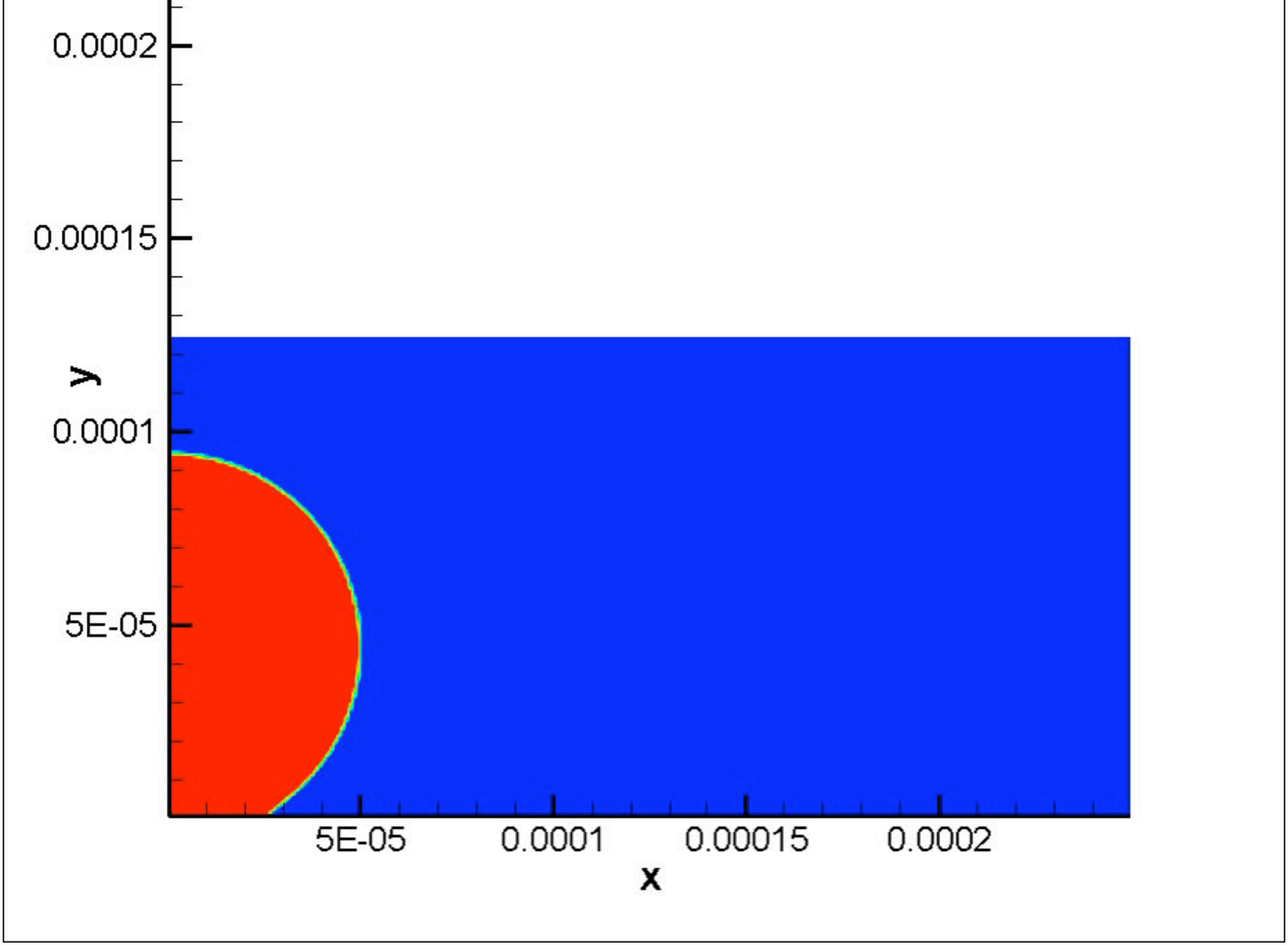
180
160
140
120
100
separation angle
0
50
100
150
200
250
Re
Present Data
Taneda



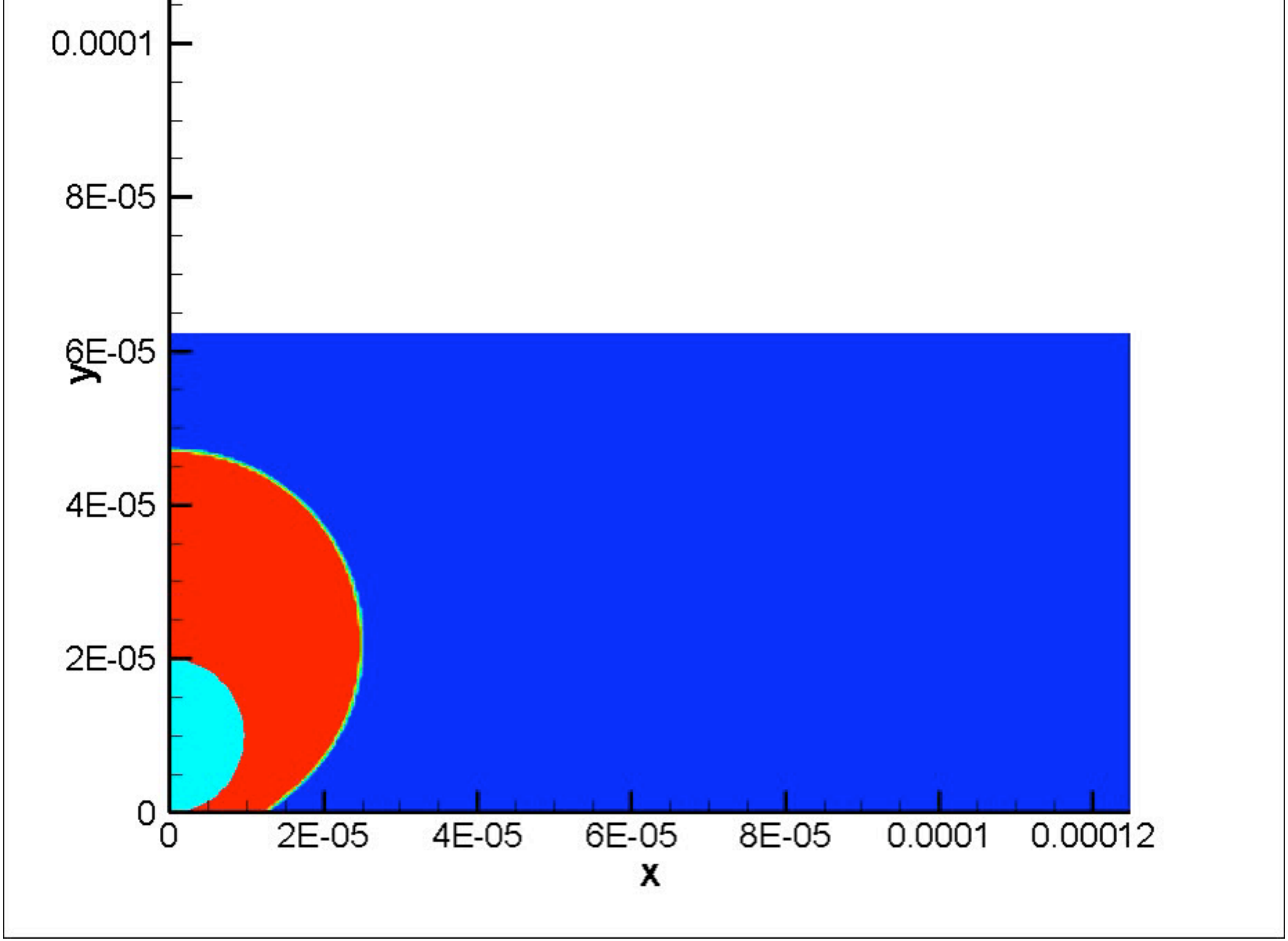
10^3
10^2
10^1
10^0
Cd
10^{-1}
10^0
10^1
10^2
10^3
Re
Clift and Gauvin
Present Data

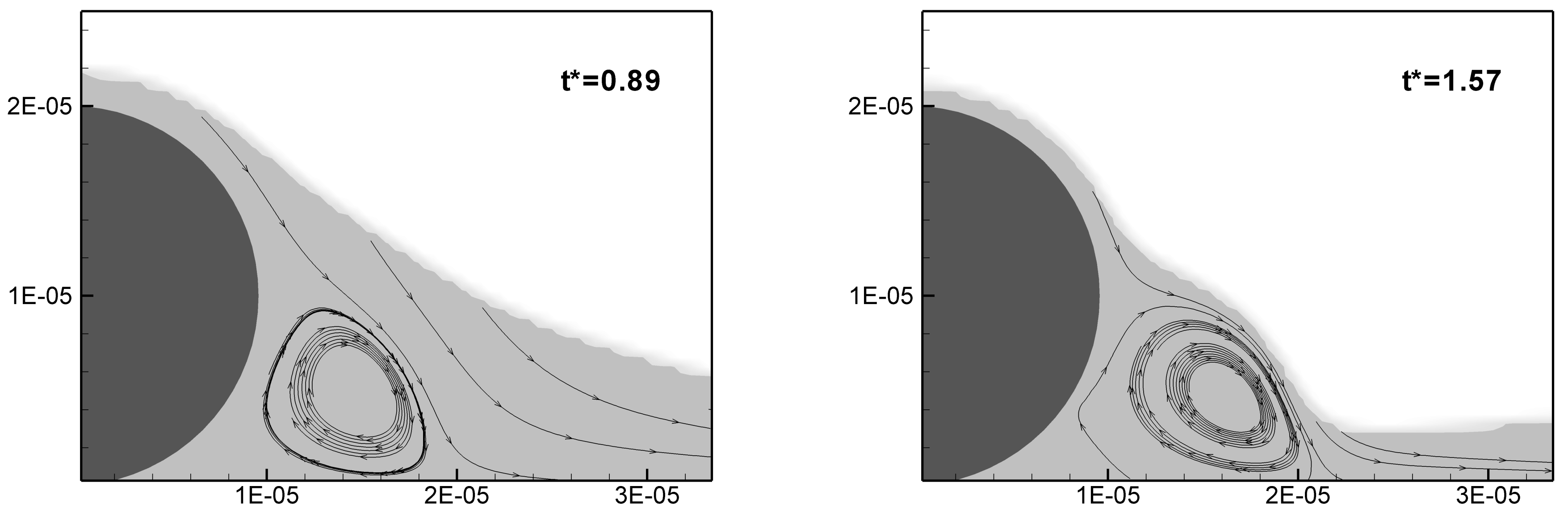
YSZ sims

	overall particle diameter	solid core diameter	impact velocity (m/s)
1	100 μm	0 μm	100 m/s
2		20 μm	
3		40 μm	
4	50 μm	10 μm	
5		20 μm	
6		30 μm	
7	100 μm	50 μm	100 m/s
8			200 m/s
9			250 m/s

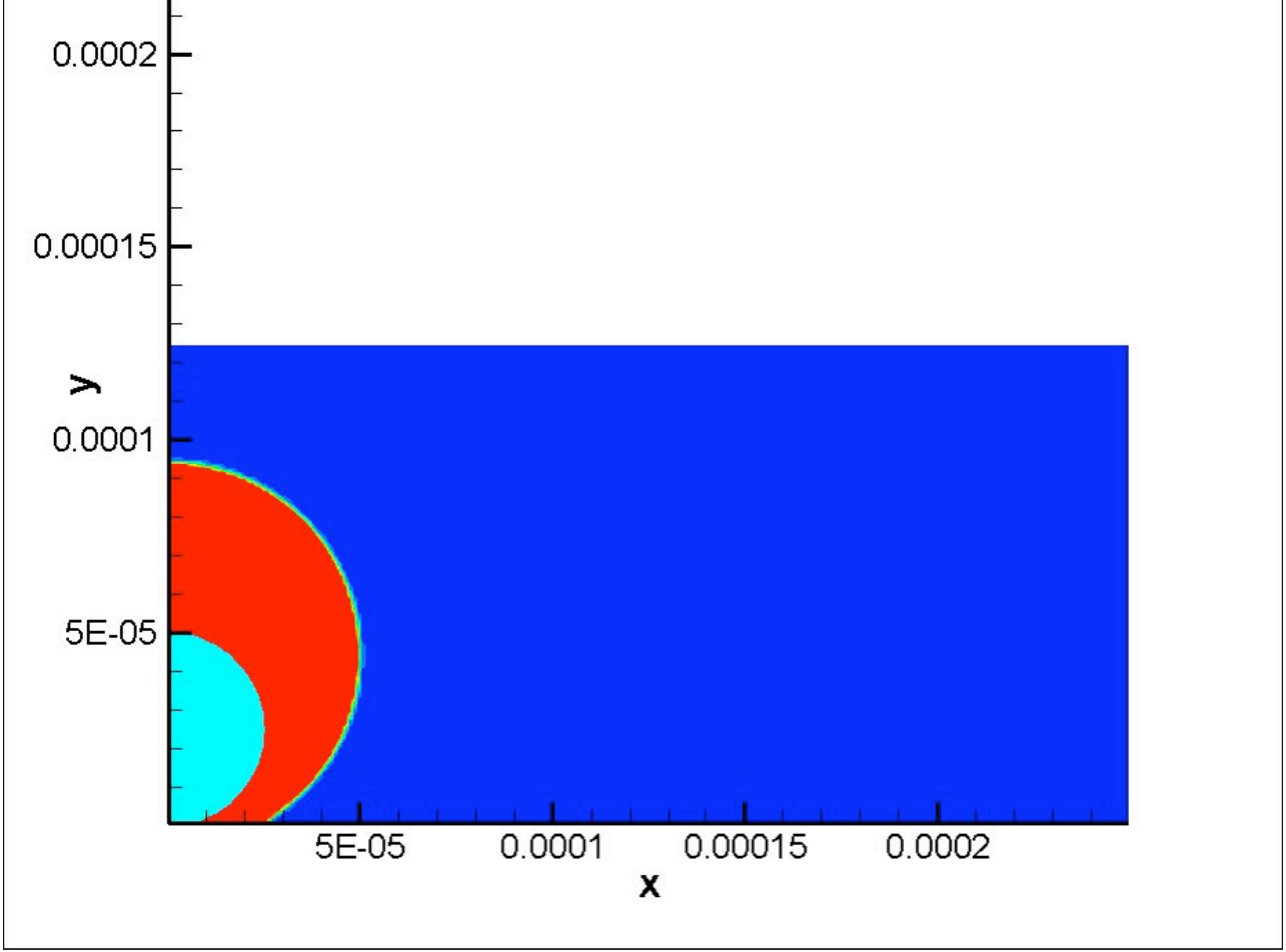


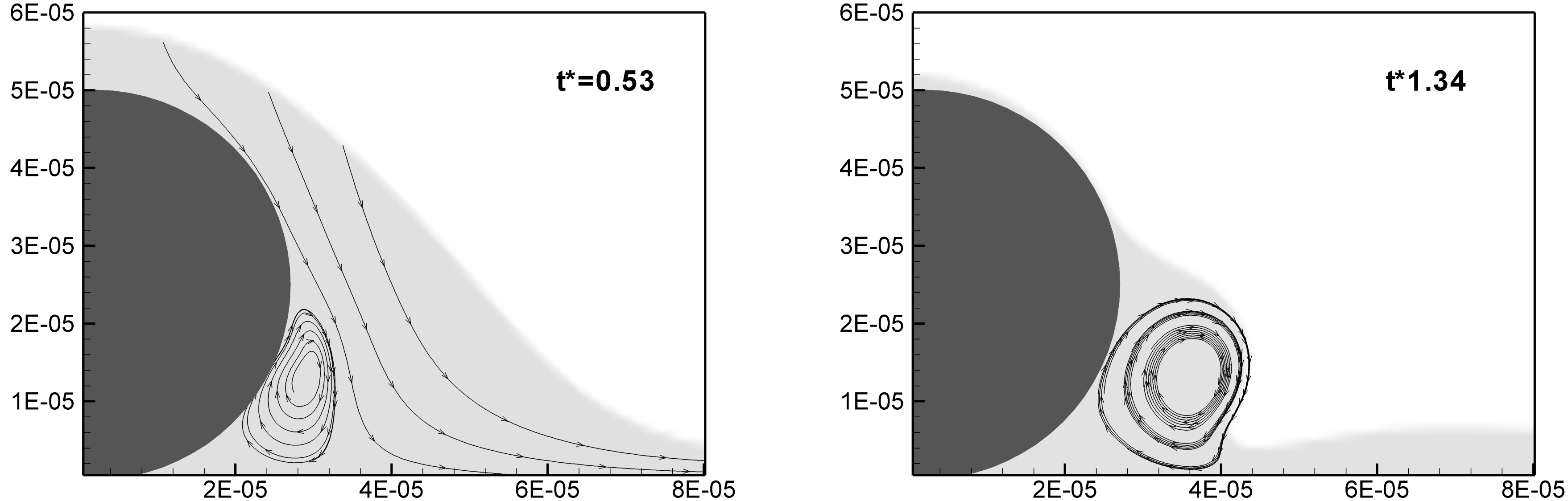
0.0002
0.00015
y
0.0001
5E-05
5E-05
0.0001
0.00015
0.0002
x


0.0001
8E-05
6E-05
4E-05
2E-05
0
y
0
2E-05
4E-05
6E-05
8E-05
0.0001
0.00012
x



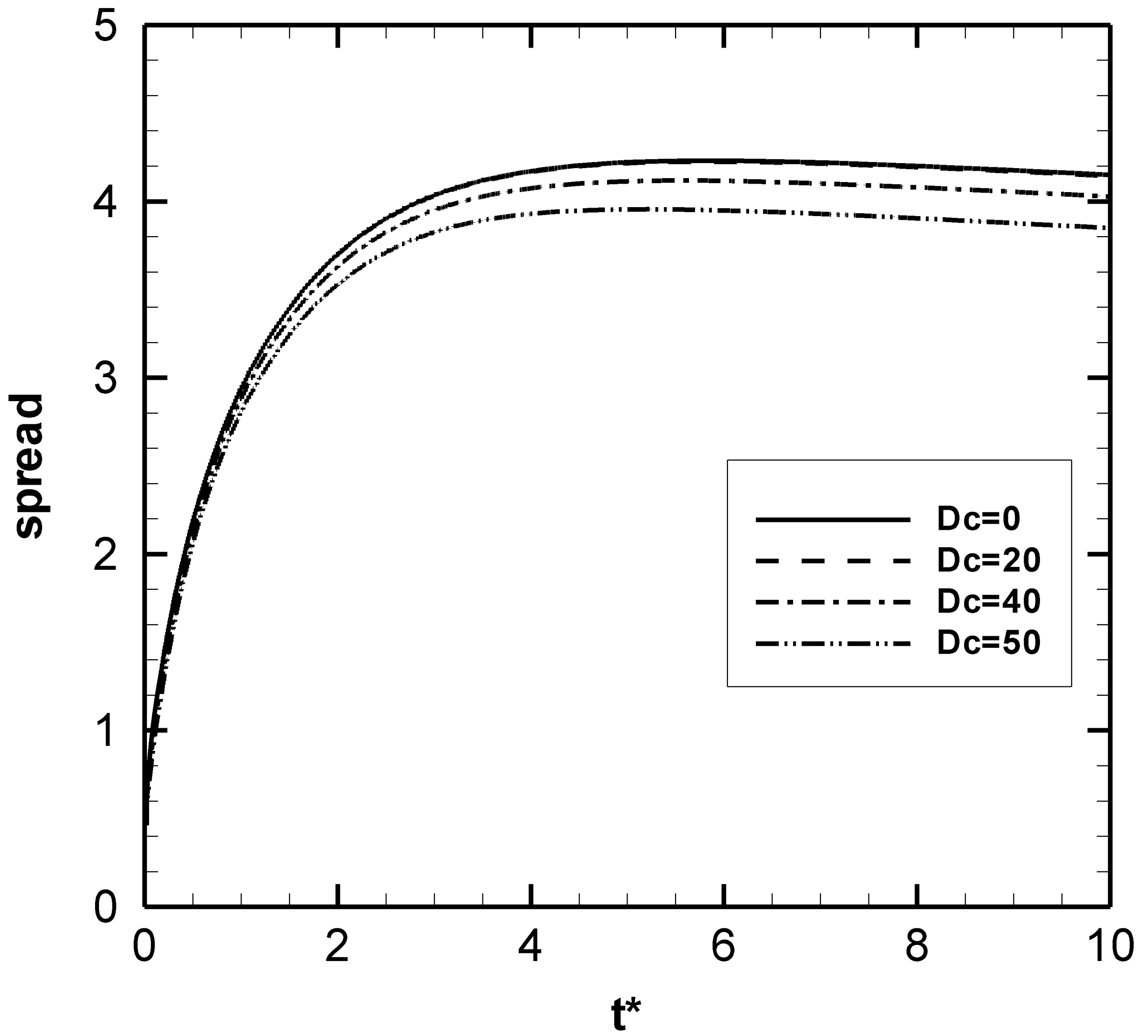
t*=0.89
2E-05
1E-05
1E-05
2E-05
3E-05
t*=1.57
2E-05
1E-05
1E-05
2E-05
3E-05


0.0002
0.00015
y
0.0001
5E-05
5E-05
0.0001
0.00015
0.0002
x



6E-05
5E-05
4E-05
3E-05
2E-05
1E-05
2E-05
4E-05
6E-05
8E-05
t*=0.53
t*1.34

Spread – 100 μm, 100 m/s



Spread – 50 μm, 100 m/s