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What's sour and what's sweet in modelling and validating metal processing

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University of Leicester, UK

Third International workshop on validation of computational mechanics models,
12th June, 2014 at the Neus Rathaus, Munchen

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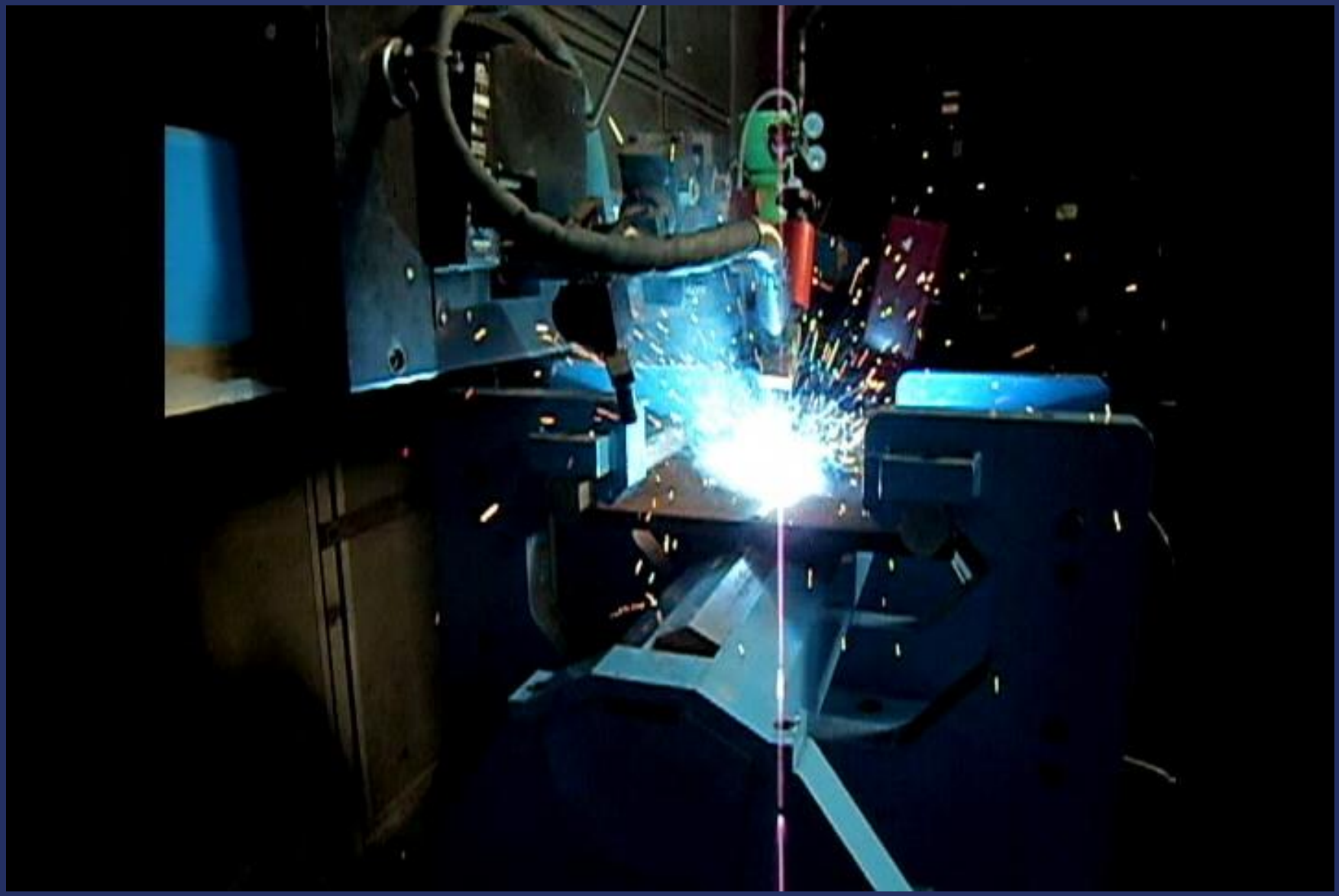
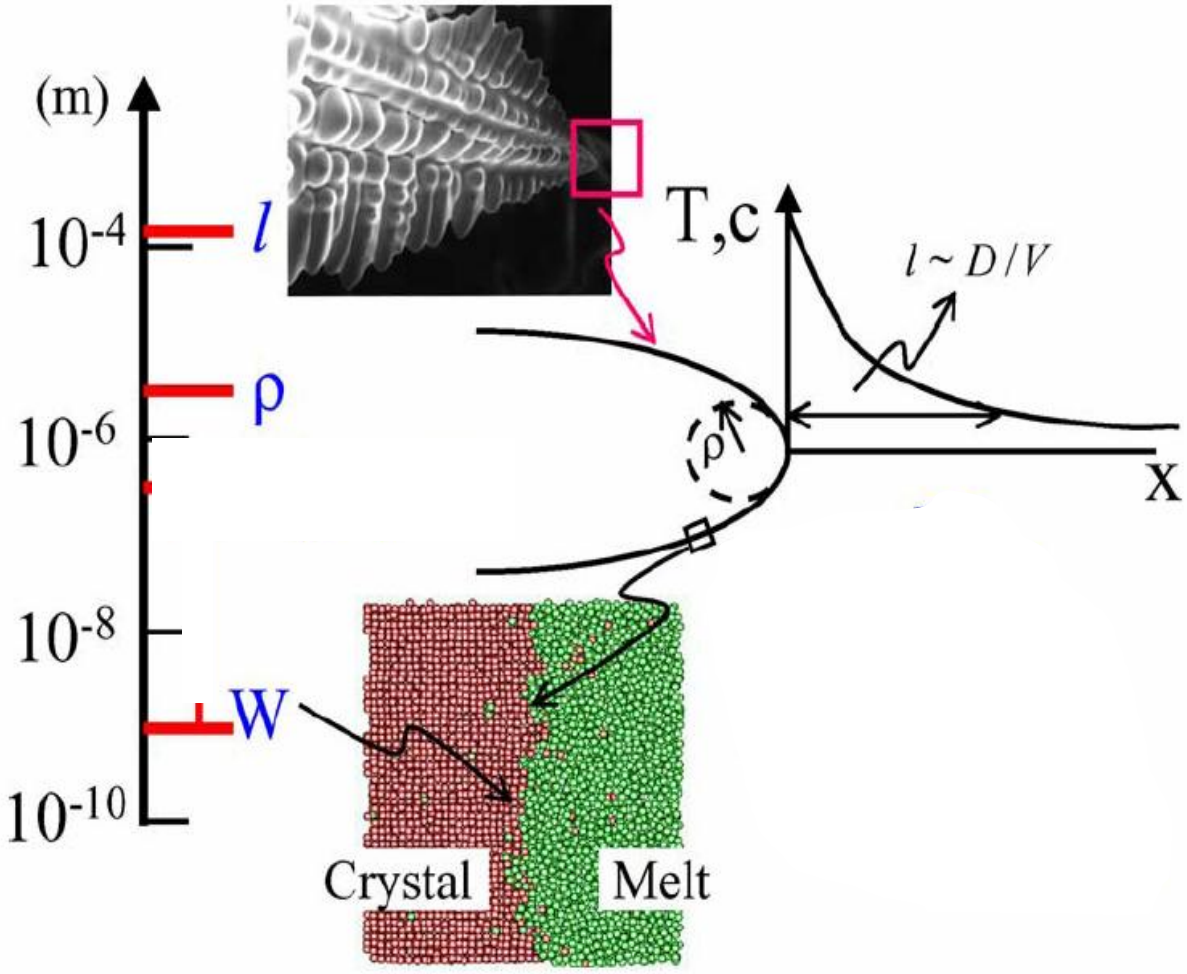
Welding Process



Multi-scale challenge of metal processing (solidification and its application in casting and welding)



energetic and kinetic properties of S/L are determined by atomic scale processes acting over the nano-meter scale with width *W* of the real S/L interface.

W is three-orders of magnitude smaller than the curvature of the dendritic tip (ρ),

Dendritic tip radius (ρ) is one or two orders of magnitude smaller than the thickness of the solute diffusion boundary layer (*l*) .

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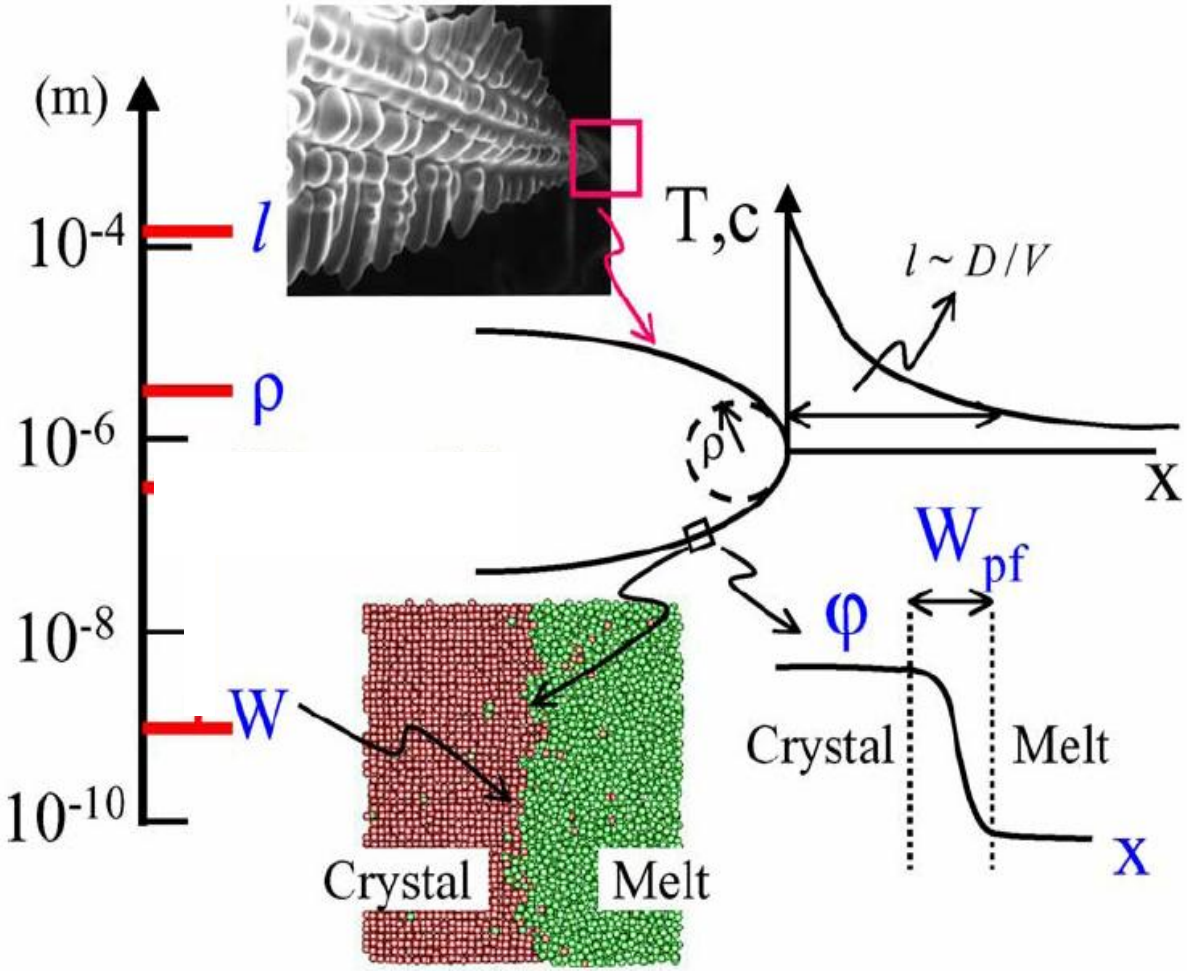

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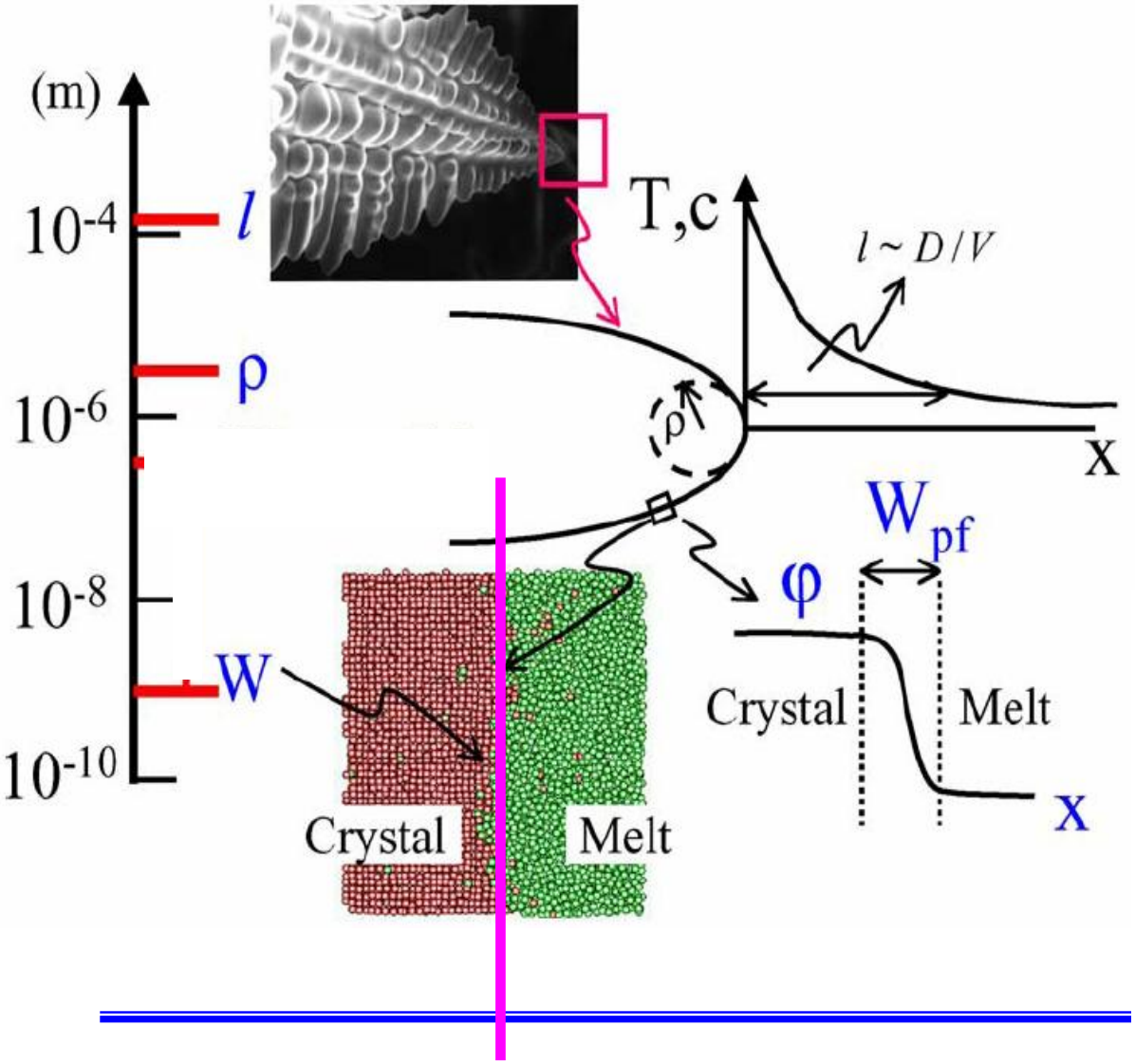

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Phase field simulations of dendritic growth use a microscopic interface width (W_{PF}).

W_{PF} >>*W* and is just small enough to resolve the curvature of the advancing crystals, but large enough to render the computations tractable.

scale (time/length)

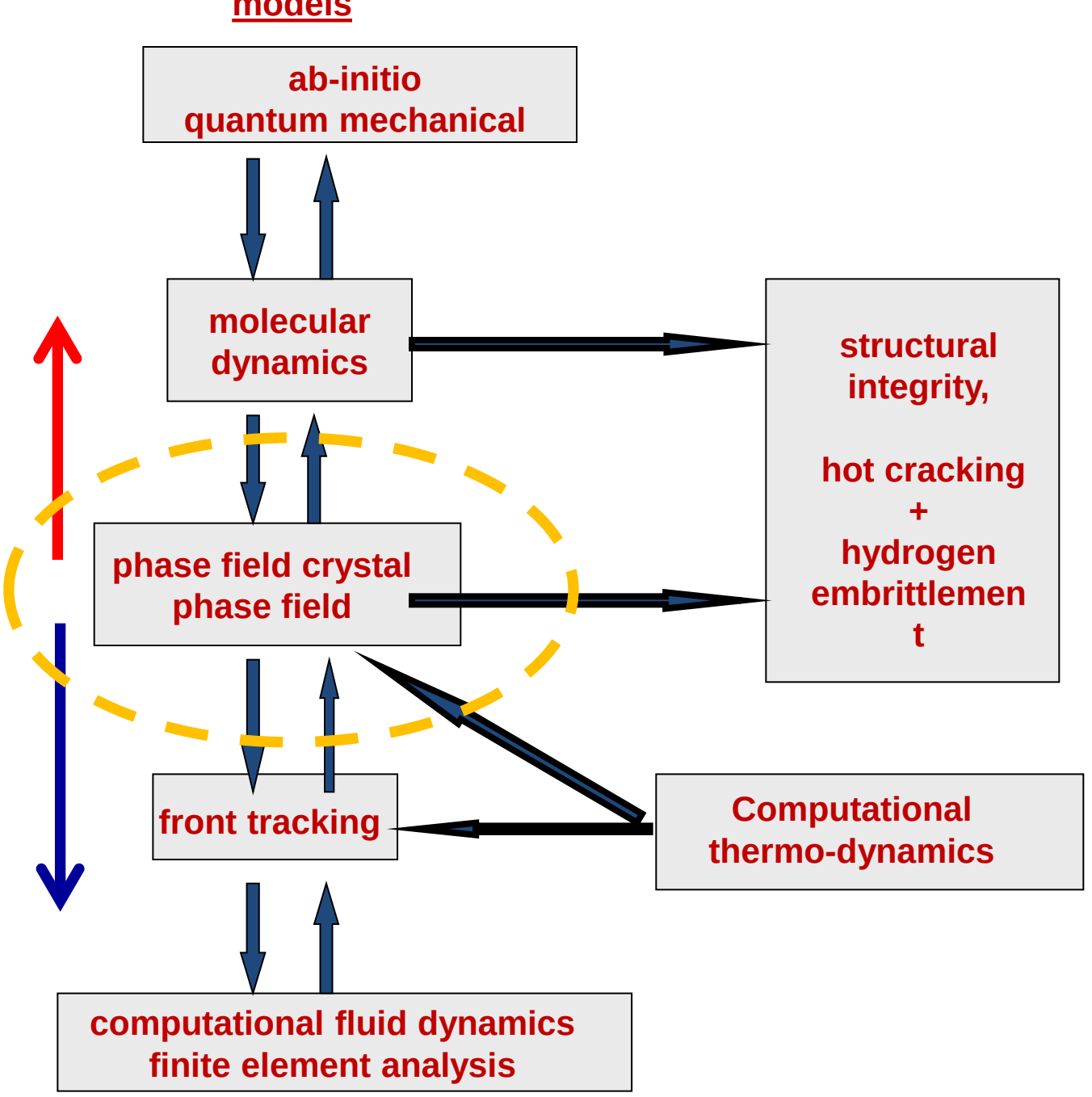
quantum
(10^{-12}s / 10^{-10} to 10^{-9}m)

classical
(10^{-7}s / 10^{-9} to 10^{-8}m)

nano-micro
(10^{-3}s / 10^{-9} to 10^{-3}m)

grain
(10^{-3} to 10^{1}s / 10^{-4} to 10^{-2}m)

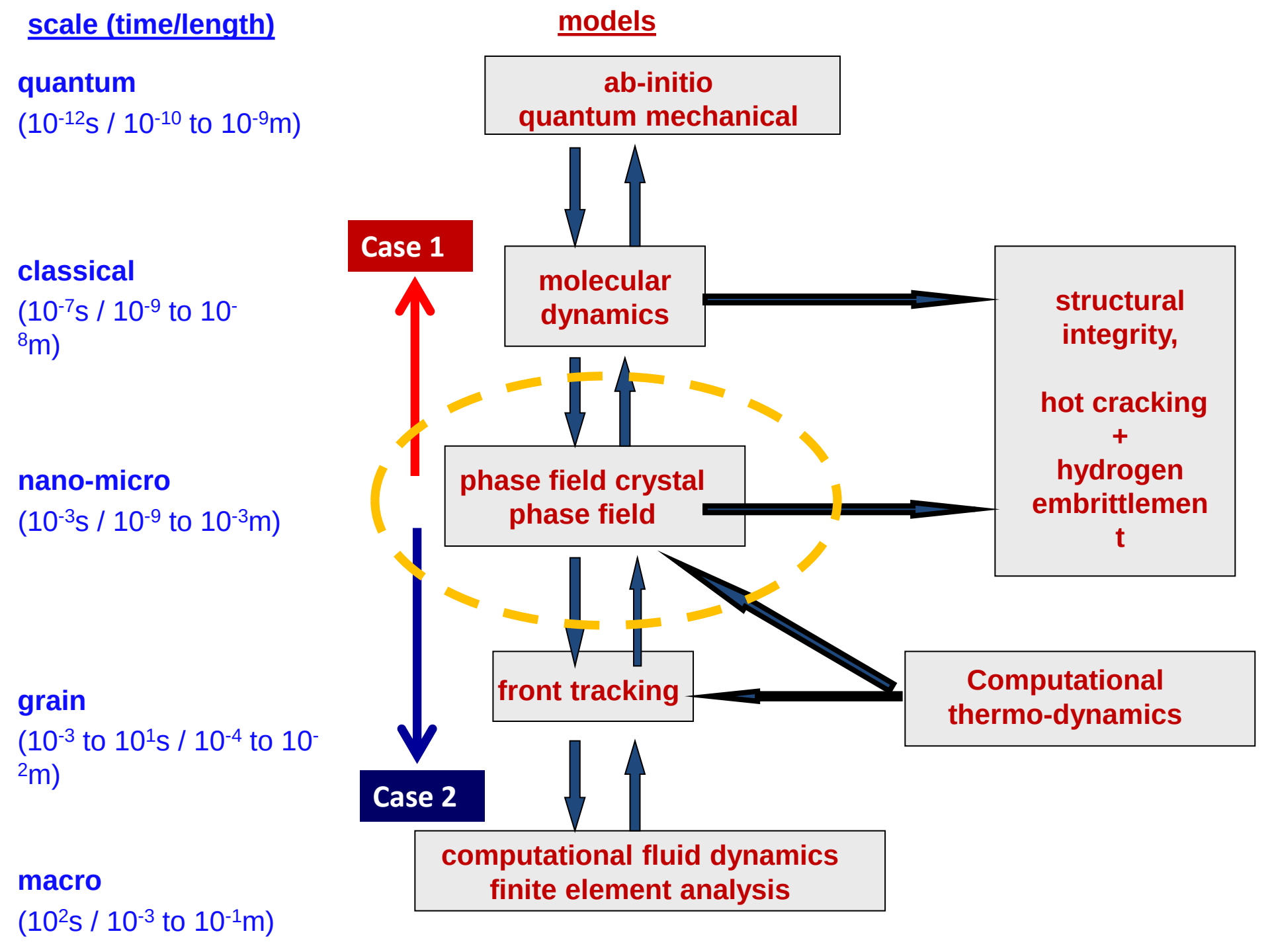
macro
(10^{2}s / 10^{-3} to 10^{-1}m)



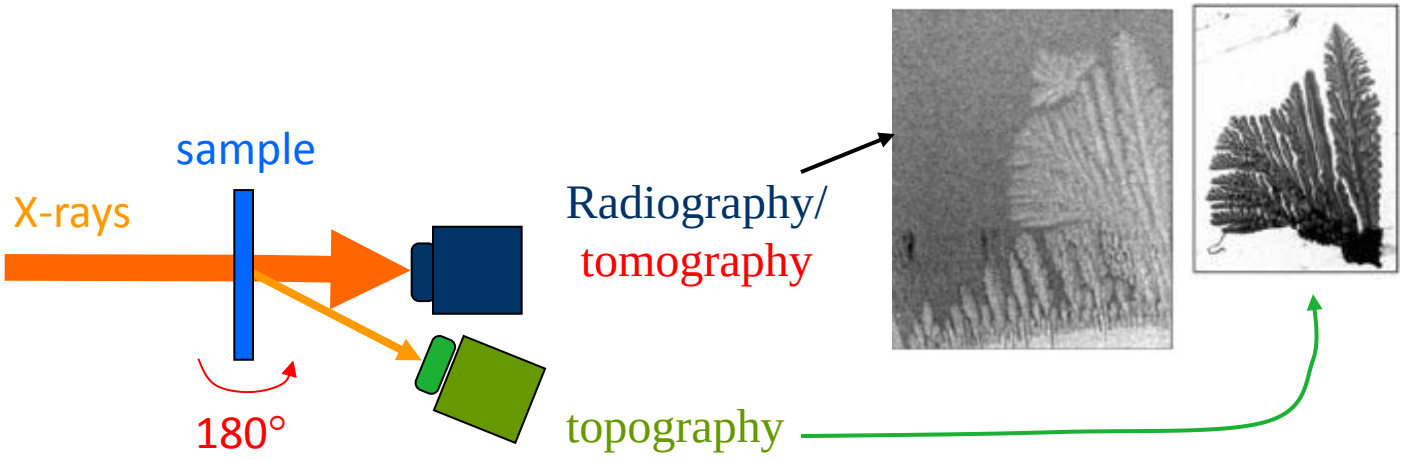
Modelling linking and Integration :
EU FP7 Project in Multi-scale Modelling of Welding

MintWeld
COOPERATION

U. Leicester, UK
UCD, Ireland
U. Oxford, UK
TUDelft , Netherlands
KTH , Sweden
NTNU, Norway
TWI, UK
Tata Steel
ISPL, Poland
FRENZAK, Poland
EPFL , Switzerland


scale (time/length)
models
quantum
(10-12s / 10-10 to 10-9m)
classical
(10-7s / 10-9 to 10-8m)
nano-micro
(10-3s / 10-9 to 10-3m)
grain
(10-3 to 101s / 10-4 to 10-2m)
macro
(102s / 10-3 to 10-1m)
ab-initio quantum mechanical
Case 1
molecular dynamics
structural integrity,
hot cracking + hydrogen embrittlement
phase field crystal phase field
front tracking
Computational thermo-dynamics
Case 2
computational fluid dynamics finite element analysis

Phenonmena can be validated (2 examples)

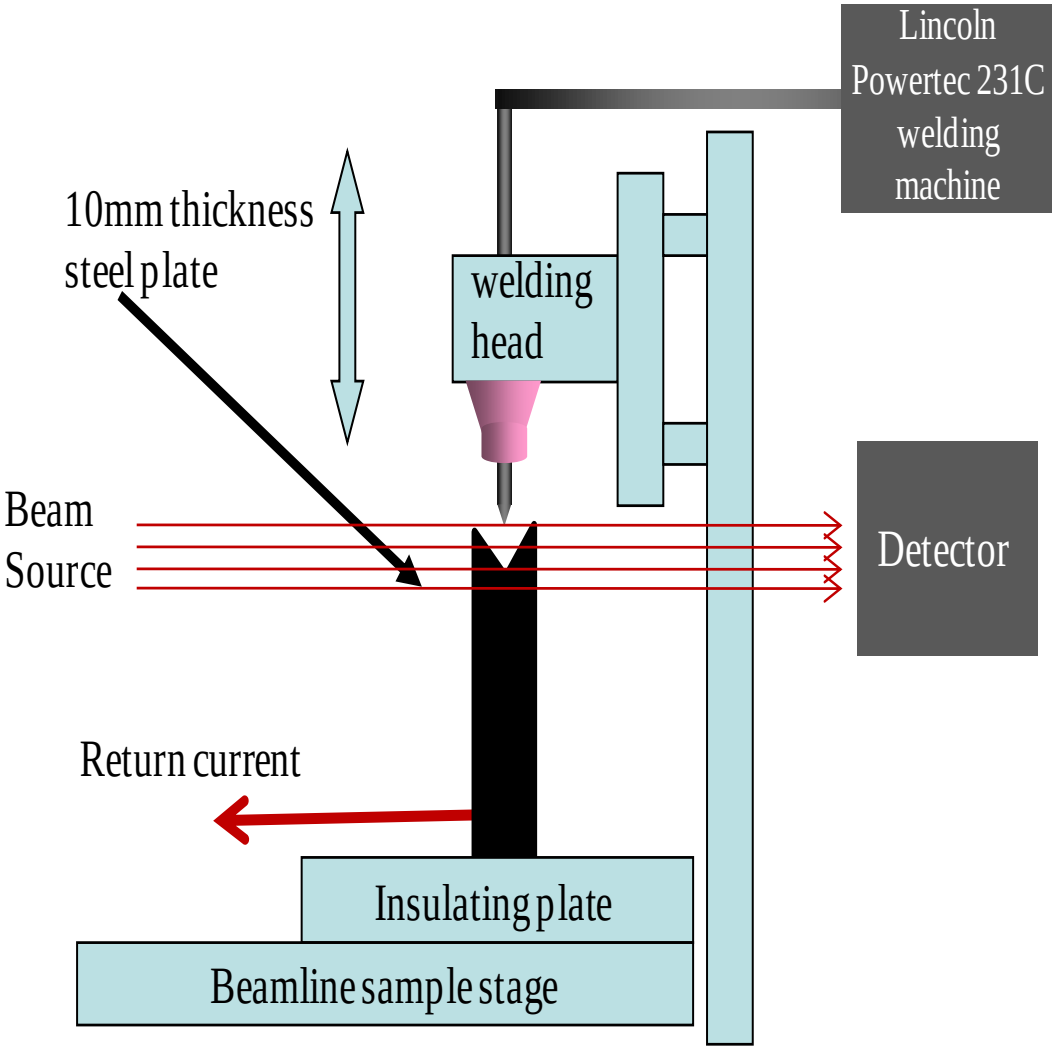


- In-situ SR radiography (1998 – NTNU (**ESRF**))
  - 2D, direct, Δr_n ~ 1.2 µm/ Δt_e ~ 0.1 s, good dynamic absorption/refraction contrast, alloys
  - s/l-interface, solute boundary, hydrodynamics
  - 2008: Performed by > 12 groups world wide

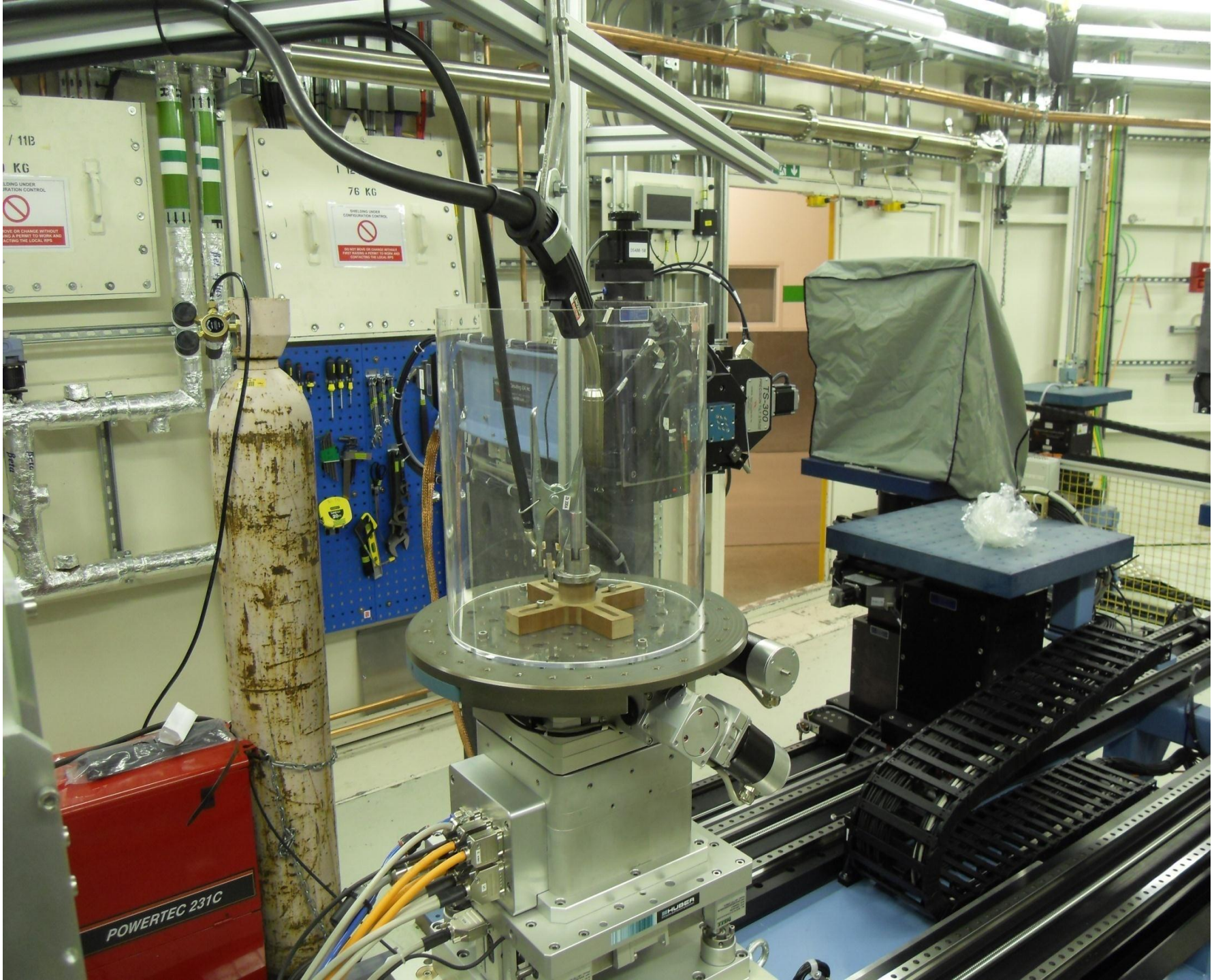
- Ultra-fast in-situ SR tomography (2004 - INPG (**ESRF**))
  - 3D indirect, Δr_n ~ 3 µm/ Δt_e ~ 10 s, absorption/refraction contrast, alloys, f_s > 0.3
  - s/l-interface, final stages of solidification (hot tears, porosity, precipitates)

X-ray imaging techniques

An industrial-scale arc-welding setup



remotely controlled metal active gas (MAG)


76 KG
POWERTEC 231C
HUBER

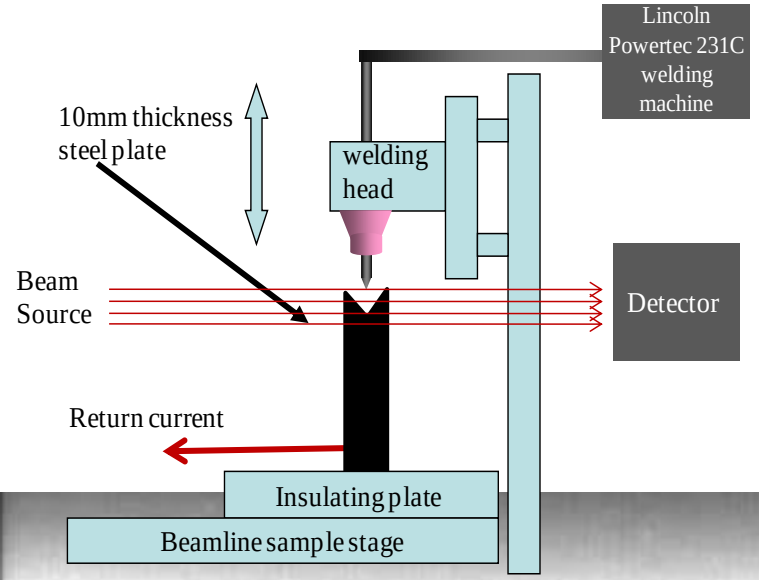
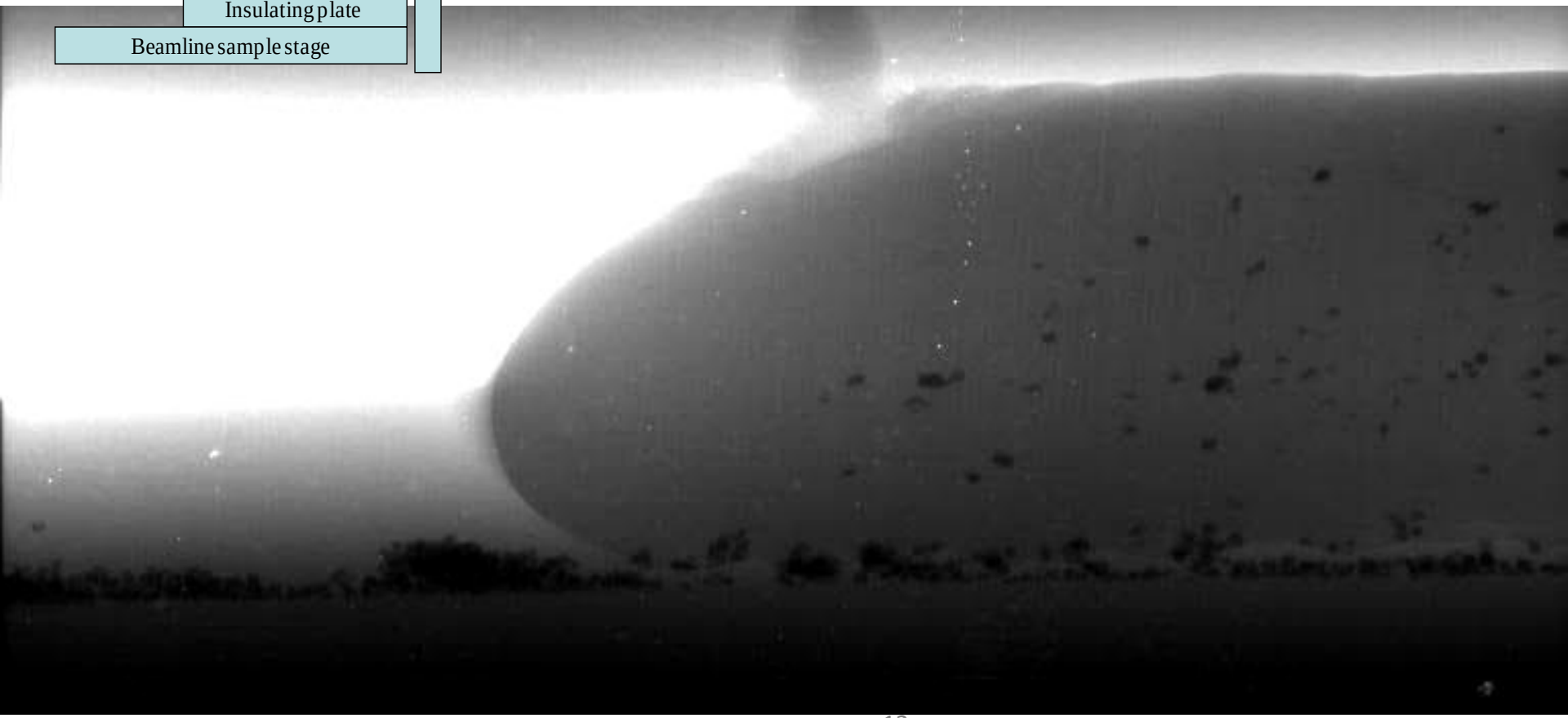
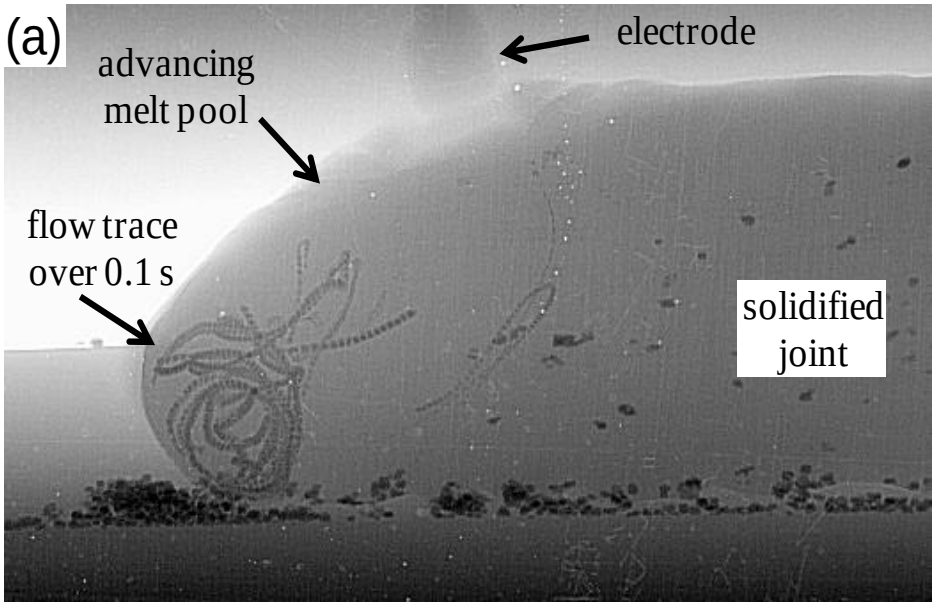
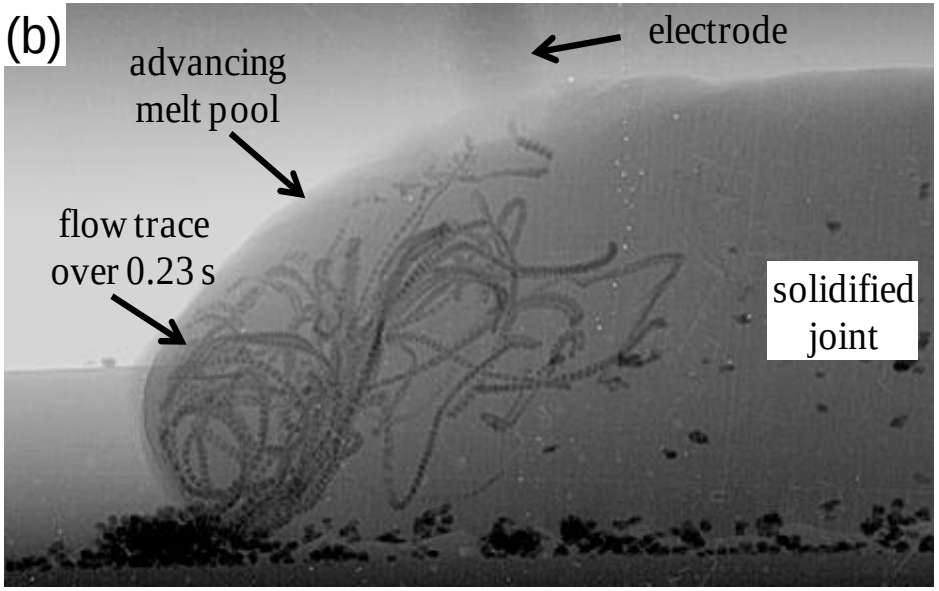


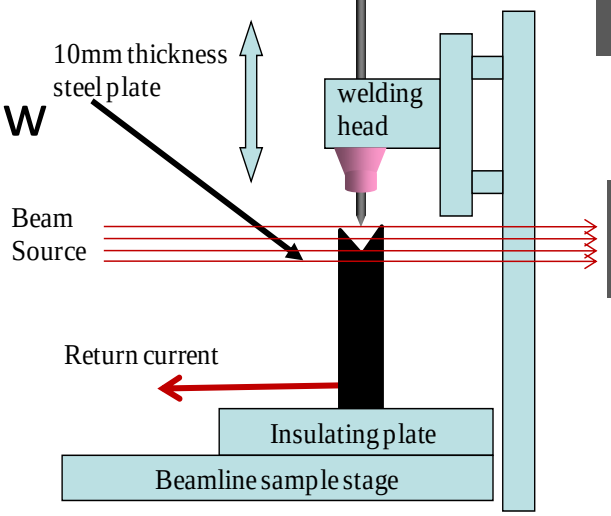
Image rate: 1000fps
Video rate: 30 fps



single streamlines of flow





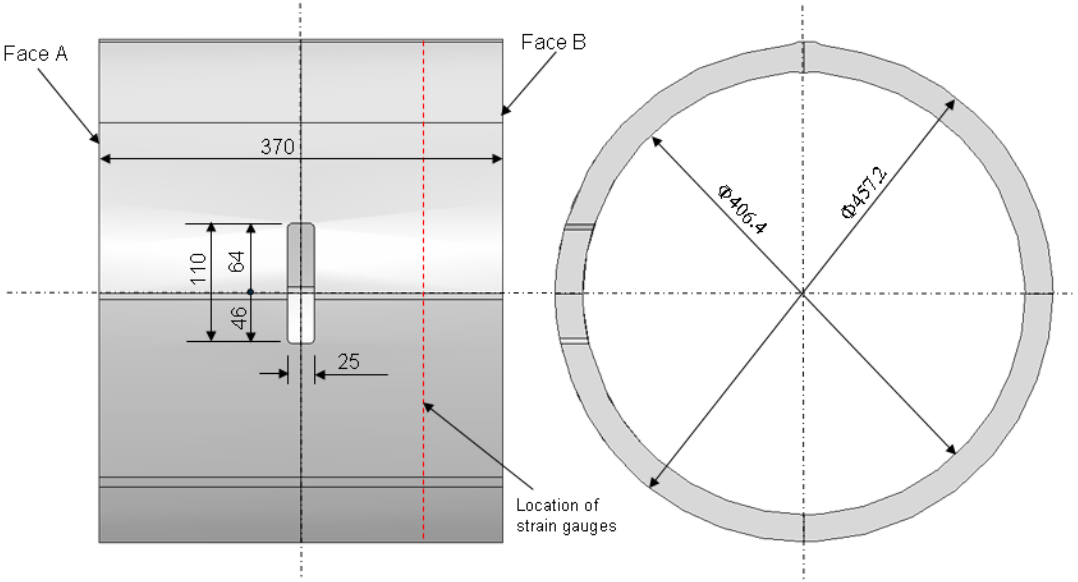


(a) over 50 mini seconds

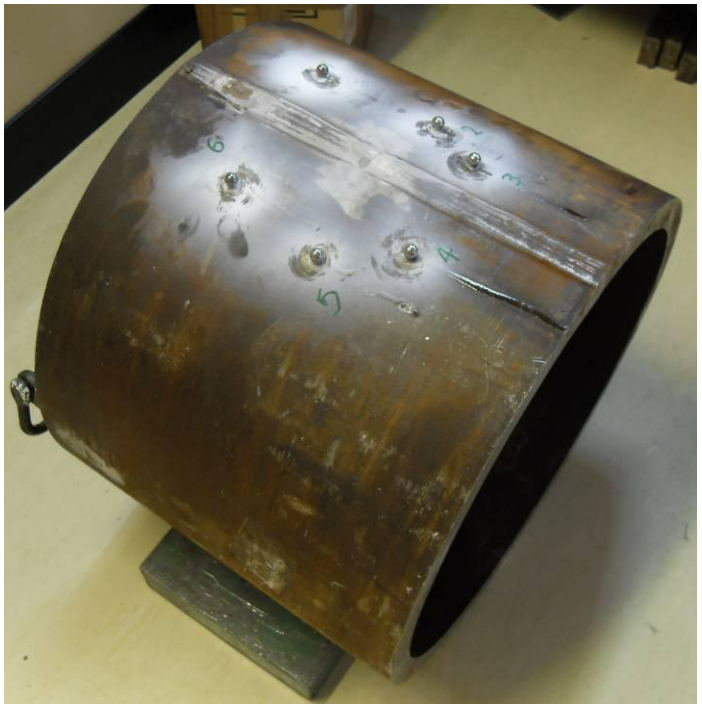
(b) over 120 mini seconds
(X-ray radiography)

Phenonmena can be validated (2nd examples)

Neutron diffraction residual stress measurement: UOE pipe

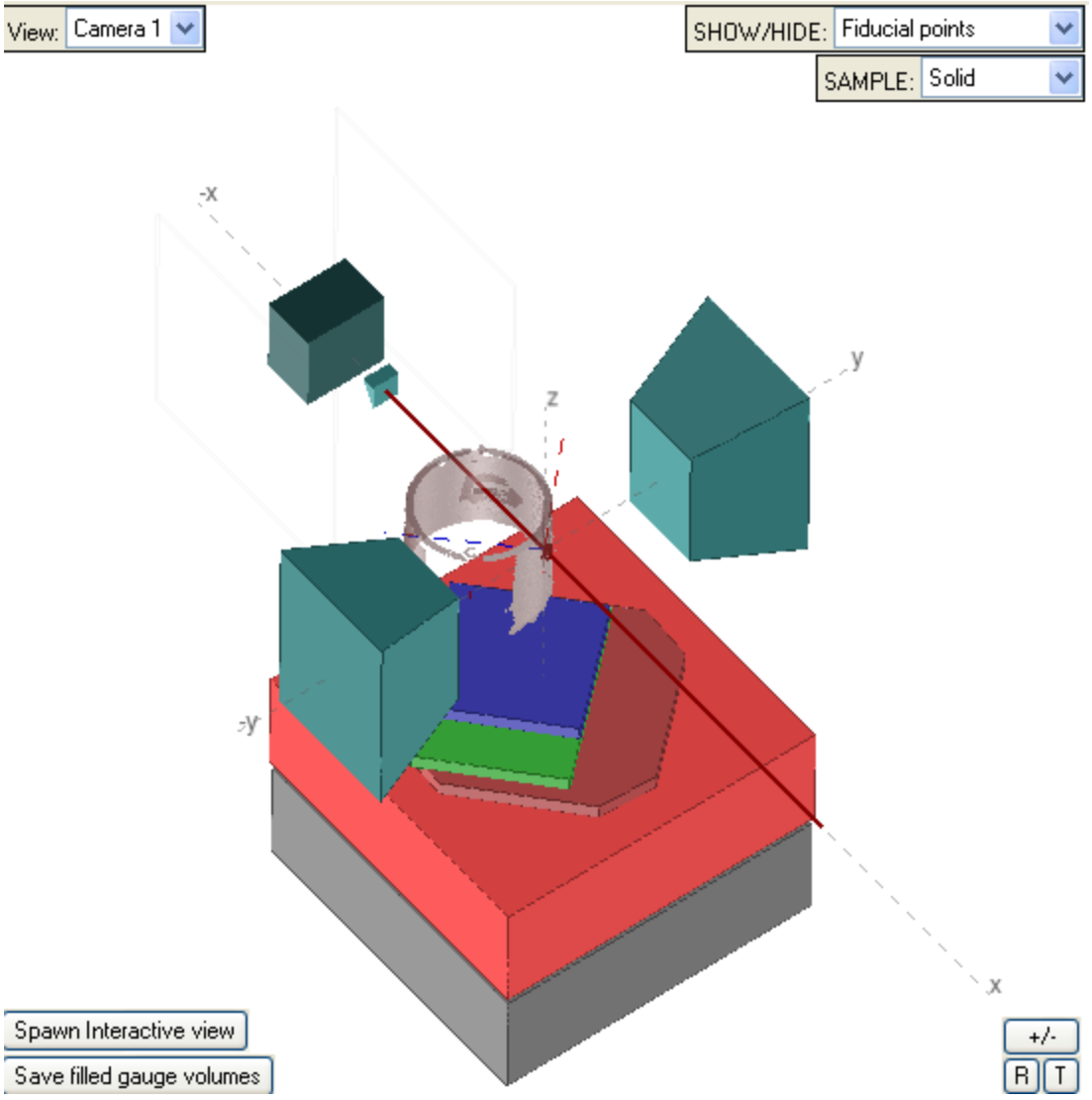


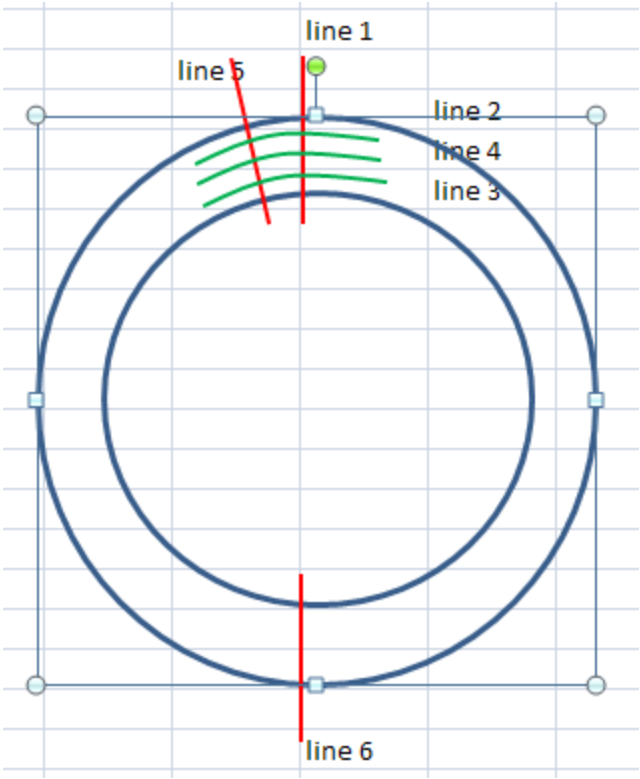
Pipe sample design & preparation



Actual pipe sample with fiducial points

Specimen design & preparation for D_0 scanning


View: Camera 1
SHOW/HIDE: Fiducial points
SAMPLE: Solid
-x
y
z
-y
x
Spawn Interactive view
Save filled gauge volumes
+/-
R
T


line 1
line 5
line 2
line 4
line 3
line 6

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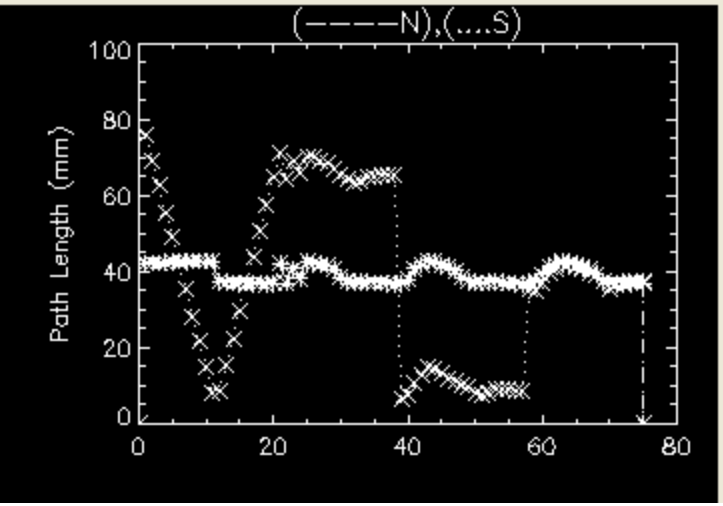
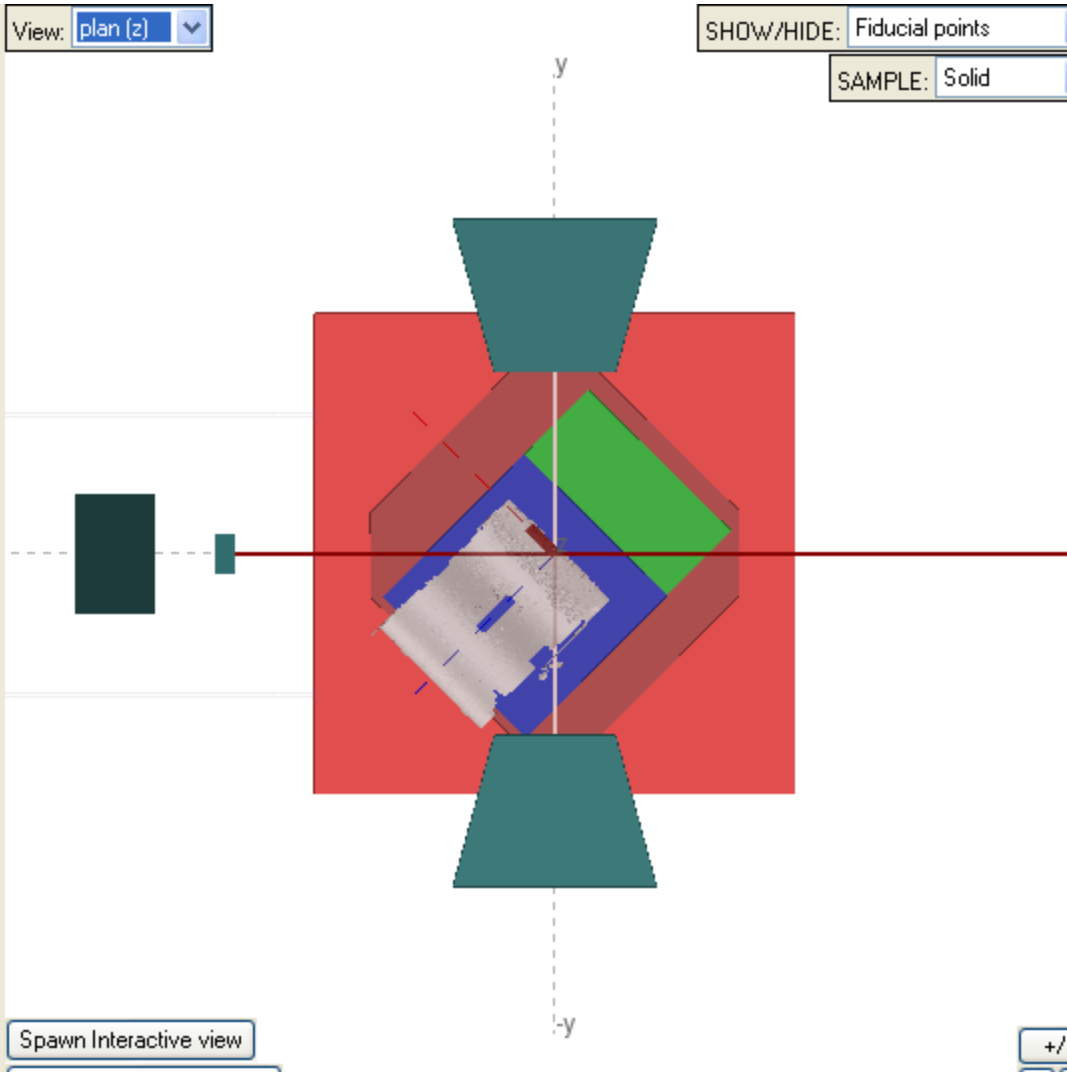
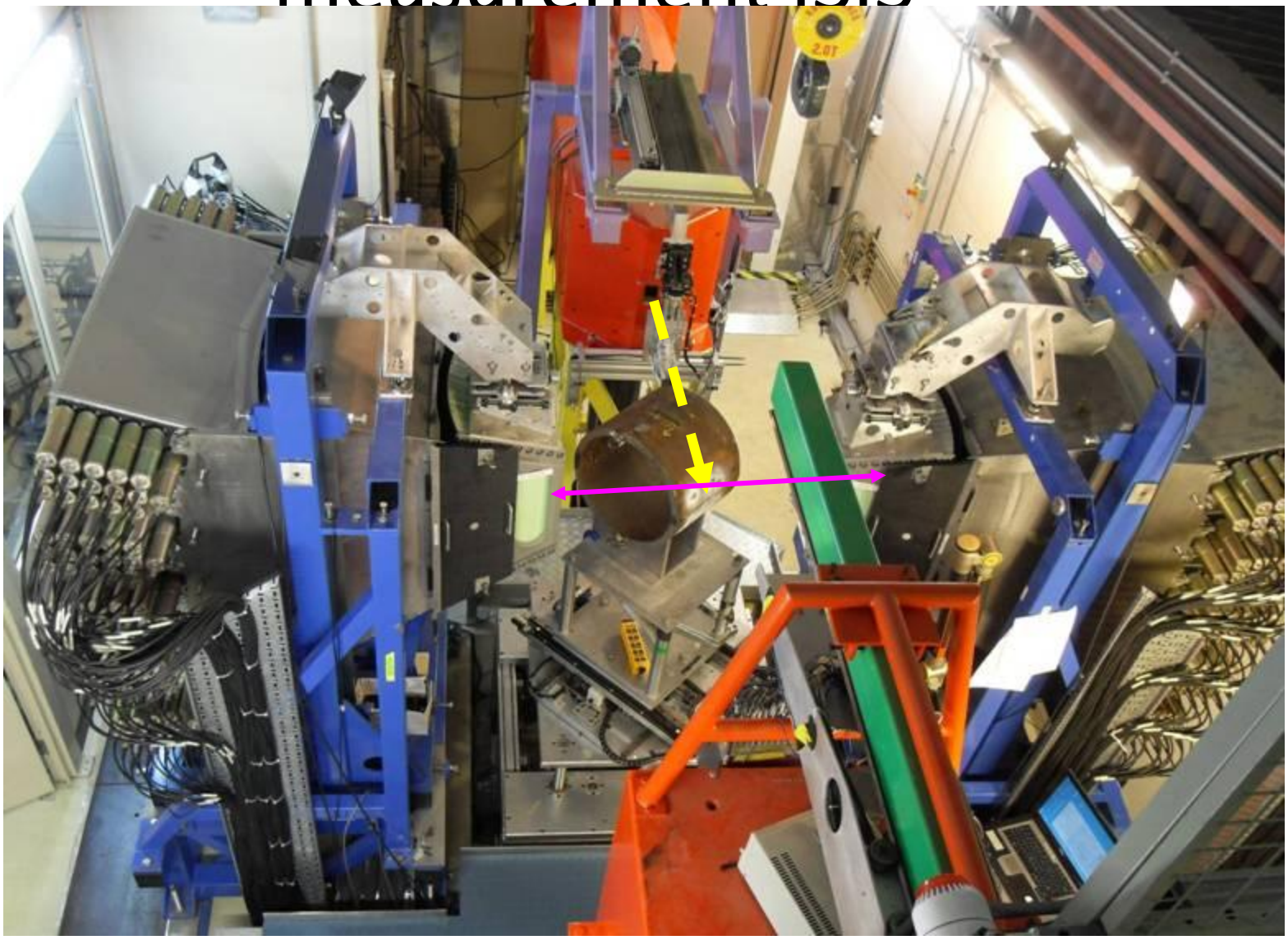
5: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
4: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
3: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
2: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
1: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
0: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
9: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
8: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
7: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
6: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
5: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
4: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
3: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
2: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg
1: Pos. Err: 0.000mm, Orient. Err (H): 0.000deg, Orient. Err (V): 0.493deg

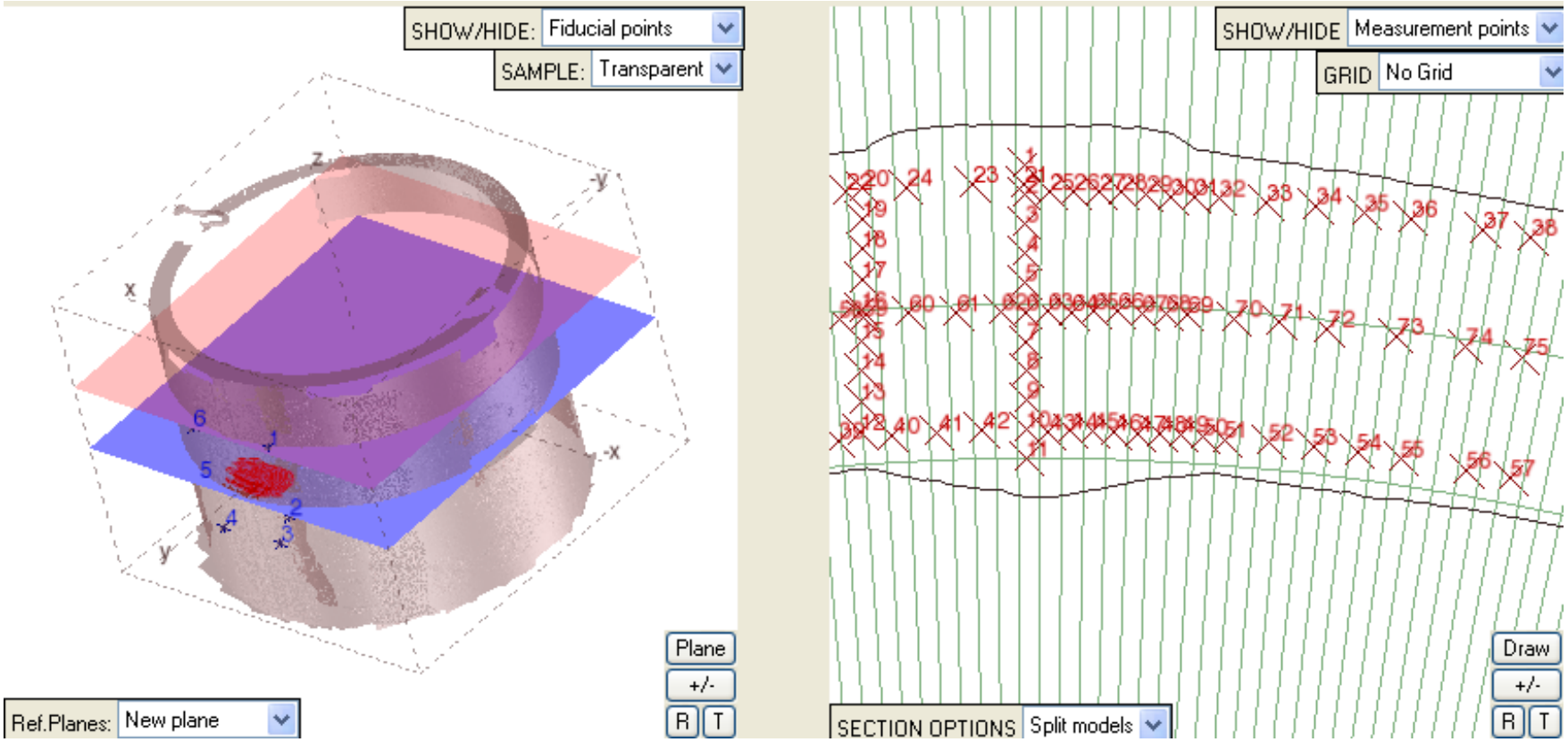




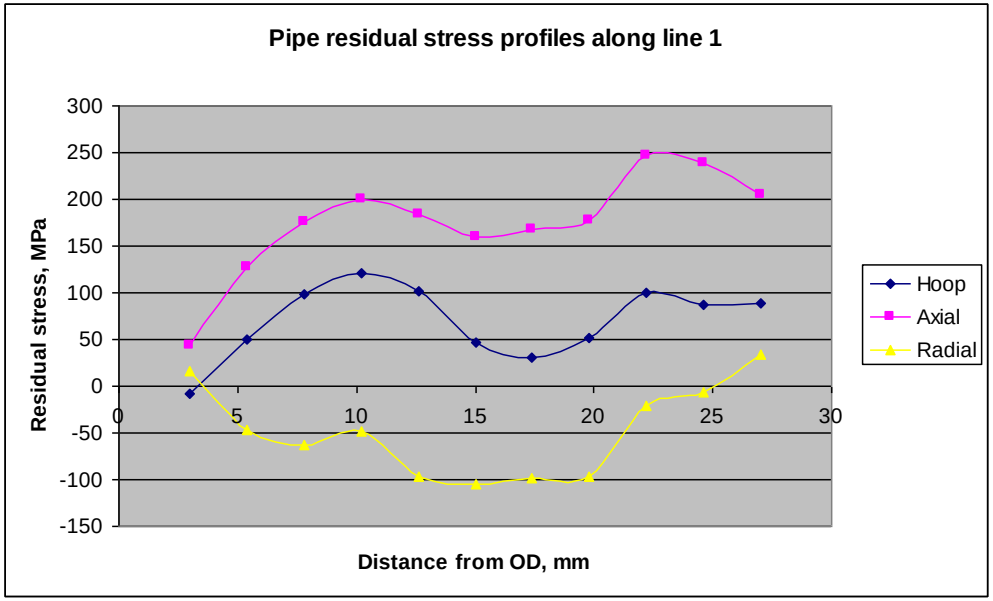
Neutron diffraction residual stress measurement ISIS

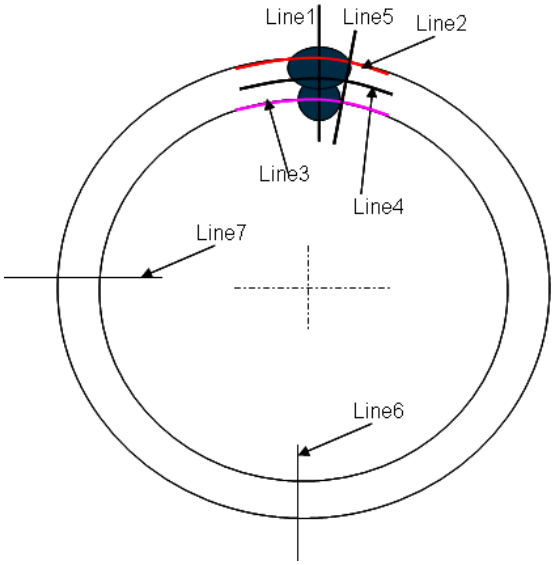


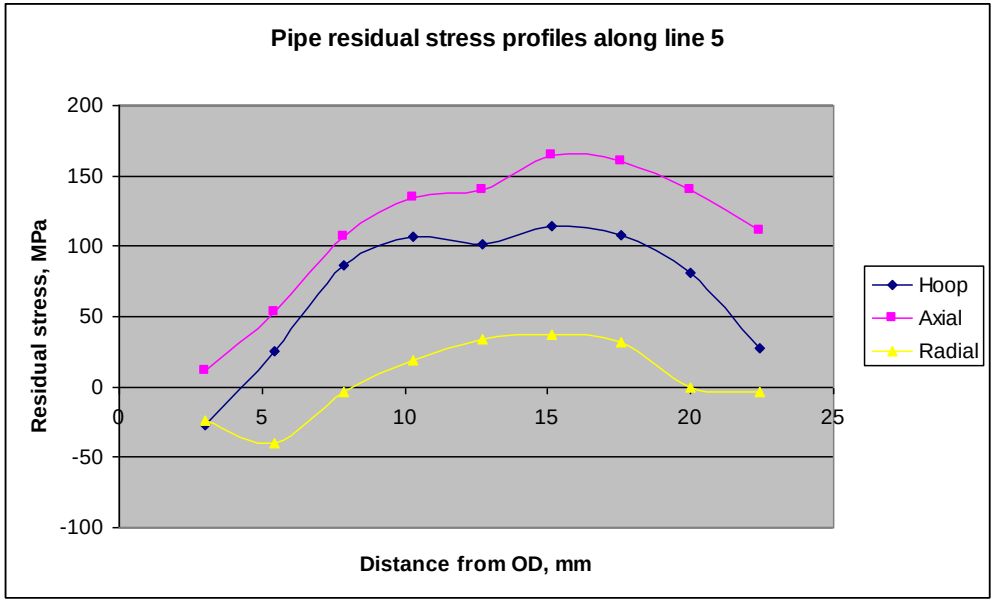
ISIS ENGIN-X beamline


SHOW/HIDE: Fiducial points
SAMPLE: Transparent
Ref.Planes: New plane
Plane
+/-
R
T
SHOW/HIDE Measurement points
GRID No Grid
SECTION OPTIONS Split models
Draw
+/-
R
T

Neutron diffraction residual stress measurement: preliminary results





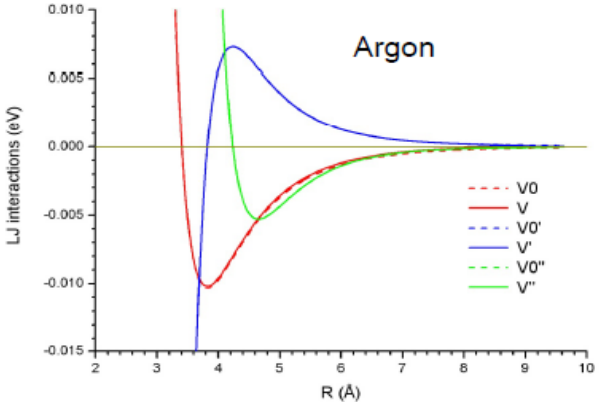


Data is difficult to be validated (prediction) from Molecular Dynamics Simulation

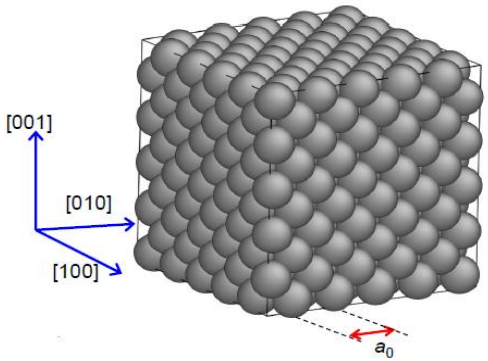
- Thermodynamic and kinetic Data (Fe)
  - Melting Temperature
  - Density
  - Enthalpy, latent heat and specific heat
  - Diffusion coefficient
  - **Solid-liquid interfacial energy and its anisotropy**
  - Anisotropy of kinetic coefficient

MD Simulation Procedure

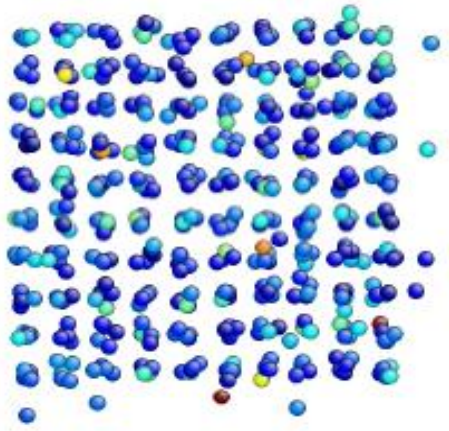
Selection of Potentials
Pair Or Multi-Body, e.g. EAM



Construction of system Model
Initial positions of atoms,
T, P, V, and Boundary Condition



System Equilibrium
Long time relaxation – to reach equilibrium



Result Evaluation
Statistic Analysis, etc.

EAM Potentials for BCC Fe

H(x): Heaviside function

- Pair potential:

$$\phi(r) = \sum_k a_k (r - r_k)^{n_k} H(r_k - r) H(r - r_2)$$
$$+ H(r_2 - r) H(r - r_1) \exp(B_0 + B_1 r + B_2 r^2 + B_3 r^3)$$
$$+ H(r_1 - r) \frac{Q_i Q_j}{r} \xi(r / r_s)$$

nuclear charges

- Density function:

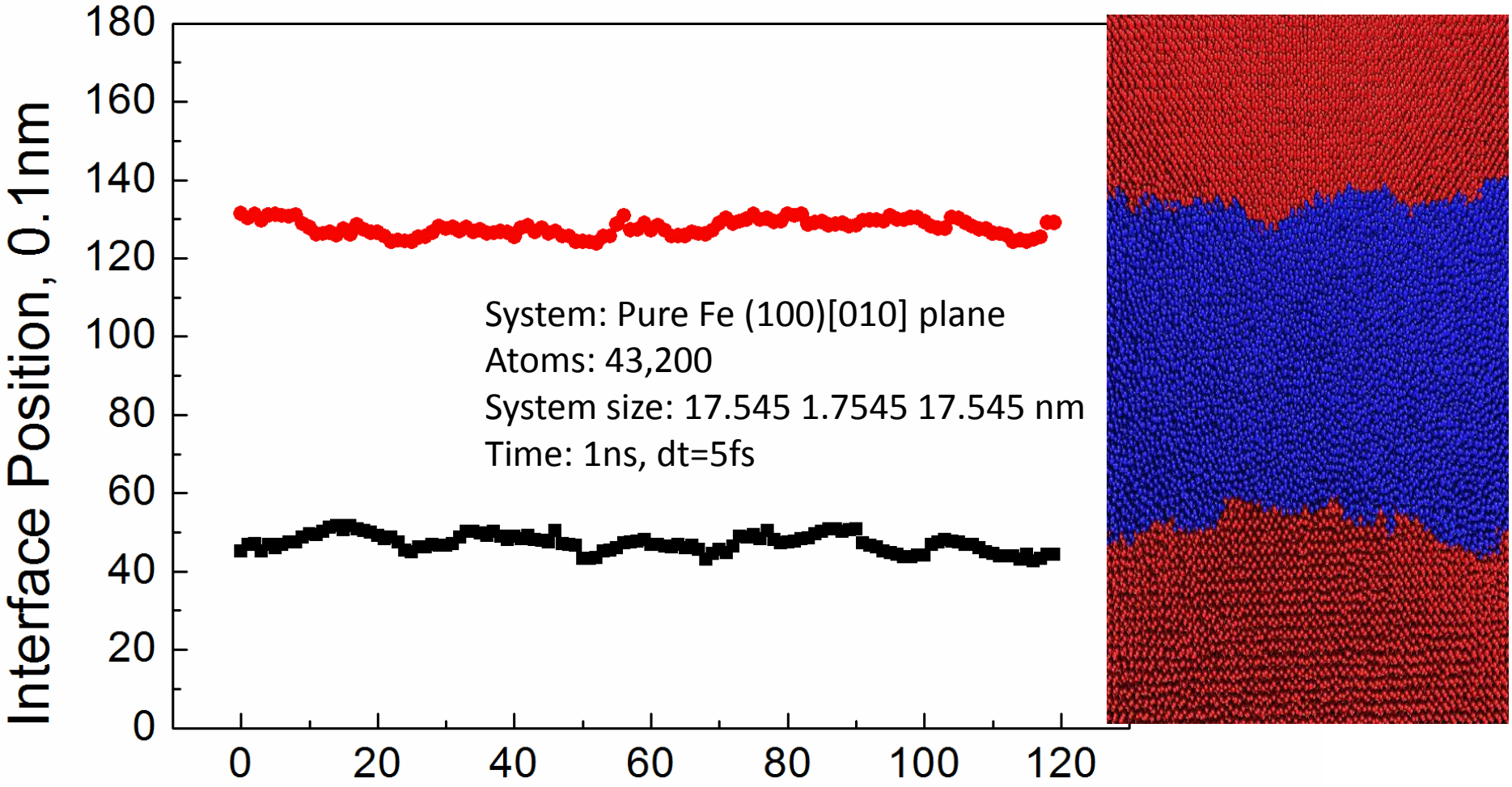
$$f(r) = \sum_K A_k (R_K - r)^3 H(R_K - r)$$

- Embedded function:

$$F(\rho) = -\sqrt{\rho} + a_2 x^2 + a_4 x^4$$

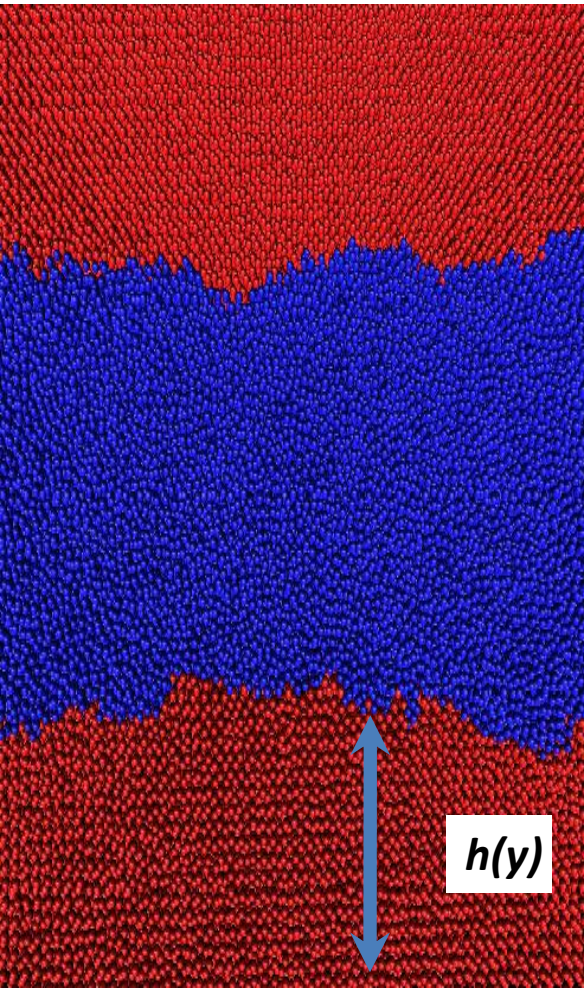
Ackland GJ, Mendelev MI, Srolovitz DJ, Han S, Barashev AV. J Phys: Condens Matter 2004;16:S2629

Solid-liquid interface fluctuation



Liu, Dong, Davidchalk, Com. Mat. Sci. 2013

Interface anisotropy - Capillary fluctuation method



Relationship between interface fluctuations and γ

$$\left\langle \left| h_q \right|^2 \right\rangle = \frac{k_B T}{A\tilde{\gamma} q^2}$$

H_q : Fluctuation spectra

Interface Position

$$h_q = \frac{1}{L}\int_0^L h(y) e^{iqy} dy = \frac{1}{N}\sum_{n=1}^{N} h(y_n) e^{iqy_n}$$

$$\tilde{\gamma}(\theta) = \gamma(\theta) + \frac{d^2\gamma}{d\theta^2}$$

interface stiffness

Interface free energy

$$\gamma(n)/\gamma_0 = 1 + \varepsilon_1\left(\sum_{i=1}^{3} n_i^4 - \frac{3}{5}\right) + \varepsilon_2\left(3\sum_{i=1}^{3} n_i^4 + 66 n_1^2 n_2^2 n_3^2 - \frac{17}{7}\right)$$

Liu, Dong, Davidchalk, Com. Mat. Sci. 2013, Davidchack, J.Chem.Phys. 125,094710 (2006)

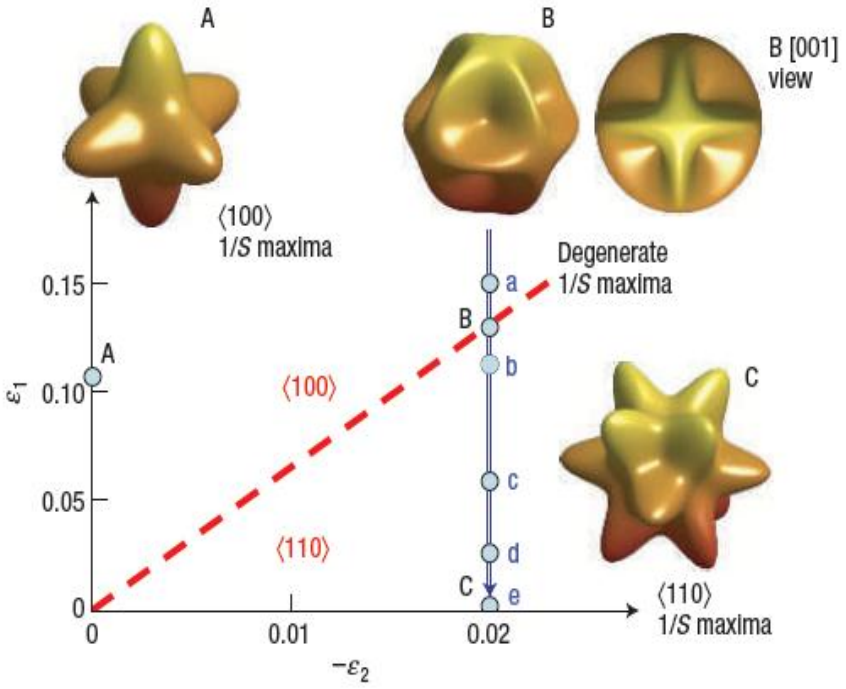
Anisotropy of interface energy

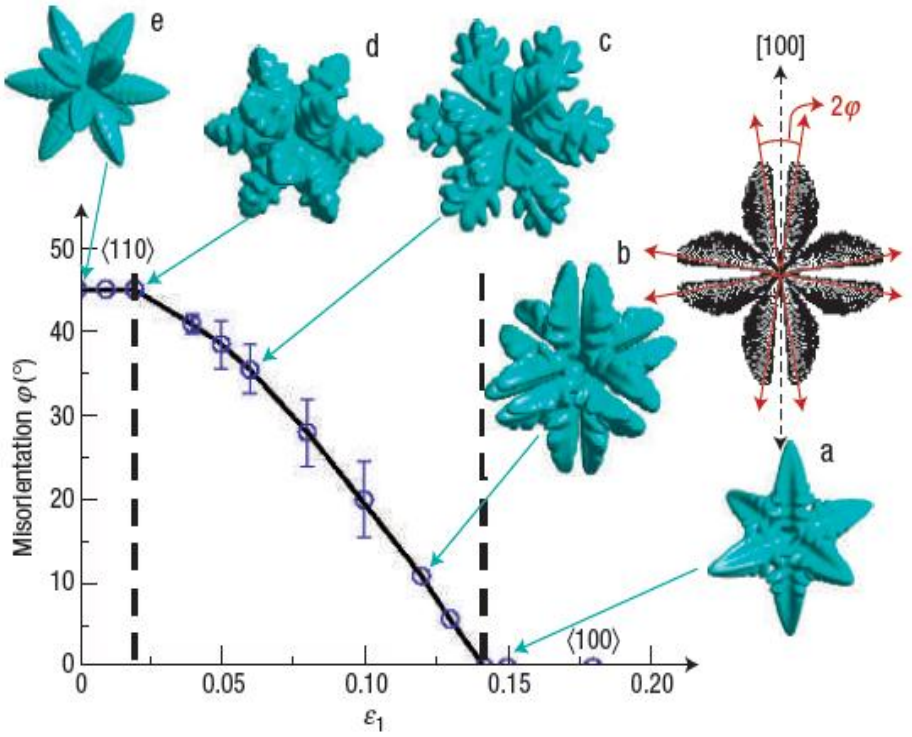
Potential:	ABCH*	Pair*	MH(SA)^{2*}	This work
Structure:	BCC	BCC	BCC	BCC
γ_0 (mJ/m^2)	206(10)	221(14)	175(11)	163.4
ε_1 (%)	1.6 ± 0.12	1.3 ± 0.18	3.3 ± 0.18	2.88
ε_2 (%)	-0.04 ± 0.28	0.26 ± 0.28	0.24 ± 0.32	-0.0612
γ_{100} (mJ/m^2)	207	222	178	165
γ_{110} (mJ/m^2)	206	220	174	163
γ_{111} (mJ/m^2)	205	221	174	162
$\frac{\gamma_{100}-\gamma_{110}}{2\gamma_0}$ (%)	0.4 ± 0.4	0.5 ± 0.5	1.0 ± 0.6	0.7
$\frac{\gamma_{100}-\gamma_{111}}{2\gamma_0}$ (%)	0.5 ± 0.4	0.4 ± 0.6	1.0 ± 0.2	1.0

Liu, Dong, Davidchalk, Com. Mat. Sci. 2013, *D.Y.Sun, M.Asta, Phys.Rev.B, 69, 174103 (2004)

Influence of Interface anisotropy

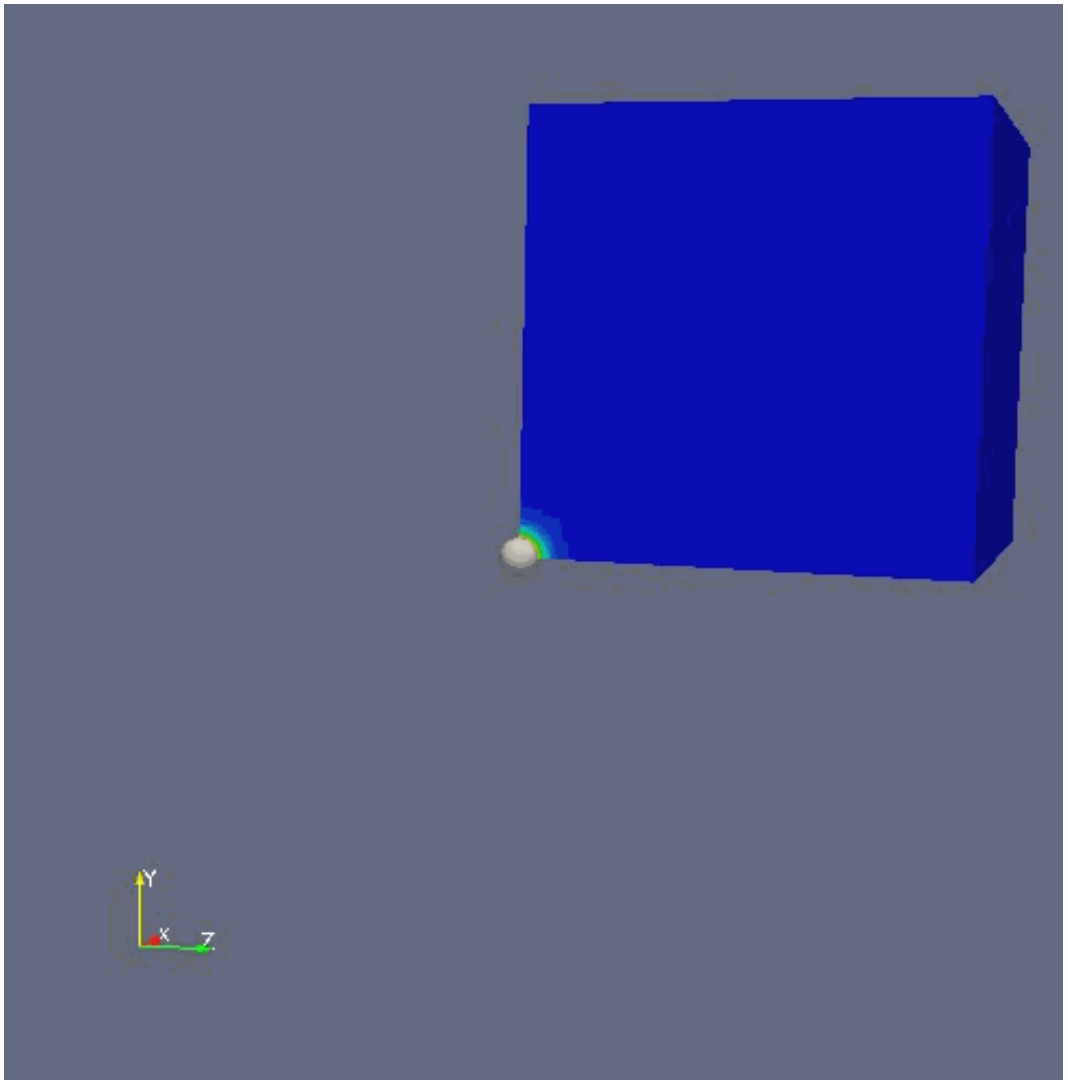
$$\gamma(\theta,\varphi)=\gamma_0\left[1+\varepsilon_1 K_1(\theta,\varphi)+\varepsilon_2 K_2(\theta,\varphi)+\cdots\right]$$





T. Haxhimali, A. Karma, F. Gonzales, M. Rappaz, Nature Mater. Vol 5, 2006, 660-664

Recent results



Input Parameter from MD:

$$\gamma_0 = 163.4\text{mJ/m}^2$$

$$\varepsilon_1 = 0.0288$$

$$\varepsilon_2 = -0.0006$$

$$T_m = 1900\text{K}$$

$$L = 0.147\text{ev}$$

One of most advanced phase field solidification modeling: including

- Adaptive meshing,
- thin interface analysis

Validated against analytical prediction….

Benchmark exercises?

Xie, Dong, Dantzig, Com. Mat. Sci. 2013

scale (time/length)

quantum
(10^{-12}s / 10^{-10} to 10^{-9}m)

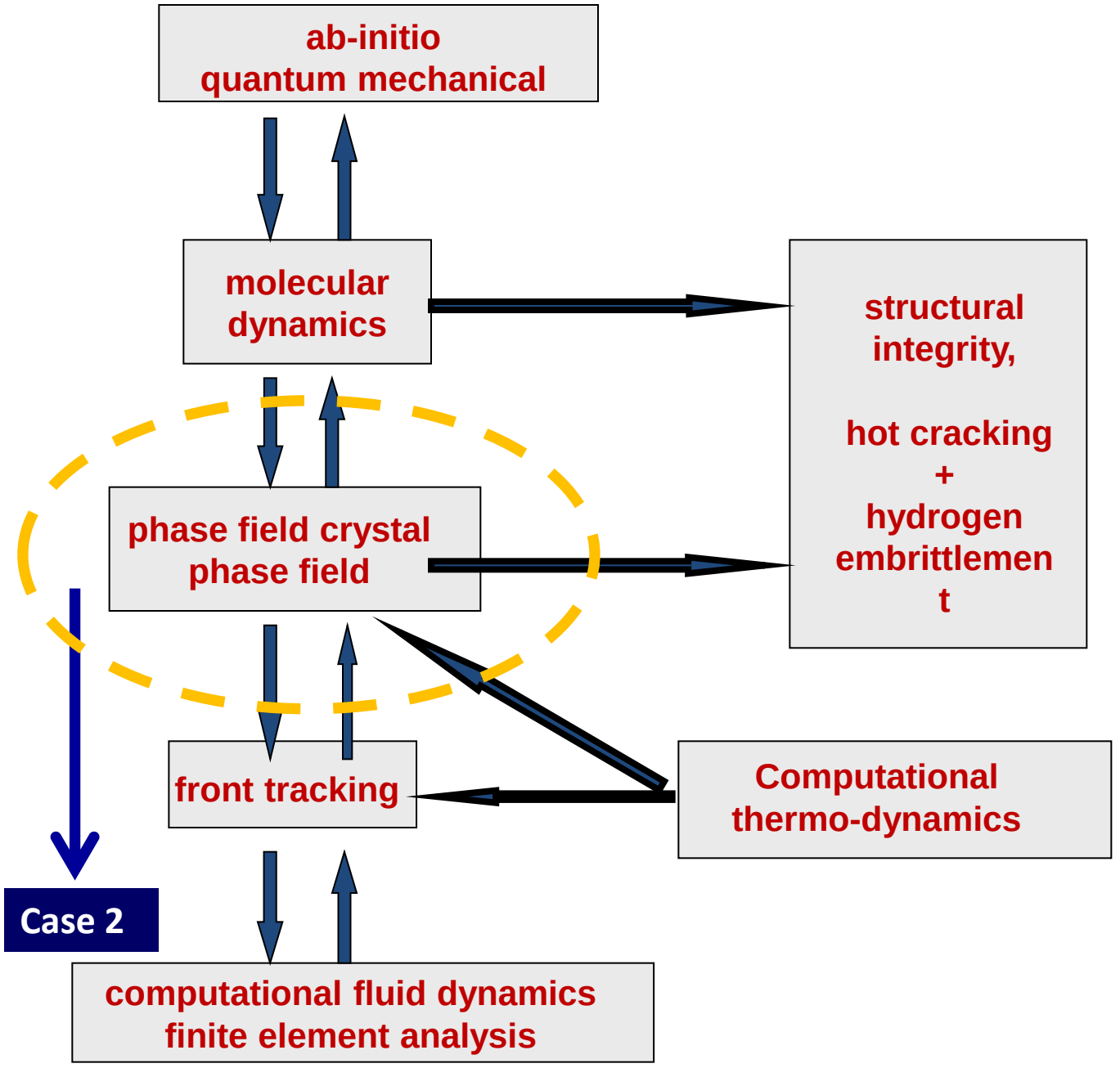
classical
(10^{-7}s / 10^{-9} to 10^{-8}m)

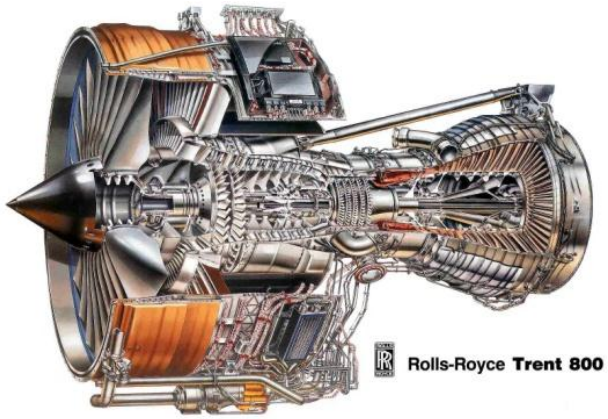
nano-micro
(10^{-3}s / 10^{-9} to 10^{-3}m)

grain
(10^{-3} to 10^{1}s / 10^{-4} to 10^{-2}m)

macro
(10^{2}s / 10^{-3} to 10^{-1}m)

models

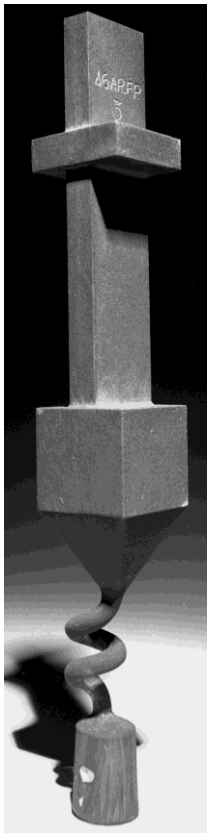


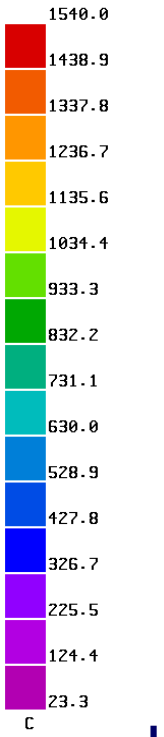


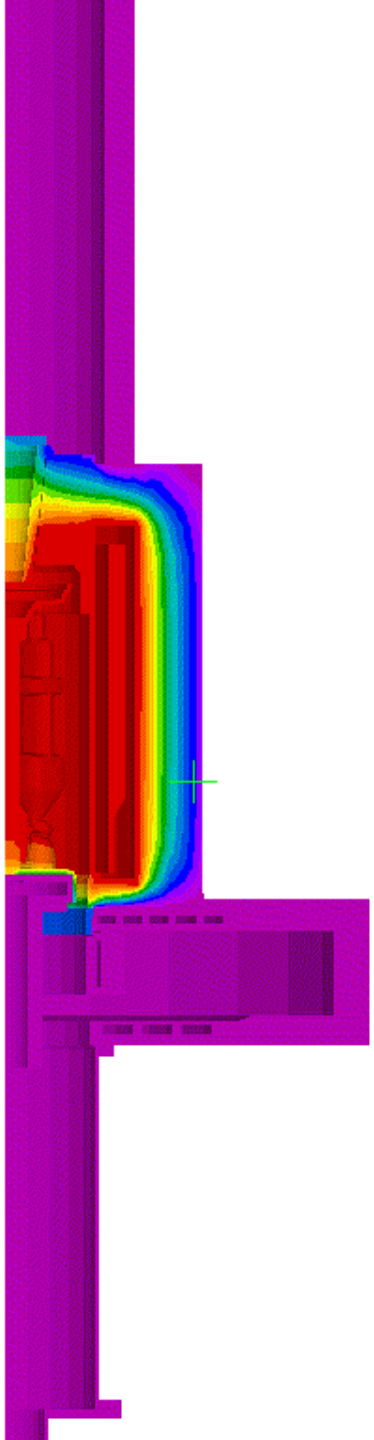
THE ROYAL SOCIETY

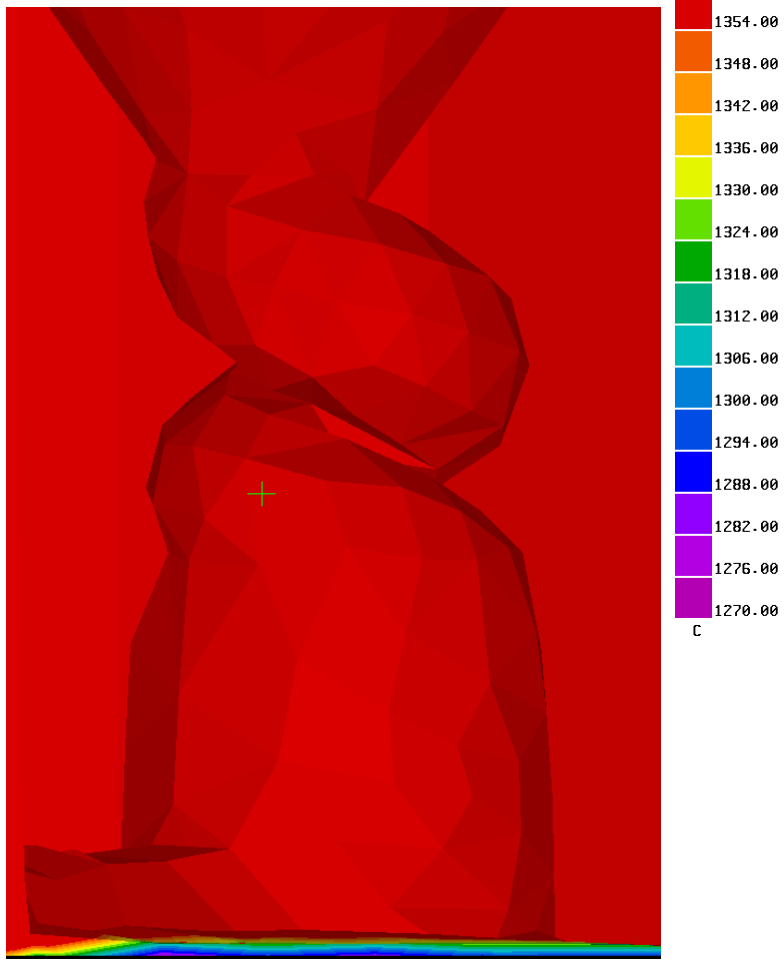
EPSRC
Pioneering research and skills

VeriCast Blade



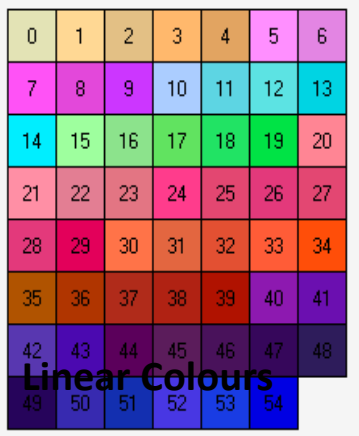




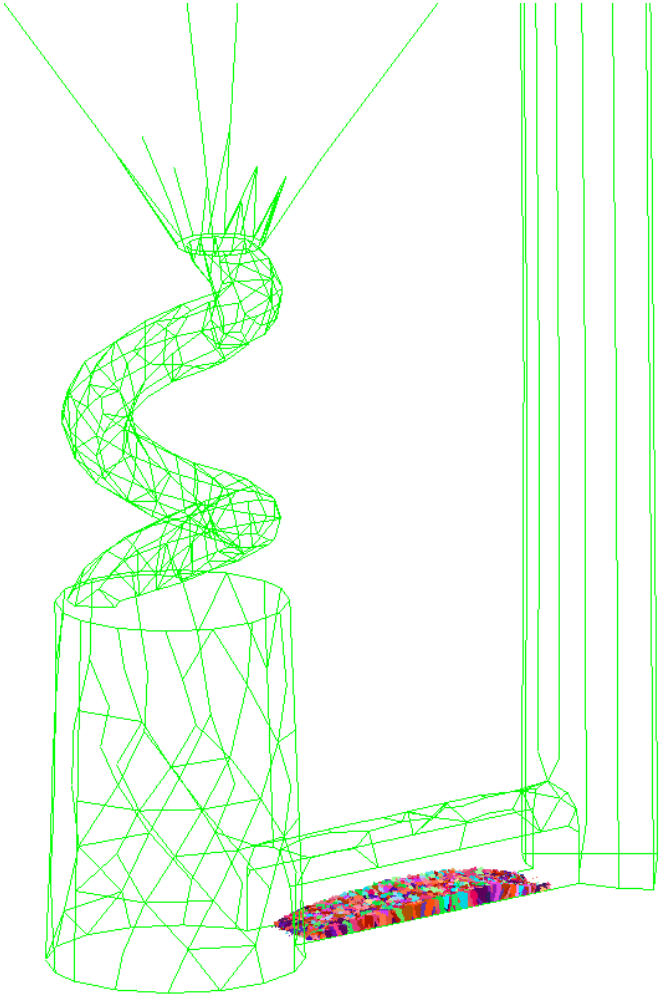


Dai, Dong, et al Met Tran A, 2011

Grain Structure Evolution



Mixed Colours

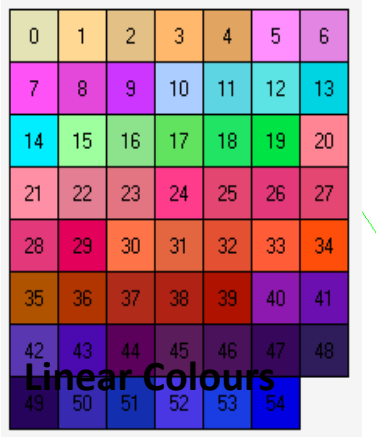


BBC TV program
April 2012
How metal works?

Dai, Dong, et al Met Tran A, 2011

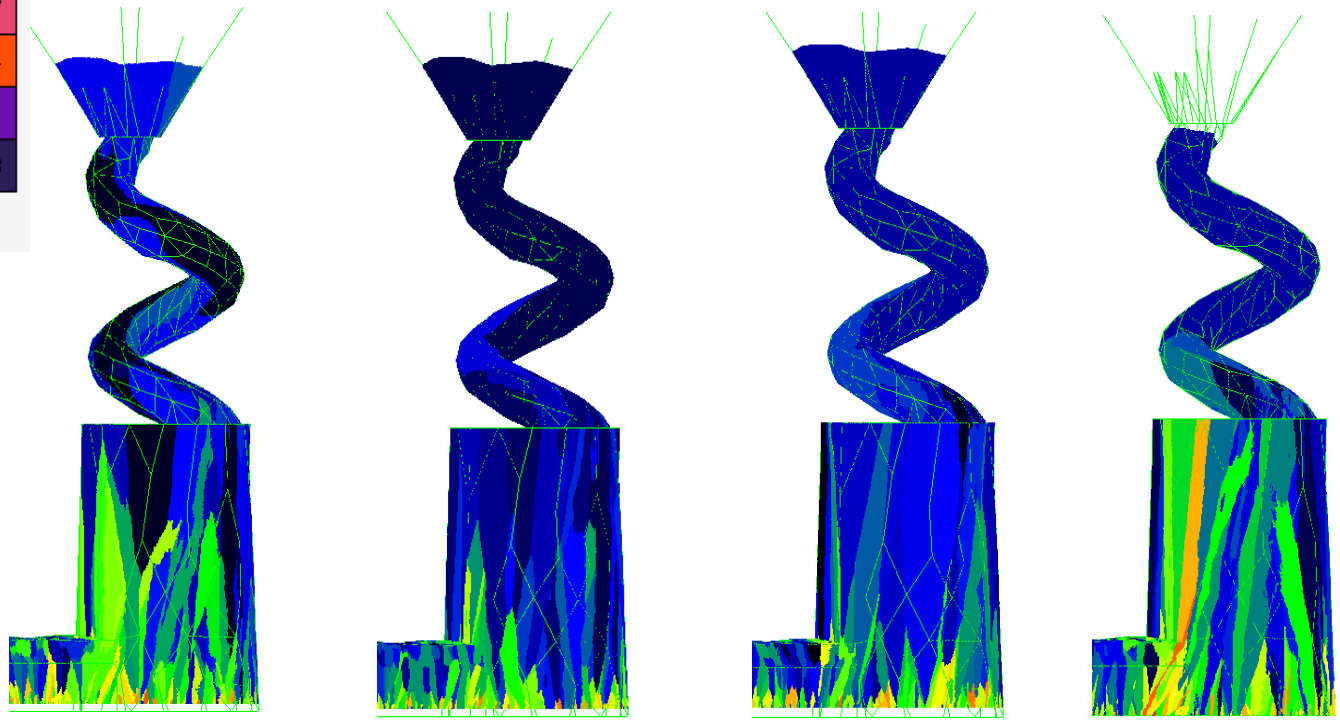
Dai, Dong, et al Met Tran A, 2011

Grain Structure Evolution



Mixed Colours

Stochastic Study



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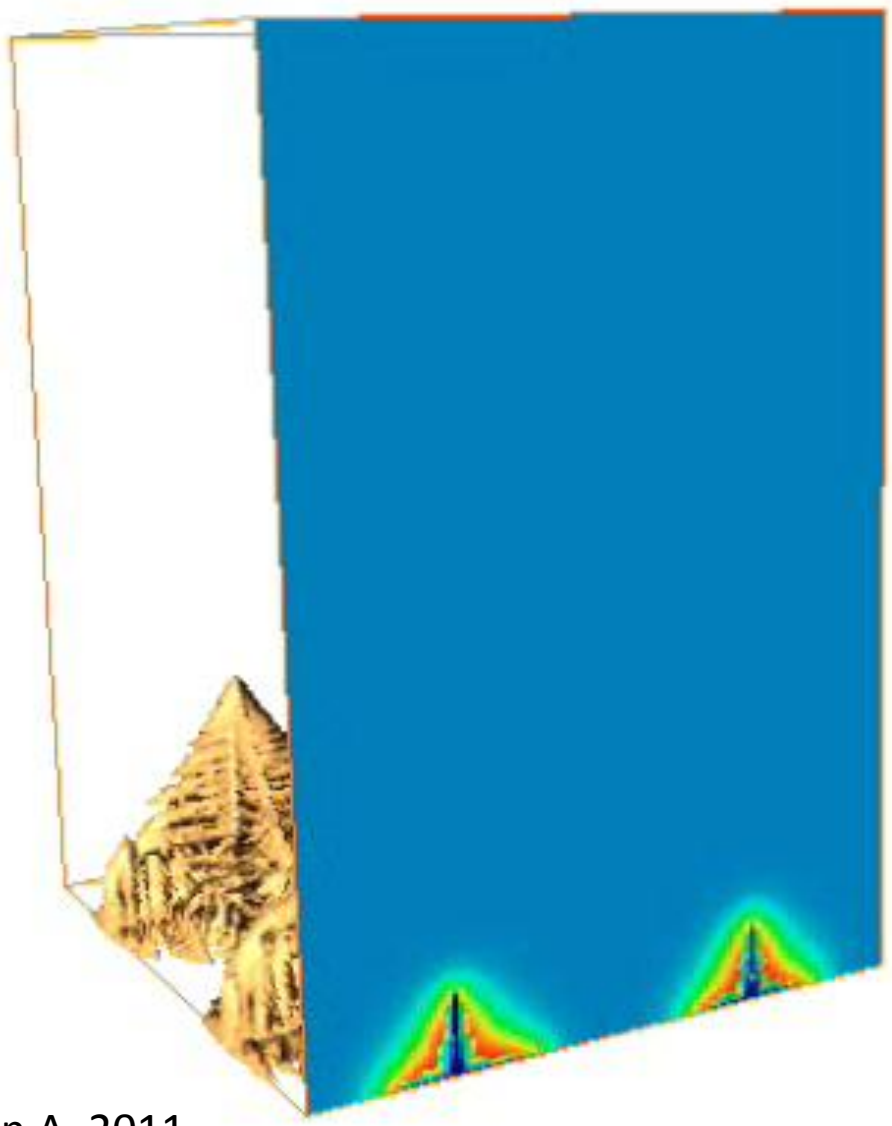
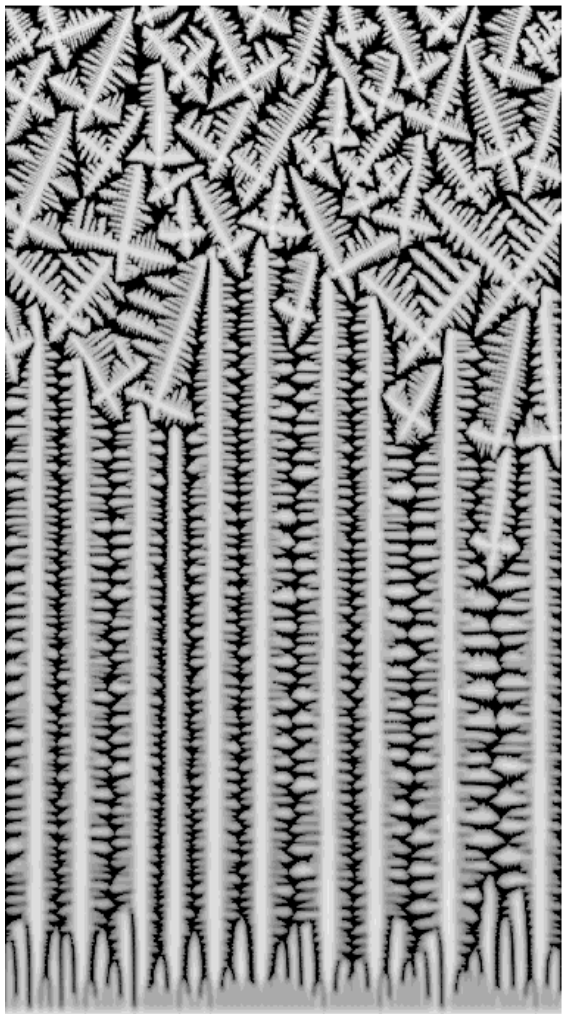
Dai, Dong, et al Met Tran A, 2011



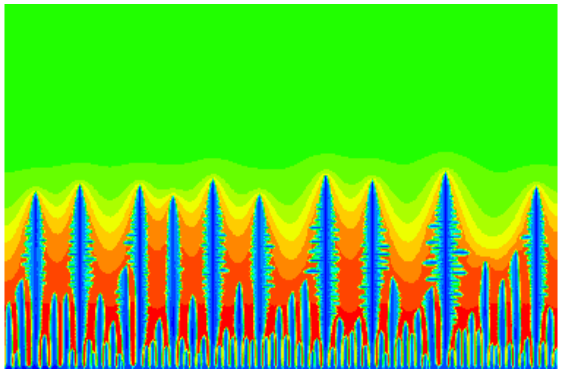
ai, Dong, et al Met Tran A, 2011

Transverse Section Views in 3D Simulations

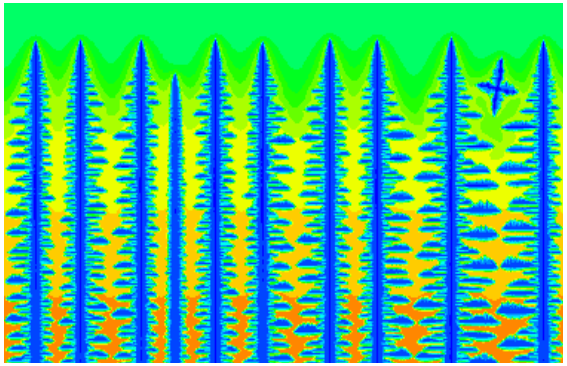


(a)

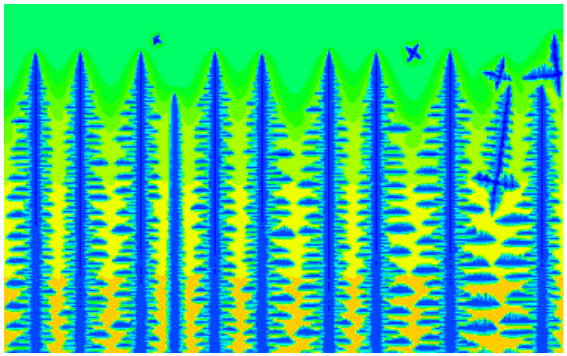
(b)



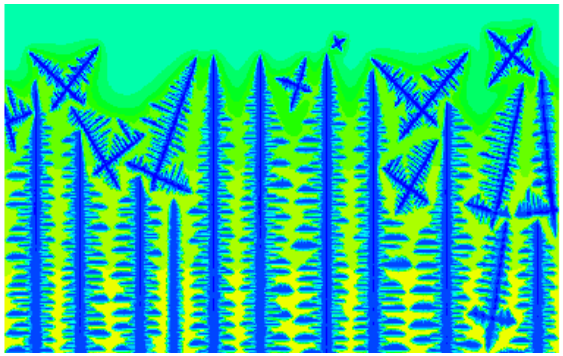
(c)



(d)

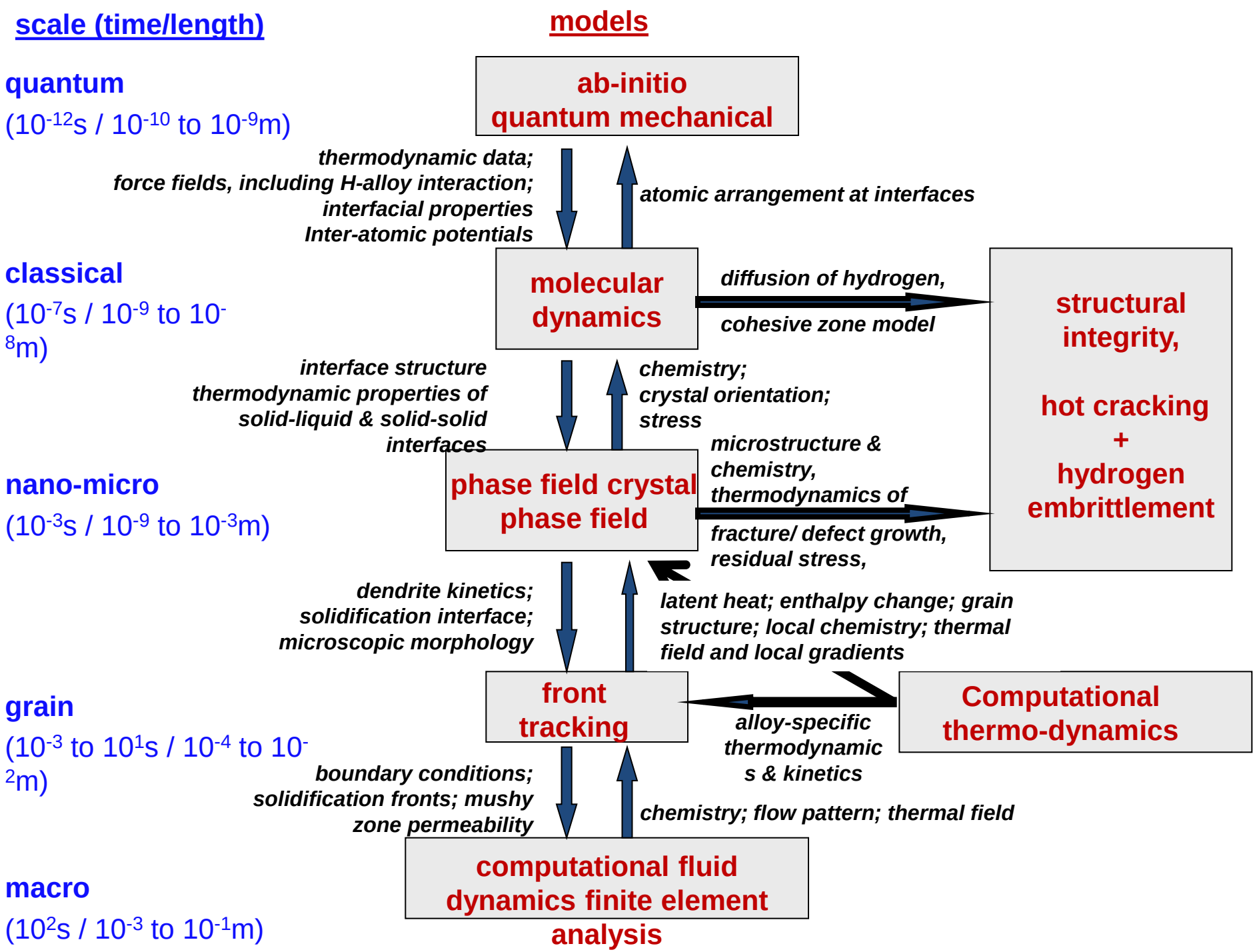


(e)



(a) 40 sec, (b) t=15 sec, (c) t=25 sec, (d) t=27 sec, (e) t=30 sec.

Dong, Lee, Acta Mat. 2005


scale (time/length)
models
quantum
(10-12s / 10-10 to 10-9m)
ab-initio quantum mechanical
thermodynamic data; force fields, including H-alloy interaction; interfacial properties Inter-atomic potentials
atomic arrangement at interfaces
classical
(10-7s / 10-9 to 10-8m)
molecular dynamics
diffusion of hydrogen,
cohesive zone model
structural integrity,
hot cracking + hydrogen embrittlement
interface structure thermodynamic properties of solid-liquid & solid-solid interfaces
chemistry; crystal orientation; stress
nano-micro
(10-3s / 10-9 to 10-3m)
phase field crystal phase field
microstructure & chemistry, thermodynamics of
fracture/ defect growth, residual stress,
dendrite kinetics; solidification interface; microscopic morphology
latent heat; enthalpy change; grain structure; local chemistry; thermal field and local gradients
grain
(10-3 to 101s / 10-4 to 10-2m)
front tracking
Computational thermo-dynamics
alloy-specific thermodynamic s & kinetics
boundary conditions; solidification fronts; mushy zone permeability
chemistry; flow pattern; thermal field
macro
(102s / 10-3 to 10-1m)
computational fluid dynamics finite element analysis

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Factories of Future (FOF): ICT Innovation for manufacturing SMEs

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