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Predicting Microstructure-Property Relationships in Structural Materials via Multiscale Models Validated by In-Situ Synchrotron Observation

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Predicting Microstructure-Property Relationshops via multiscale models

Nature versus Nurture in the MGI…

validated by synchrotron observations

Peter D. Lee, Lang Yuan, Chedtha Puncreobutr, S. Karagadde

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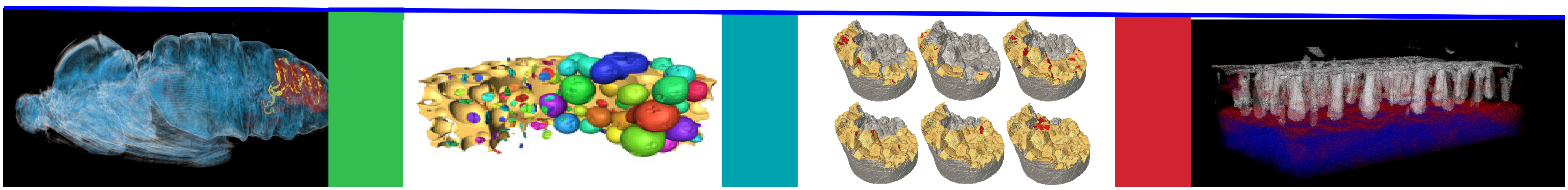
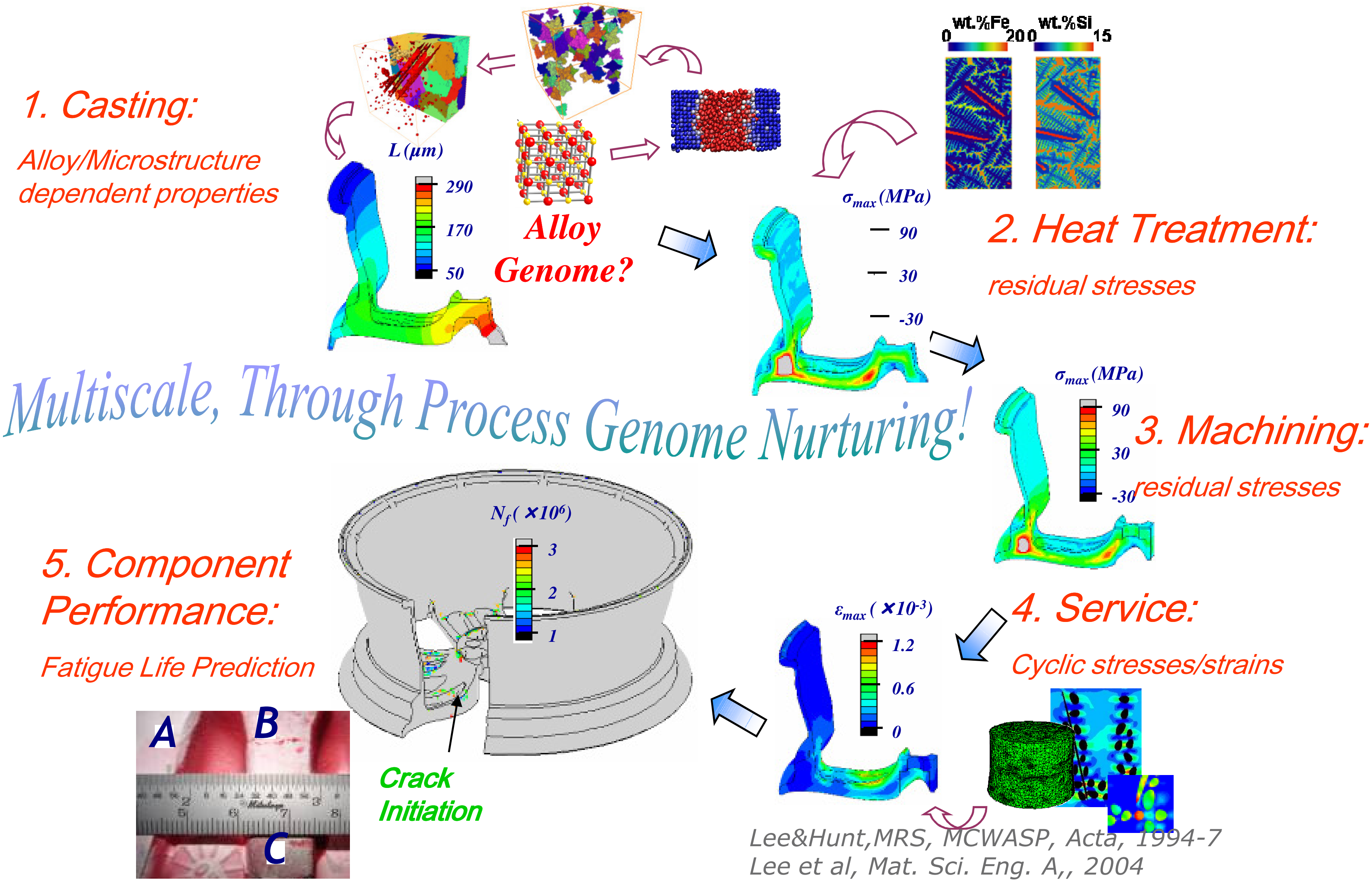
www.mxif.manchester.ac.uk



Why simulate Microstructural Evolution (ICME)?
To track genome evolution across length scales and processes



Lee&Hunt,MRS, MCWASP, Acta, 1994-7
Lee et al, Mat. Sci. Eng. A,, 2004
Maijer, Lee et al, Met. Trans, 2004
John Allison, ICME. JOM, 2006

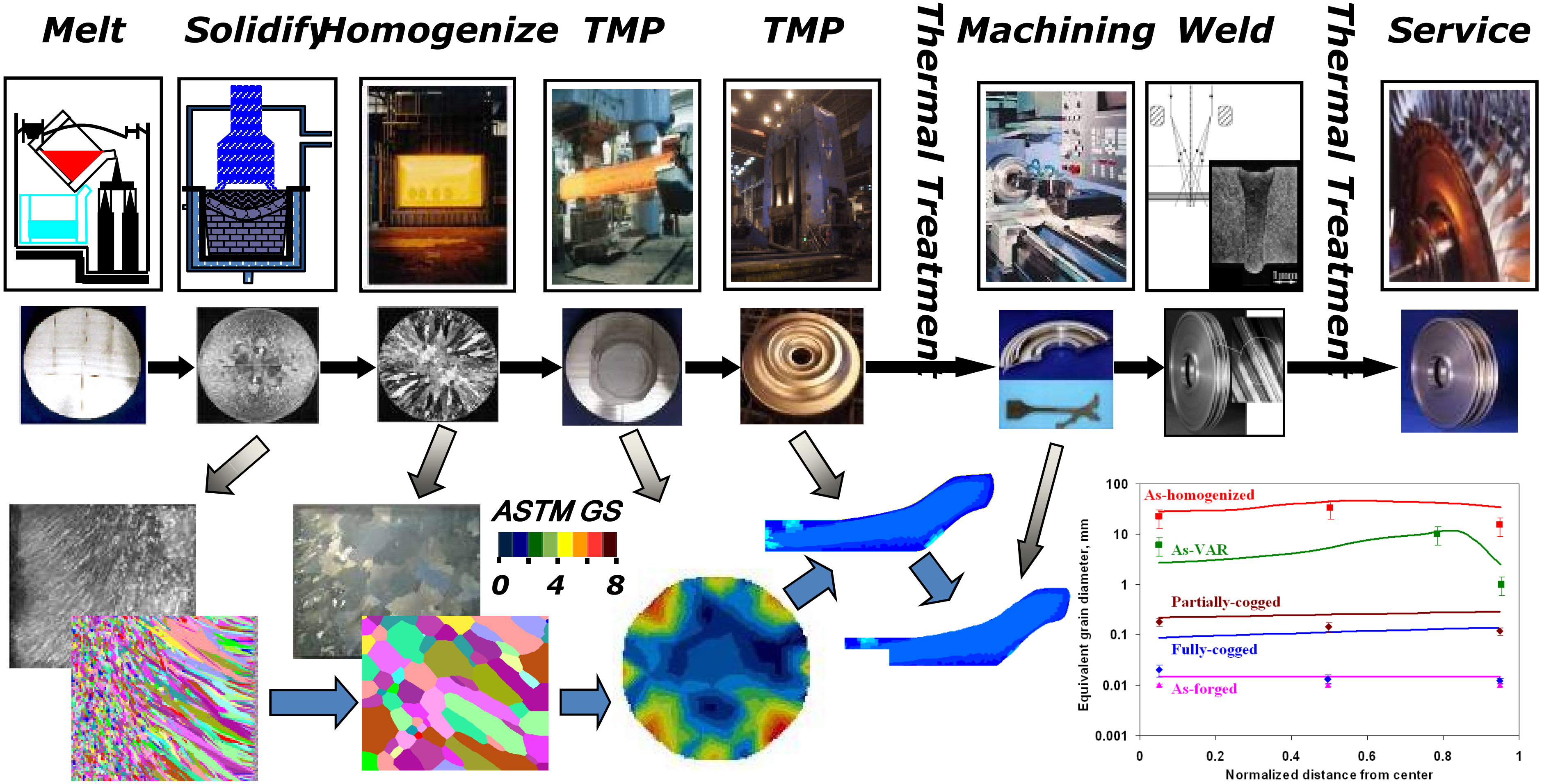
I've modelled alloy processing for 25 years - What lessons have I learned?

1. When using multi-scale, through process modelling (or ICME), there are sufficient unknown parameters one can tune, you usually get the answer you want…

2. For structural materials, it is not only the innate alloy properties, but also how you manufacture the component that matters

I.e. Nurture can be more important than Nature if you want to get the most out of a Material's Genome.

Typical number of Nurturing steps...



Evolution of the Material Genome During Nurturing!

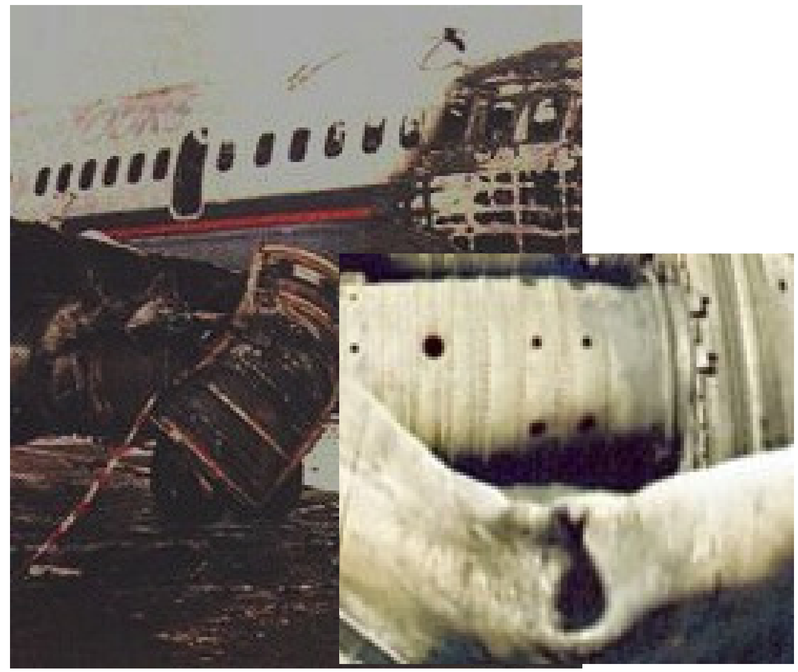
With Rolls-Royce; Special Metals & Wyman-Gordon
Univ. of Cambridge (Tin) and Birmingham (Ward)

Kermanpur, Tin, Lee, JOM 56(3) 2004, 72-78. or Tin, Lee, et al Met. Trans. A., 2005.

Is optimising *Nature*, then providing good *Nurturing* enough?

- 1989 Kegworth air crash, caused by fan blade loss, manufacturing defect

- 1985, Manchester, failed combustor weld repair - porosity



Lesson 3 - Lifing is often limited by a deviant microstructural feature, rather than the average, even though it may have the same genome...

My Conclusion…

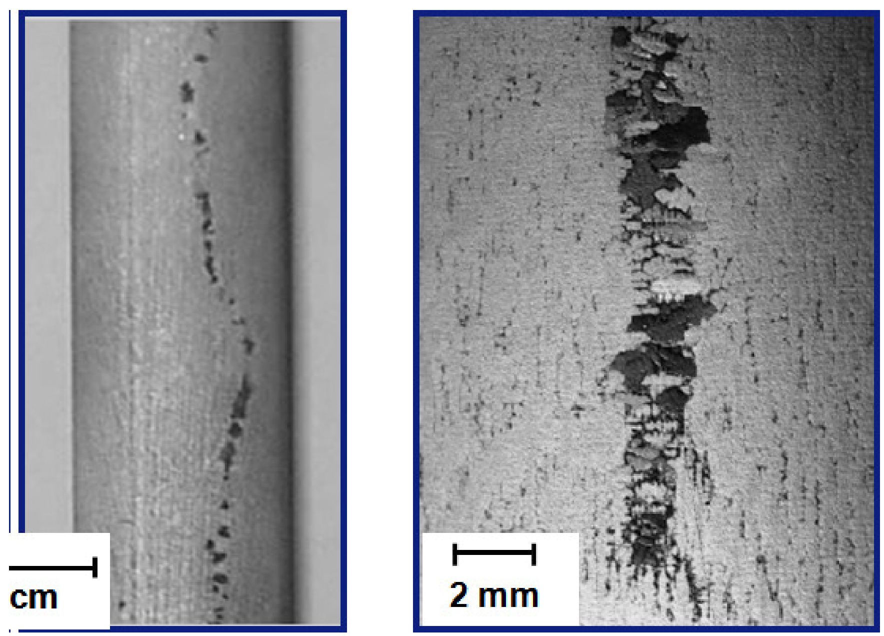
The Materials Genome Project needs to map out not only the average behaviour, but also the distribution in behaviour, including the rebels

Manchester X-Ray Imaging Facility

Research Complex at Harwell

MANCHESTER 1824 The University of Manchester

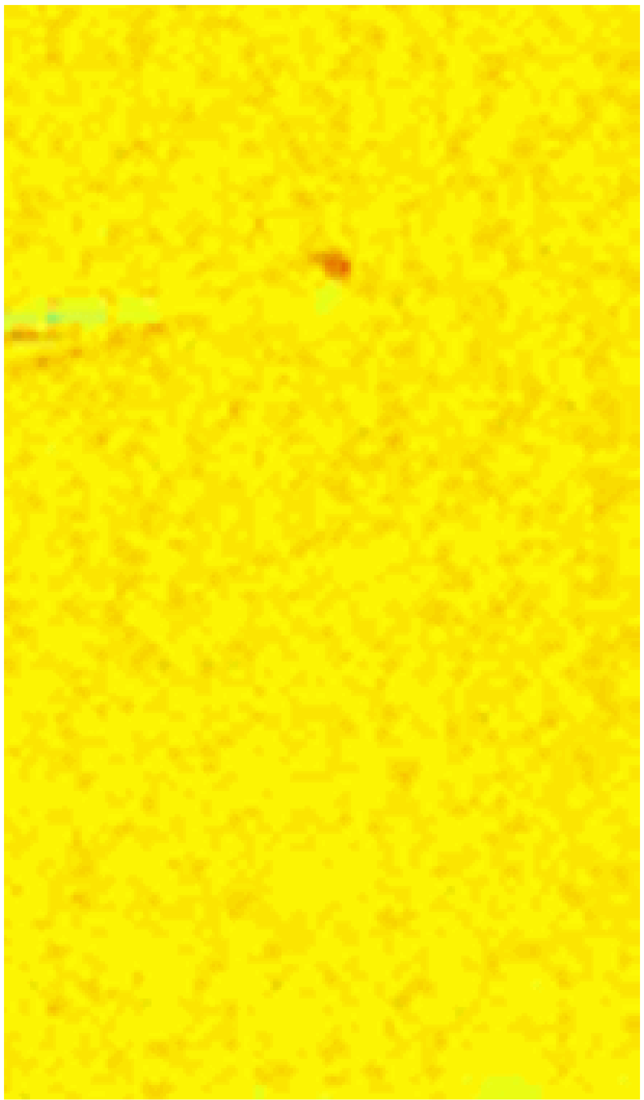
Example 1: Predicting deviant microstructures in Ni-based SX turbine blades blades: or *the Freckle Rebel*



Beckermann, Flemings Symposium, 2001

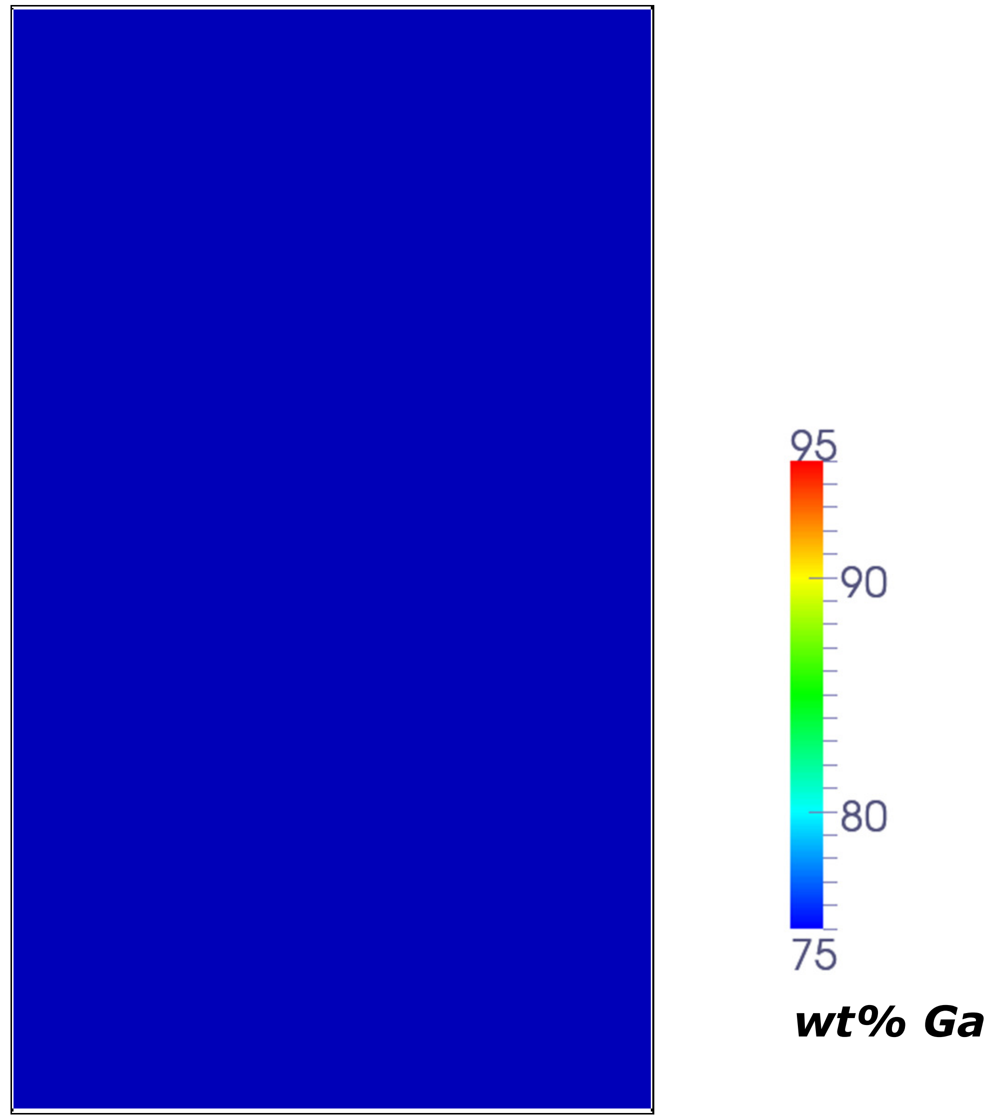
Solidification of Ga-25wt%In alloy, G .5K/mm, R 8.1 μm/s

X-ray In-situ observation, Courtesy HZDR,DE



N Shevchenko et al 2012
Mater. Sci. Eng. 33 012035

μMatIC Simulation



www3.imperial.ac.uk/advancedalloys/

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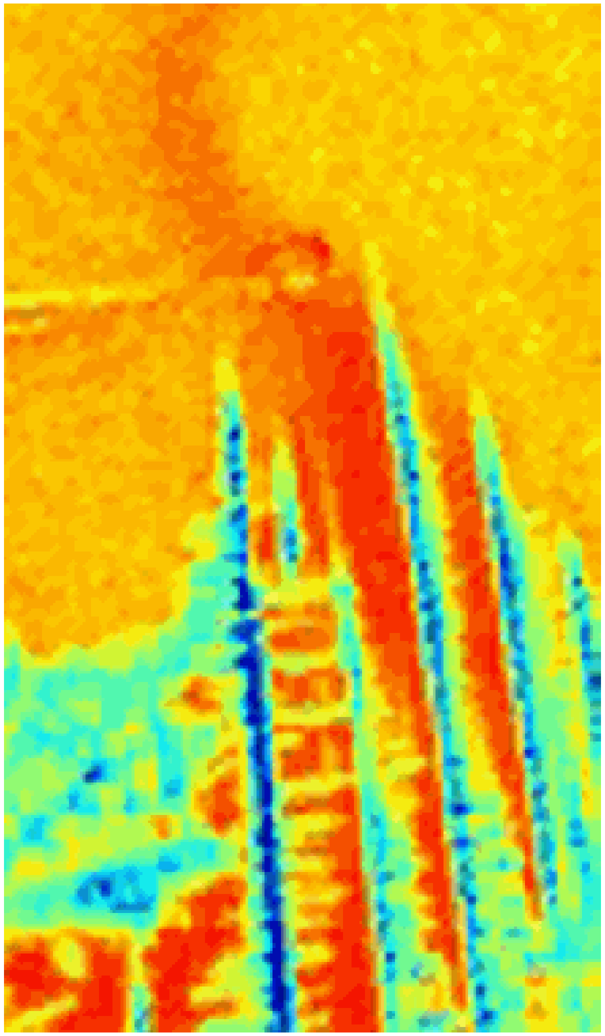
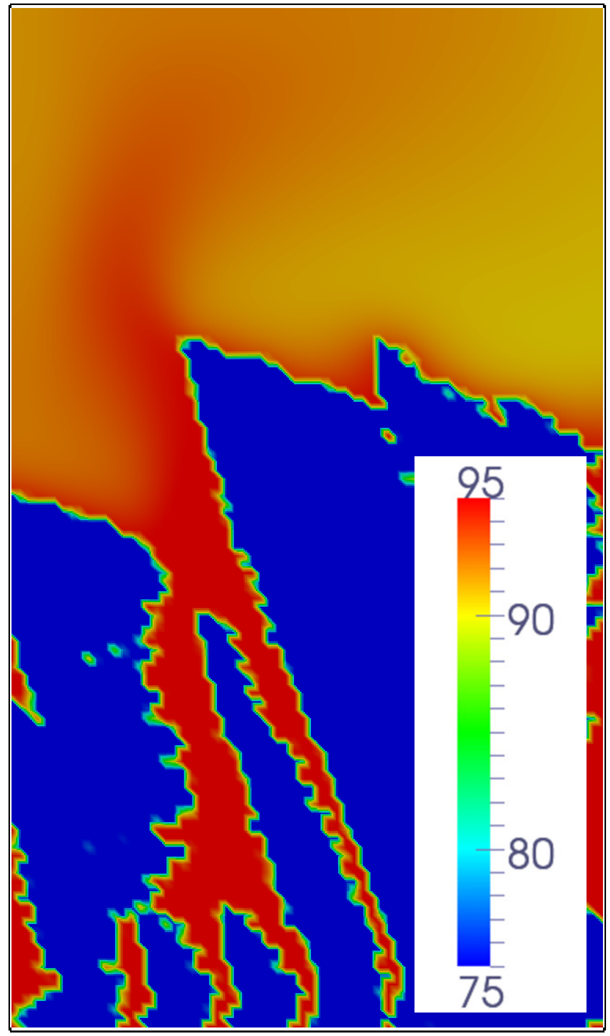


N Shevchenko et al 2012 Mater. Sci. Eng. 33 012035

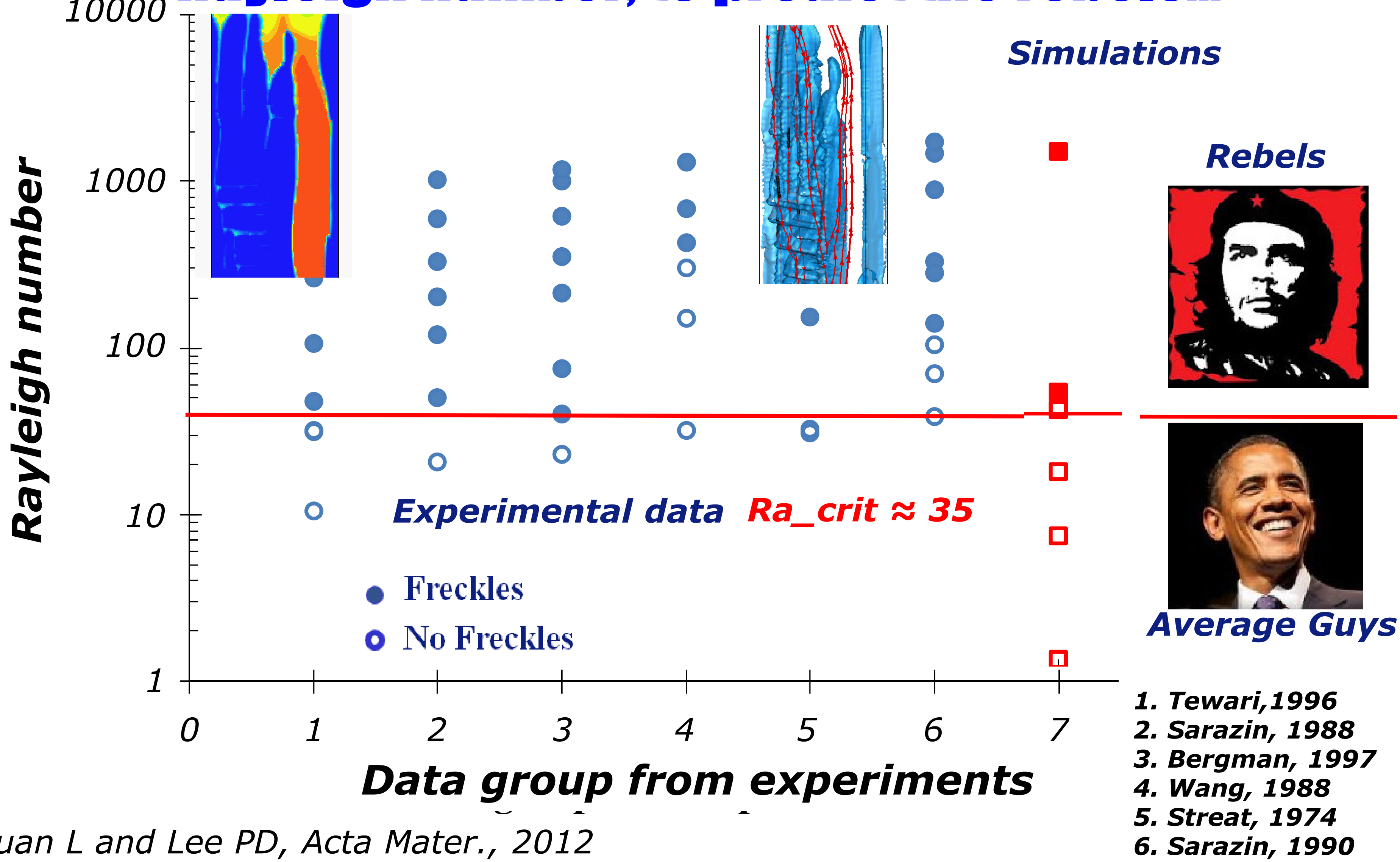


wt% Ga

www3.imperial.ac.uk/advancedalloys/

Upwards liquid flow increases solute concentration in the channel with local remelting, remelting secondary arms and stopping primary arms

To scale the microstructural model to a macroscopic level, we can approximate it via the Rayleigh number, to predict the rebels...



Yuan L and Lee PD, Acta Mater., 2012

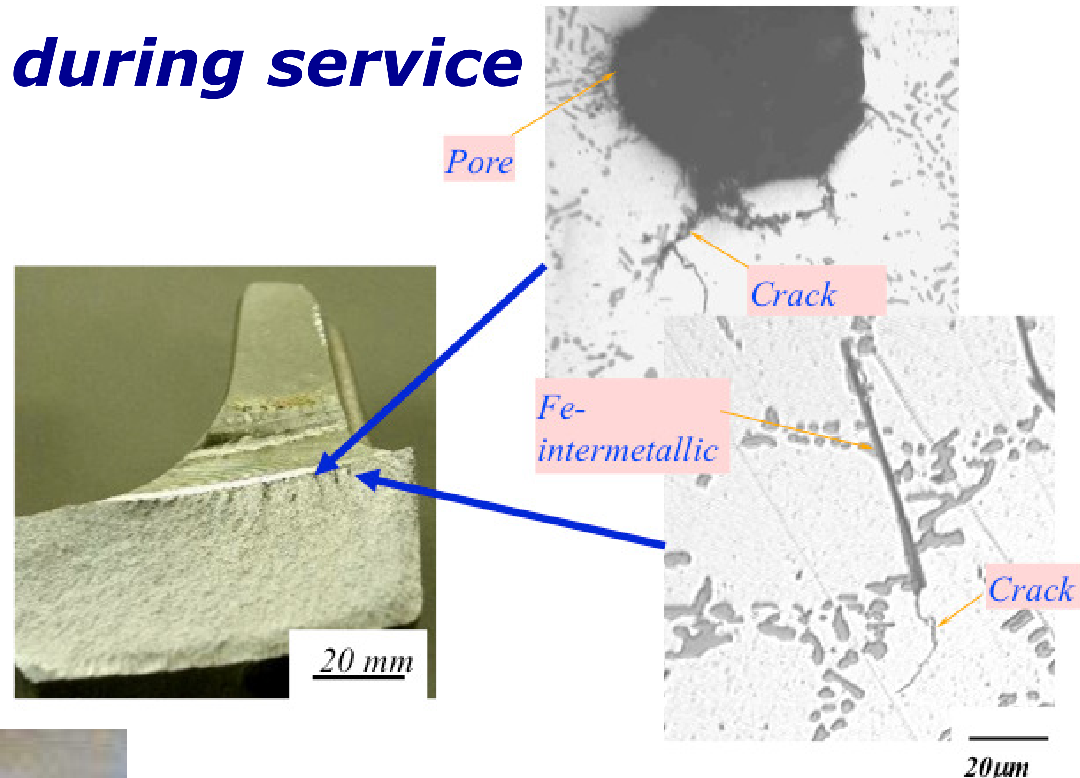
Example 2

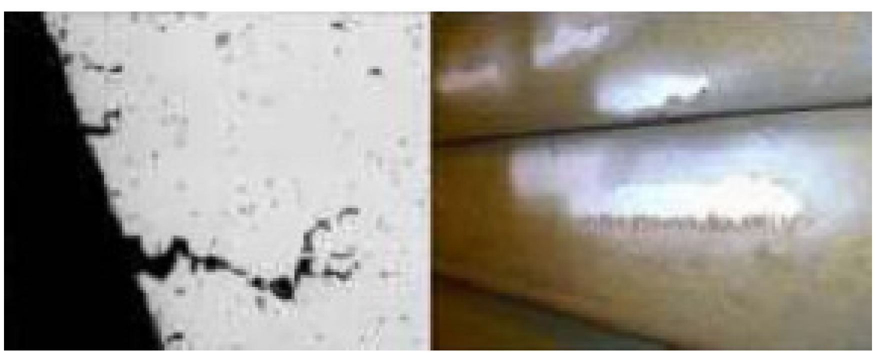
Understanding why eating your spinach is not always good for your strength, or

predicting Fe-intermetallic Rebels...

Why worry about deviant microstructures like pores and Fe-intermetallics?

They initiate failure during service





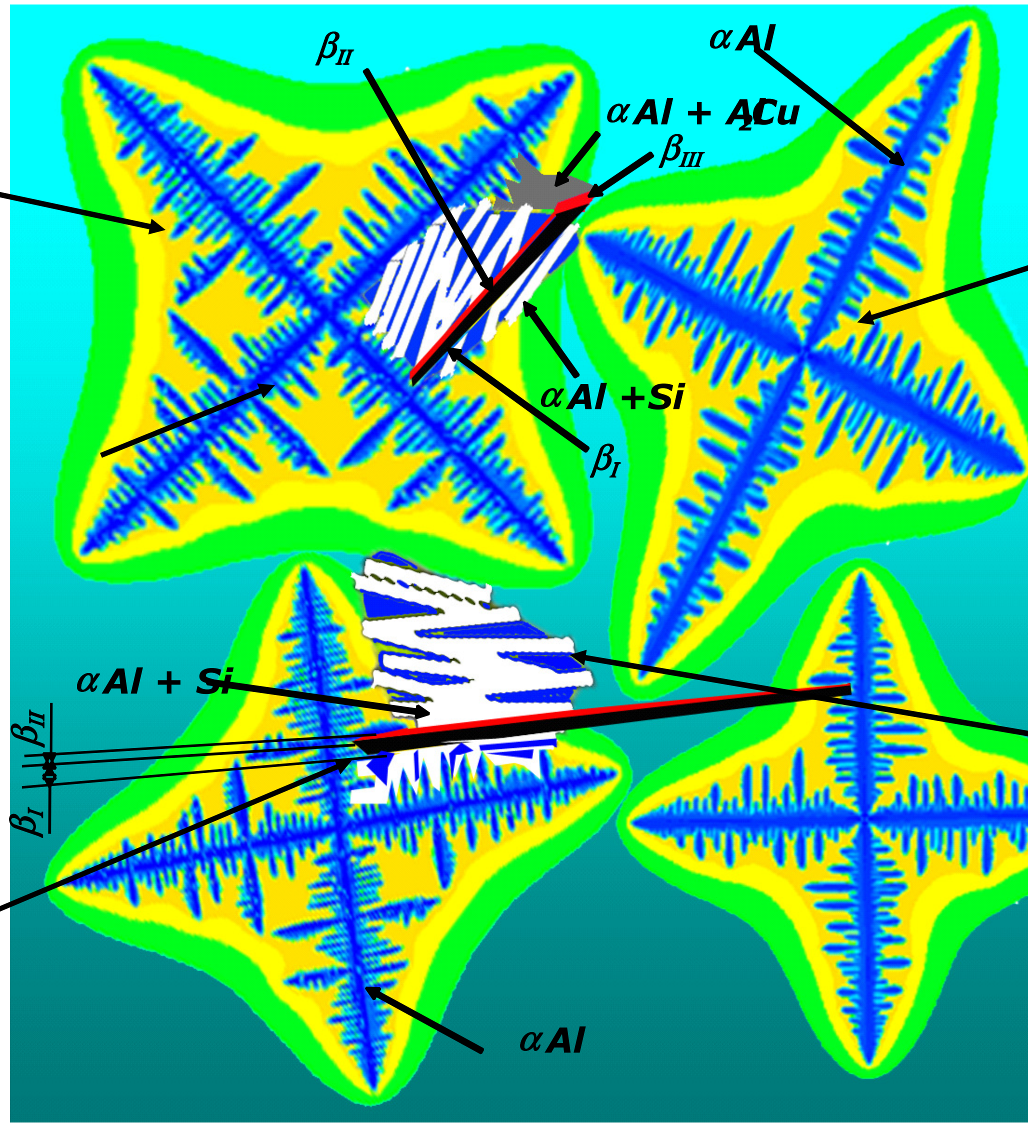
And they alter formability during manufacturing

Yi, J.Z. et al. Met. Trans. 34A, 2003.

What needs to be simulated?

Solute partitioning (Si & H) at solid/liquid front

Intermetallic nucleation And growth



Grain nucleation and Growth

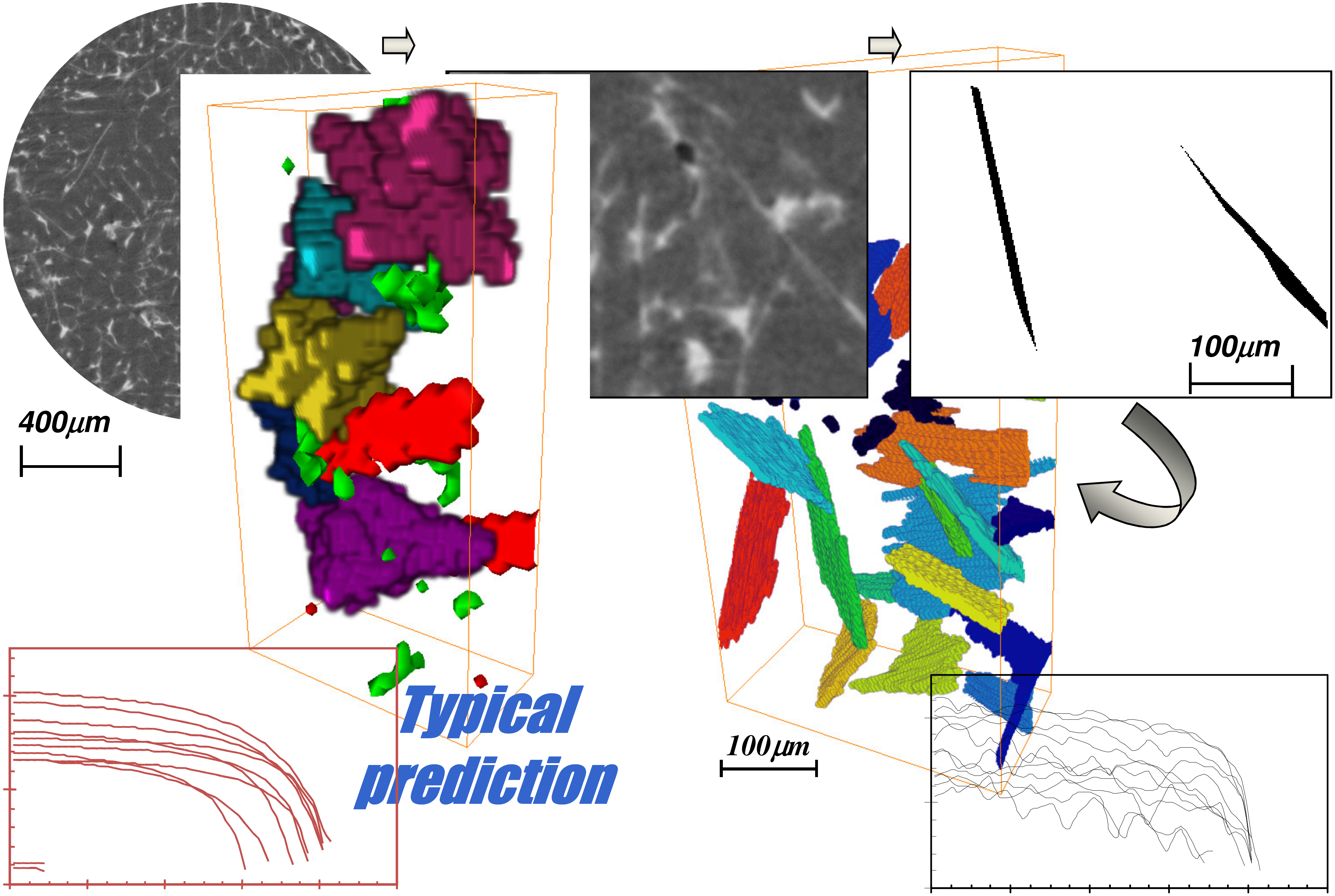
Eutectic growth

Growth restricted by solid

For speed we model with 10μm elements, and approximated anisotropy

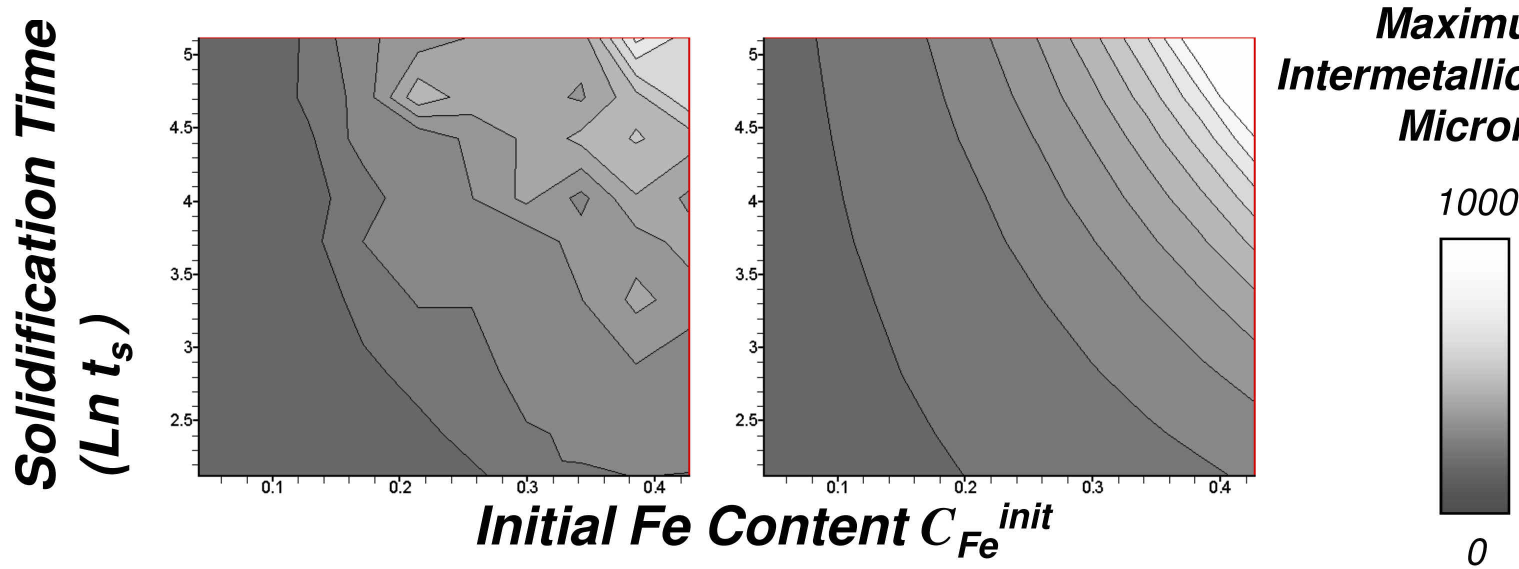
- ~~**Nucleation: nanometres**~~ → ***Empirical fn***
- ~~**Dendrite tip radius: 1 micron**~~ → ***Fs>0.5, approximate...***
- ~~**Coarsening: 10 microns**~~ → ***Borderline...***
- ~~**Solute diffusion: 10 microns**~~ → ***Fs>0.5, ~Scheil btwn dendrites***
- **H diffusion: 100 microns** ✓
- **Pores: 10-100's microns** ✓
- **Intermetallics: 10-100's microns** ✓
- **Grain size: 100-1000 microns** ✓

Synchrotron CT Characterization of Fe Intermetallic Morphology compared to model prediction



How do we capture the genome and span scales? Via model-based constitutive equations

1000's micromodel predictions ***Regression Fit***



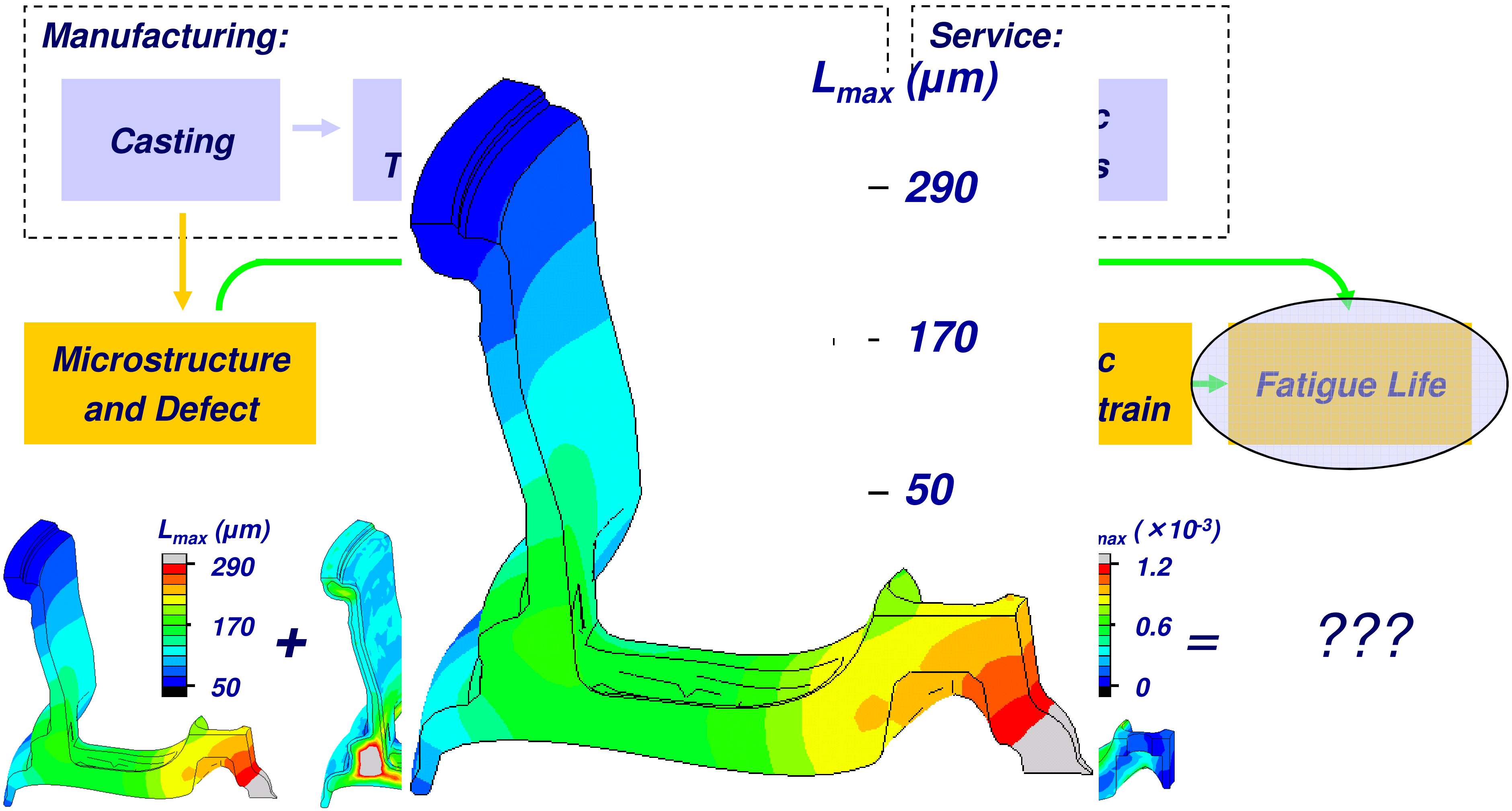
$$\ln L_{\max} = b_0 + b_1 \ln t_s C_{Fe}^{init}$$

and statistical variation

Challenges:

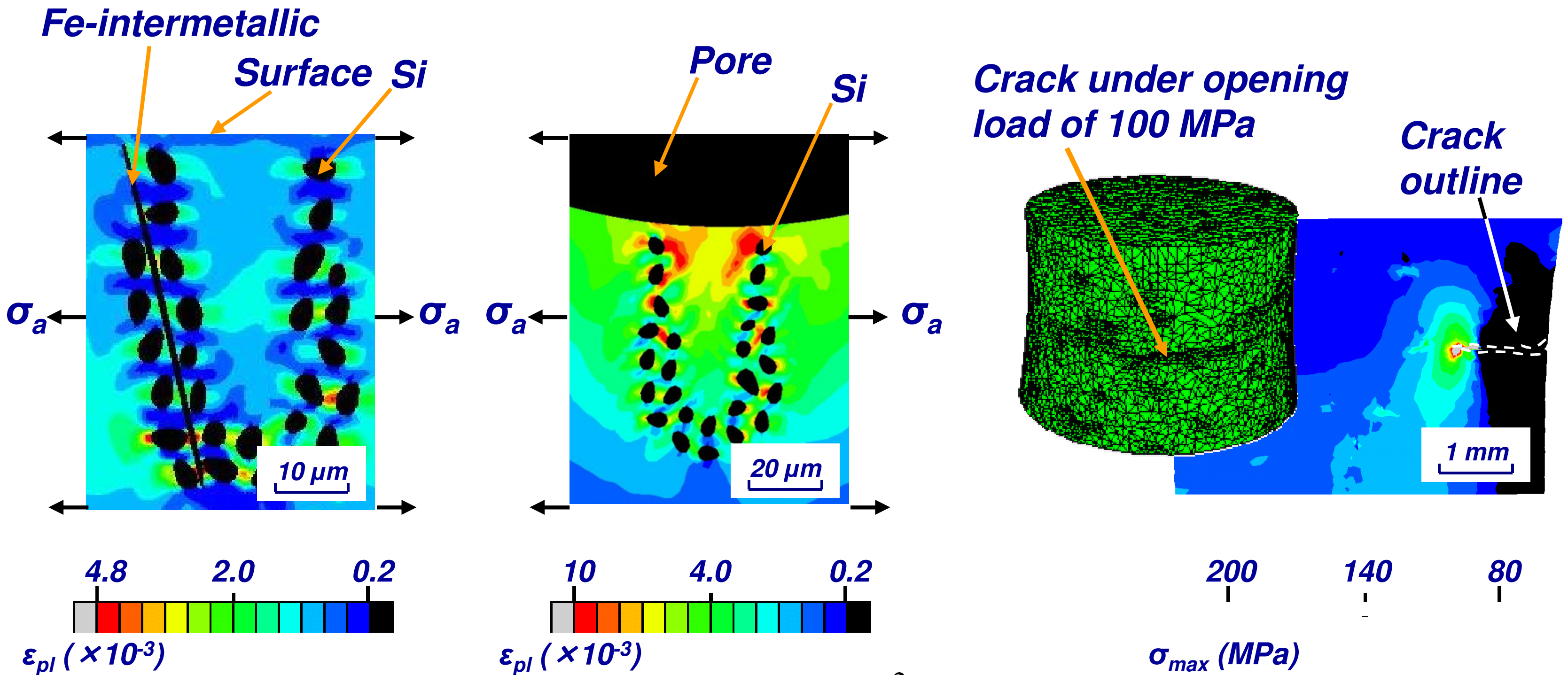
1. ***Improved statistical tracking of multi-variant distributions***
2. ***Fitting highly coupled phenomena (e.g. Pressure)***

Coupling deviant microstructure to Lifing



Li et al, MCWASP 2006, MMTA 2007

Crack Initiators



$$N_f = N_i + N_p = \frac{C_0}{\lambda_2}\left[\frac{1}{k_\sigma \sigma_a}\left(k_0 + \frac{\alpha}{\sqrt{\lambda_2}}\right)\right]^{\frac{2}{\beta}} + C_1\left(\varepsilon_{max}\frac{\sigma_a}{\sigma_y}\right)^{-s\times t}\left(a_f^{\,-t+1} - a_i^{\,-t+1}\right)$$

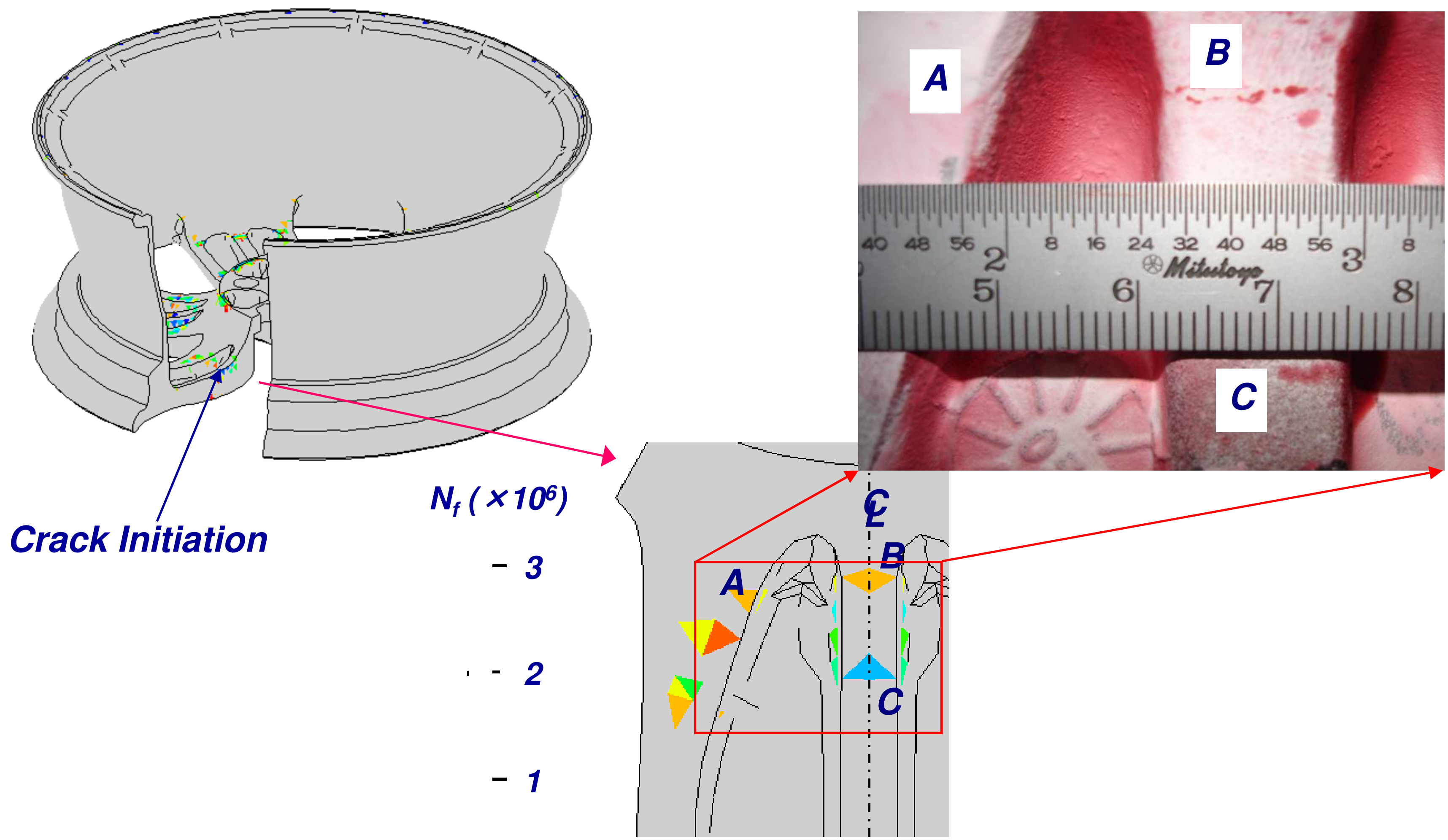
Maximum size of deviant microstructures: Pores or Fe-rich intermetallics - L_{max}

Gao YX et al., Acta Mat, 2005
Li P et al., AEM, 2006

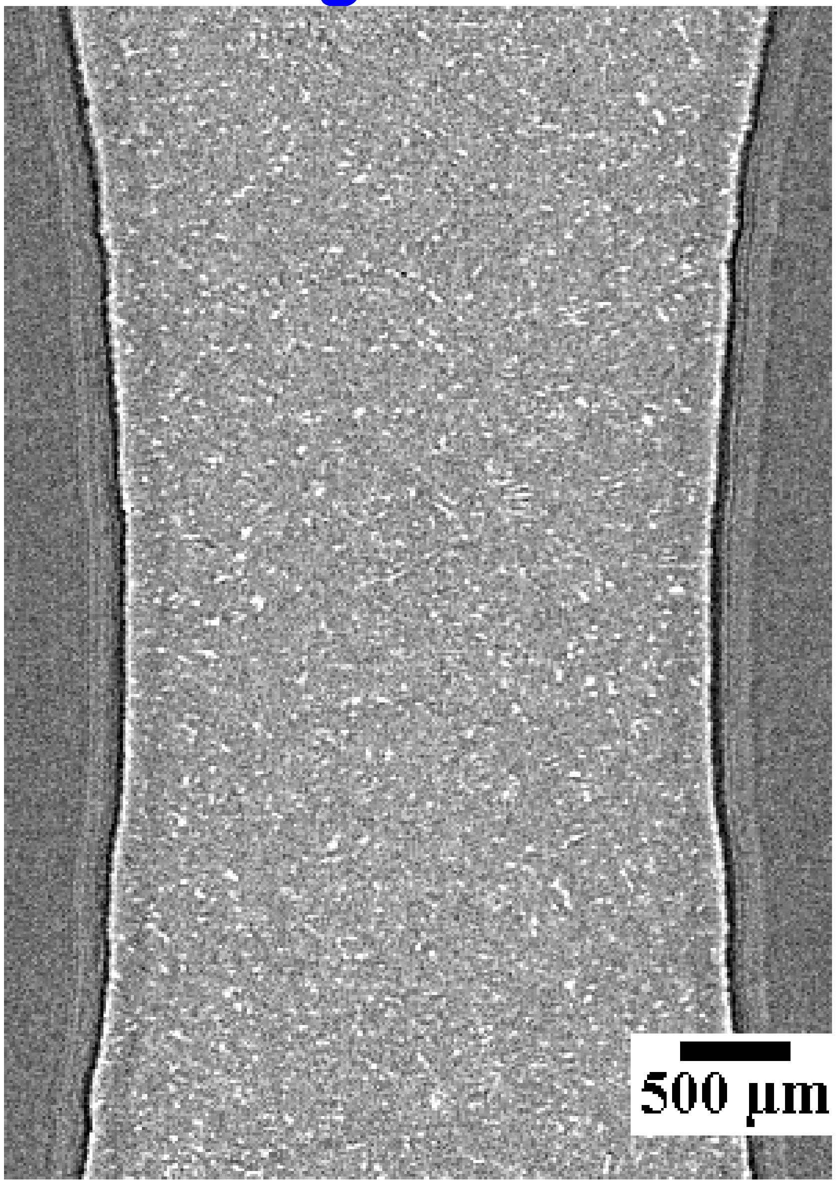
Challenges: models for flow stress of each phase, interface strength and adding debonding model, etc…

Does it work?

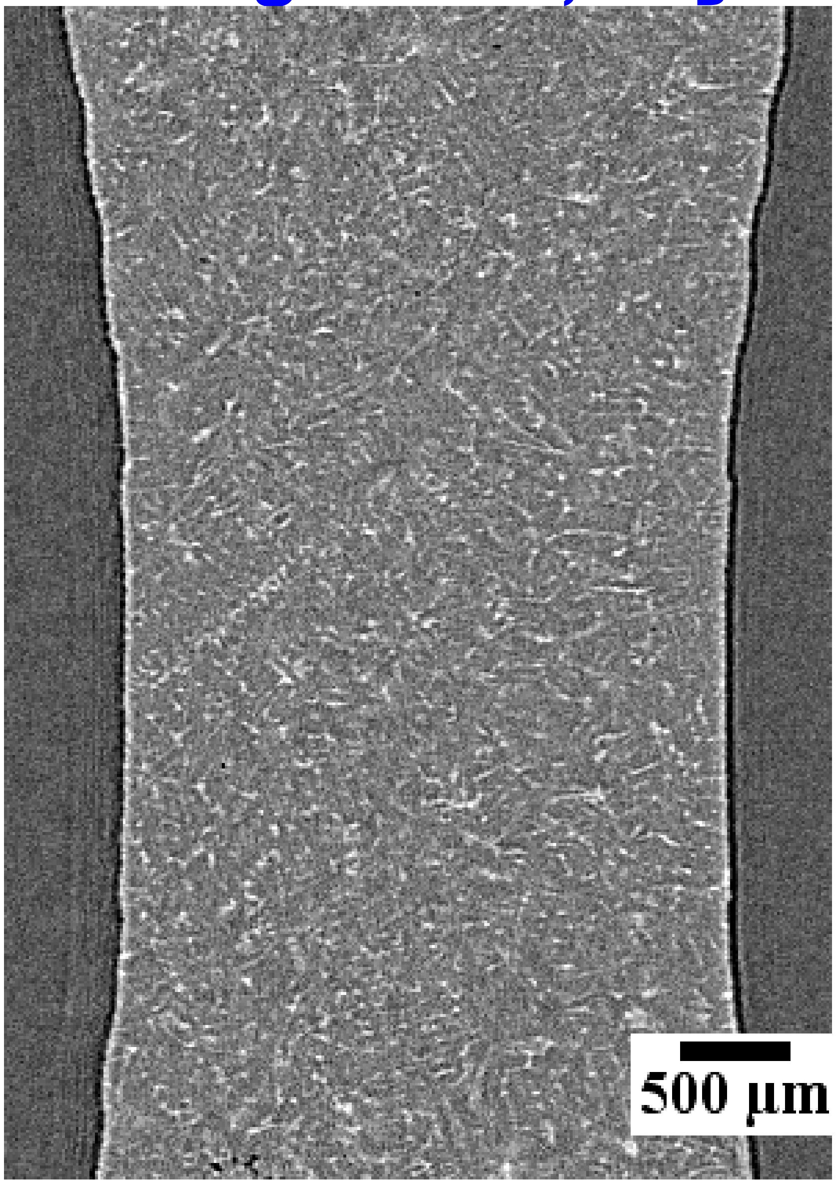
Accurate prediction of failure location was achieved (deviant feature - pores).



In situ observation shows Fe reduces hot forming/increases hot-tearing of A319, why?



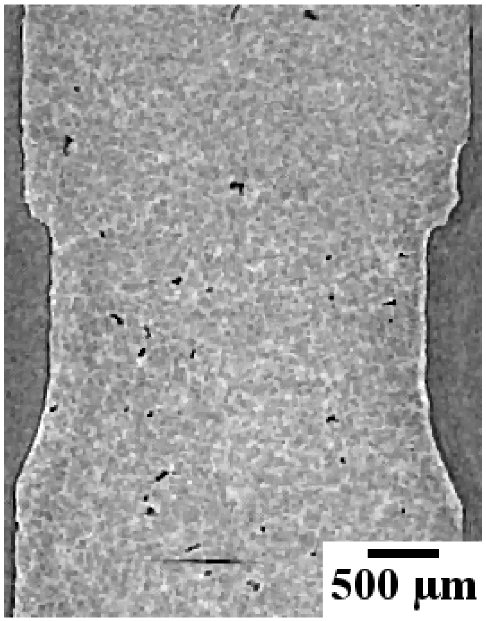
0.2wt.%Fe



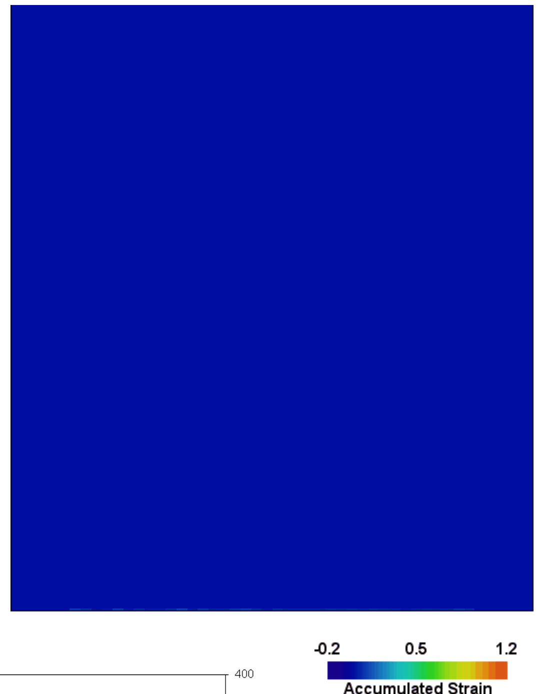
0.6wt.%Fe

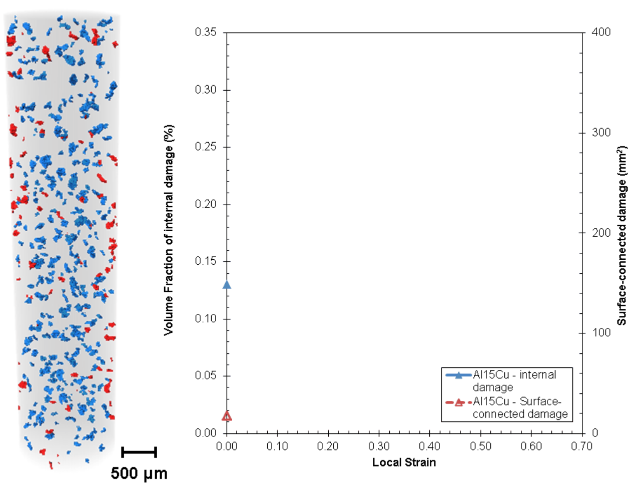
Comparison of analysis techniques

Imaging

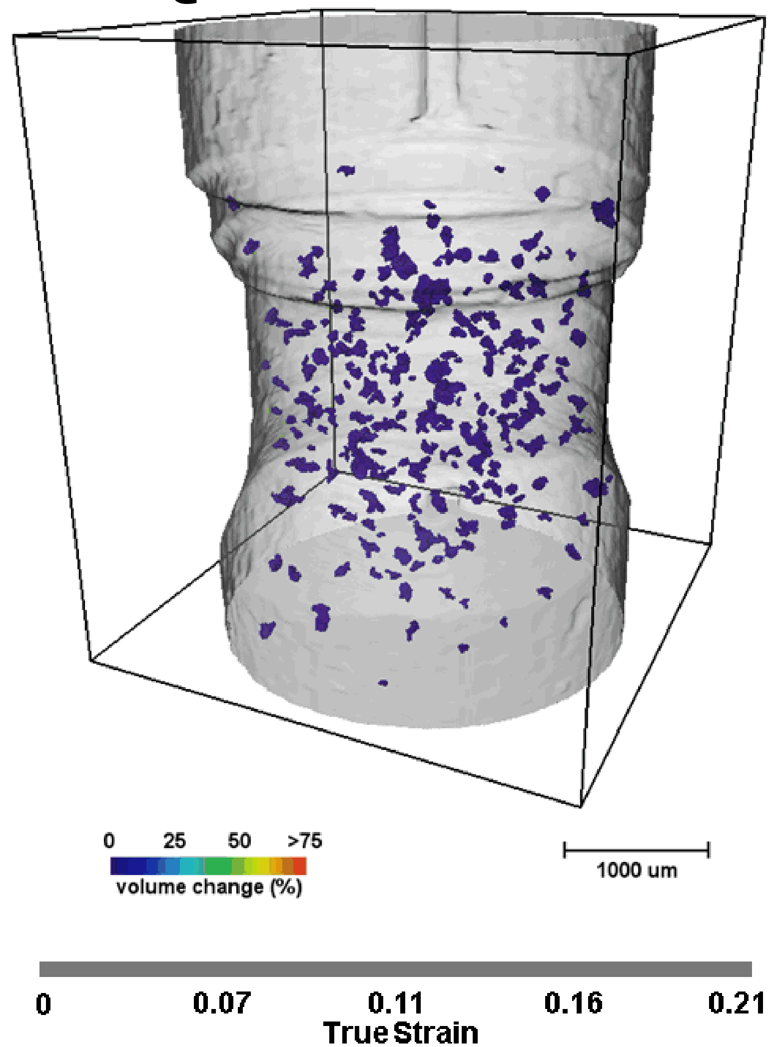


DVC

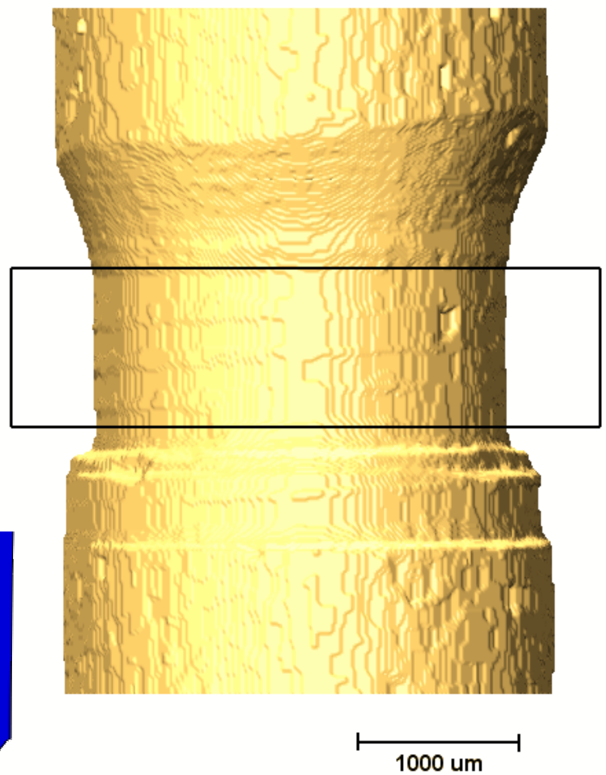


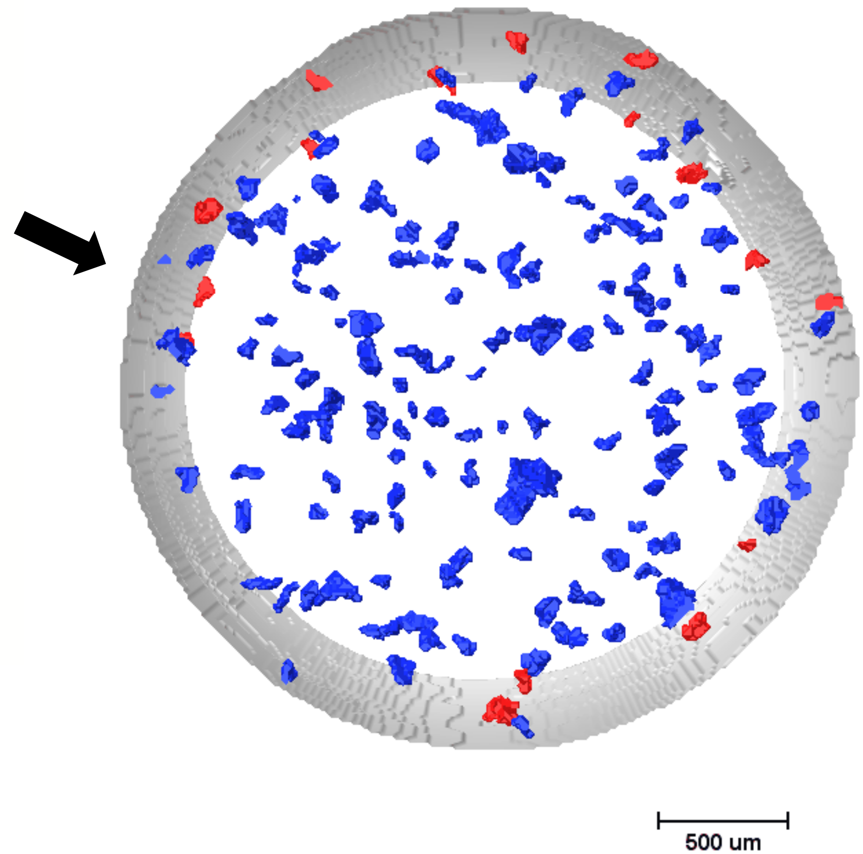


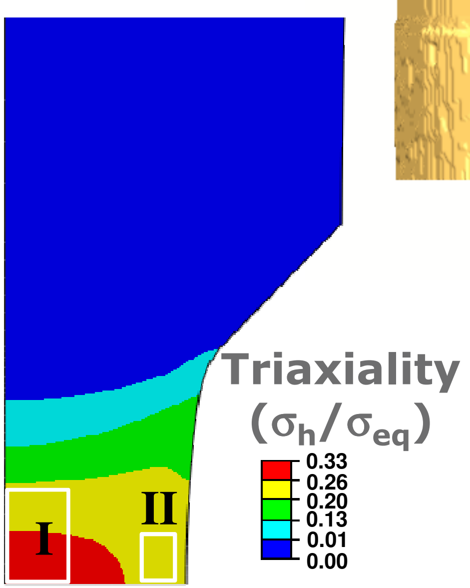
Tracked Quantification



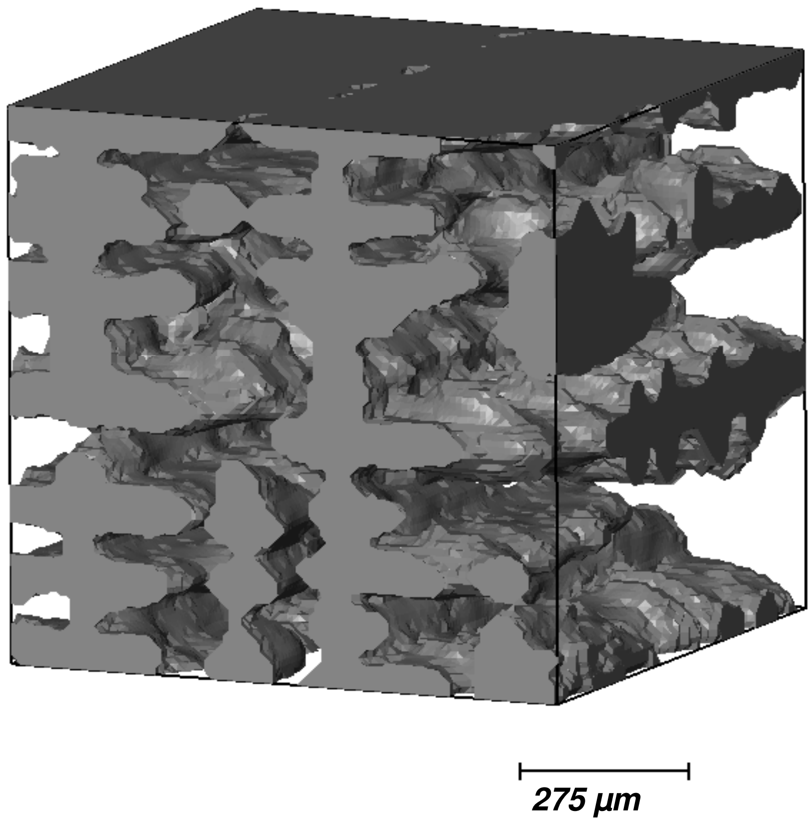
We can directly compare to predicted influence of triaxiality on localisation of damage



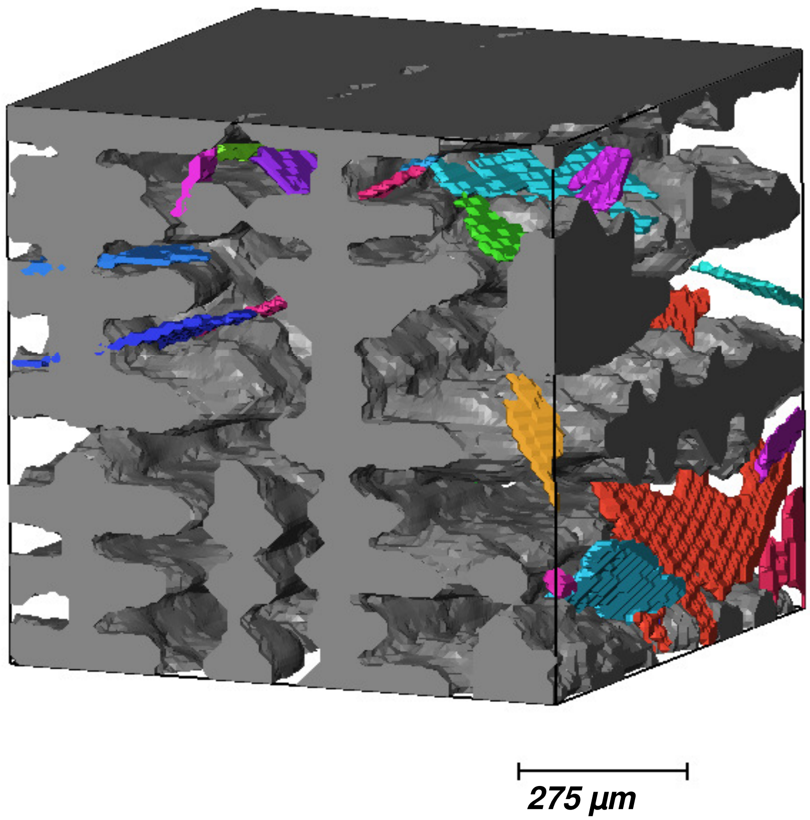




1st hypothesis, the intermetallics reduce interdendritic flow – we can use image based modelling to directly simulate the flow

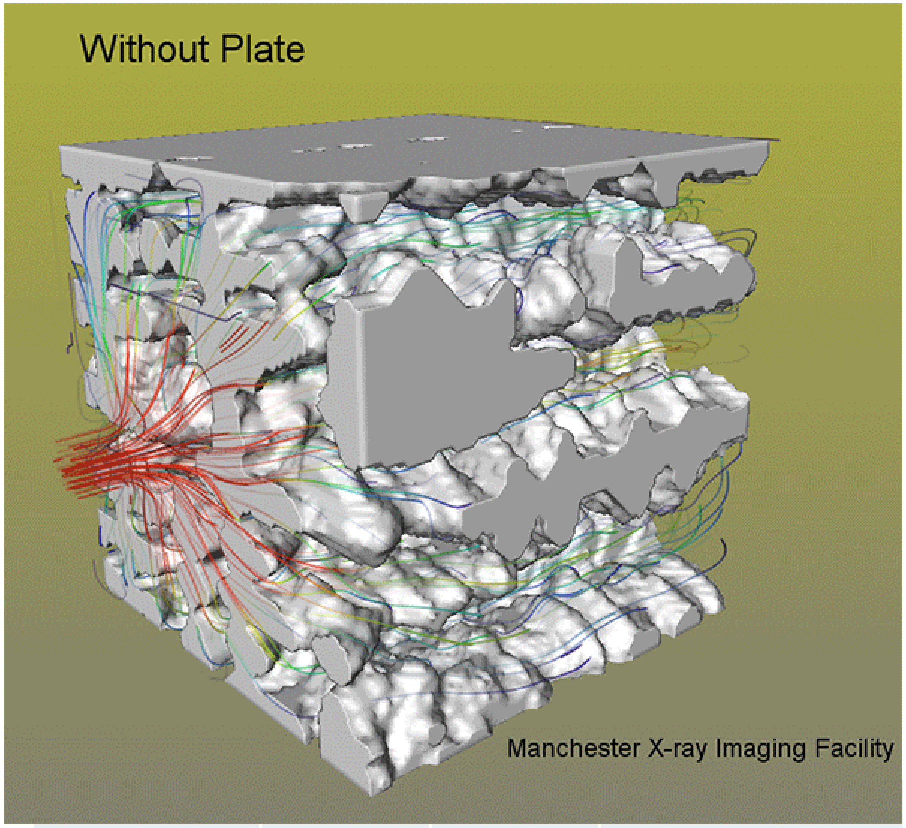


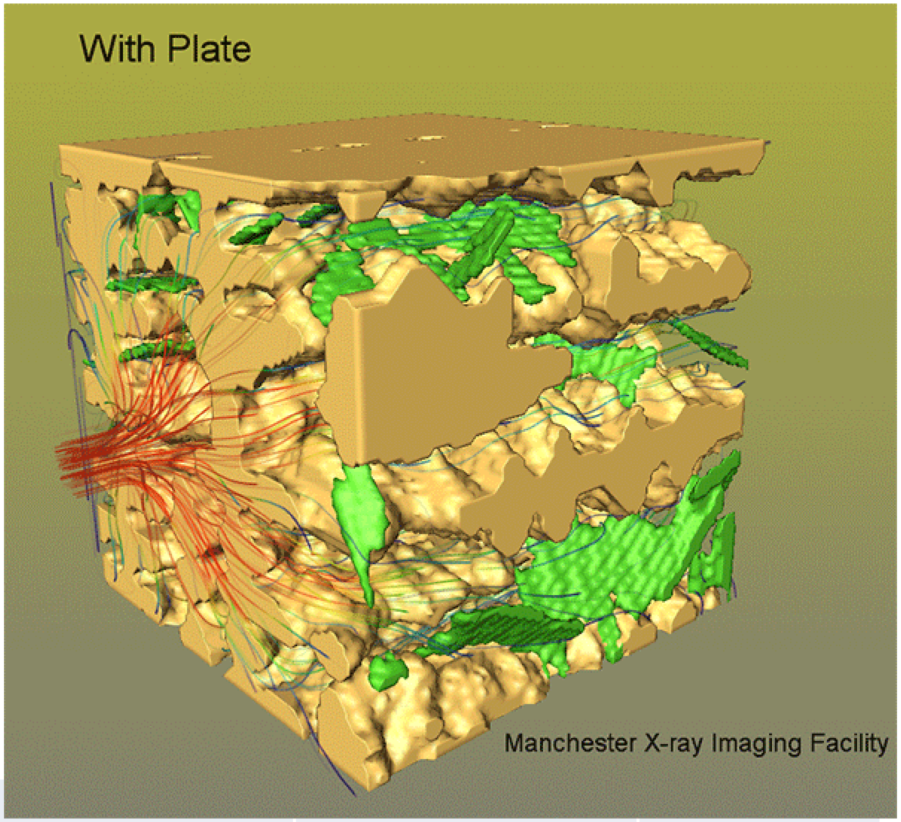
Dendrite



Dendrite + Intermetallics

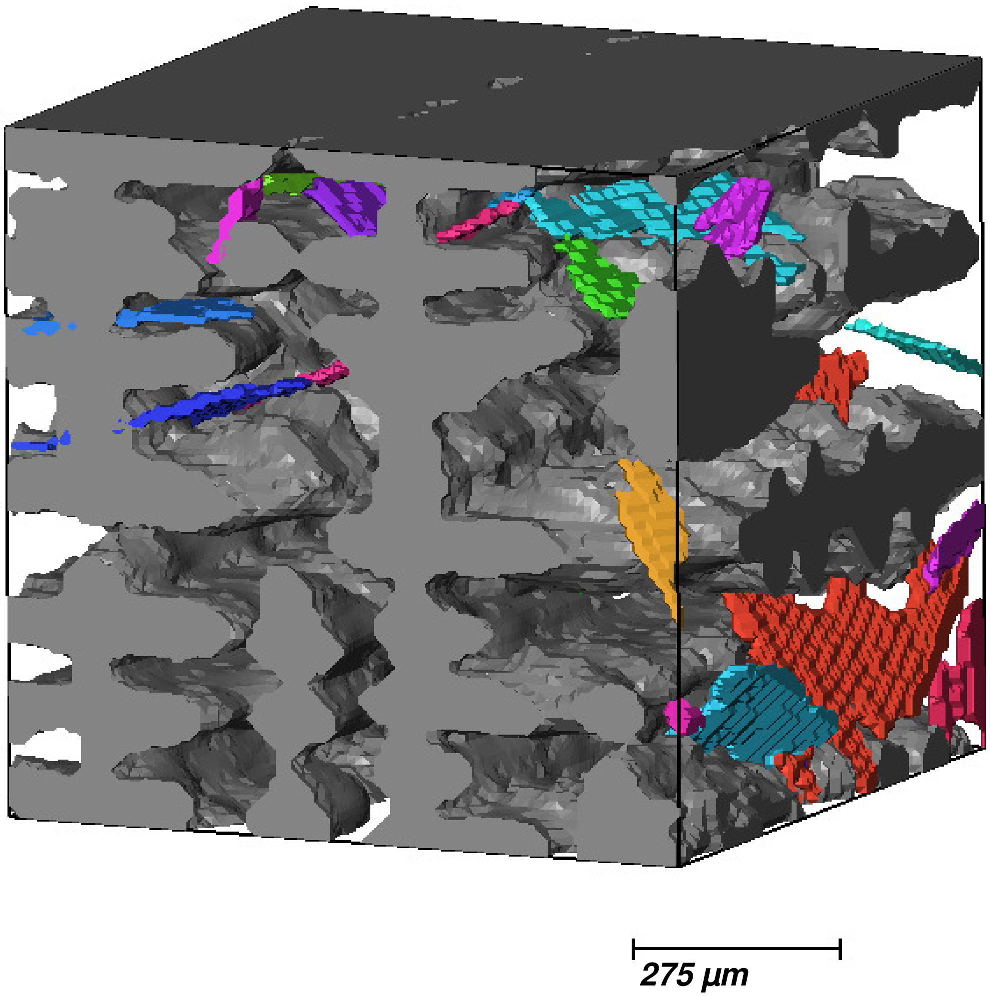
Flow Simulation results – <10% reduction in flow

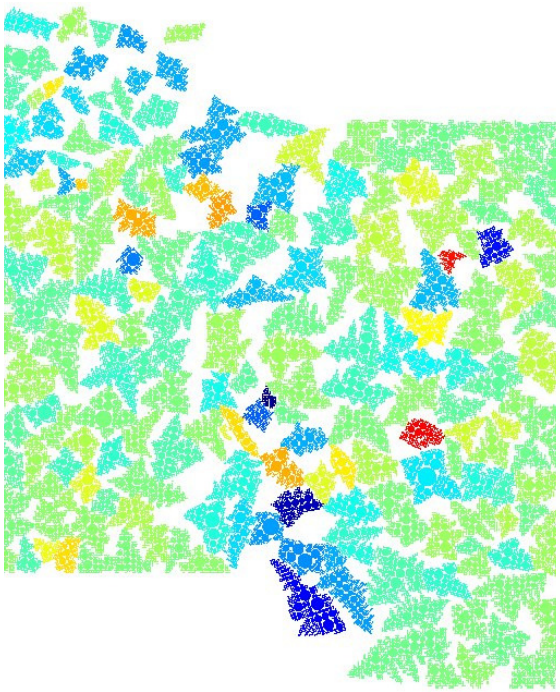




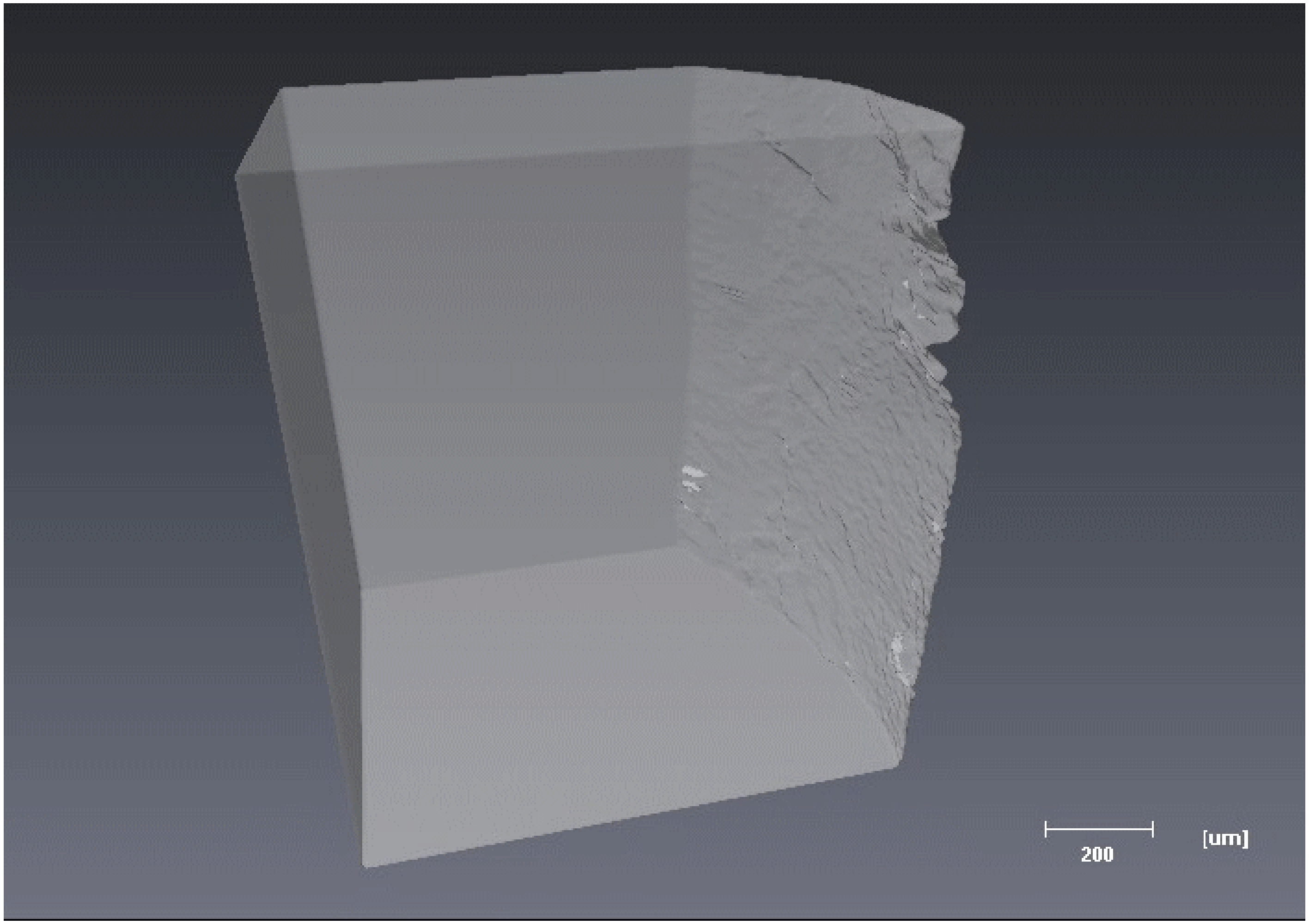
Geometry file	k [um^2]	k [d]	Input pressure [Pa]	Output pressure [Pa]	Flow rate [um^3.s^-1]	Viscosity [Pa.s]
Without Plate	178.5231	180.88853	130000	100000	4.87E+11	0.001
With Plate	167.14487	169.35954	130000	100000	4.86E+11	0.001

Synchrotron imaging with direct simulations demonstrated flow is only a minor effect, so now we need another hypothesis!



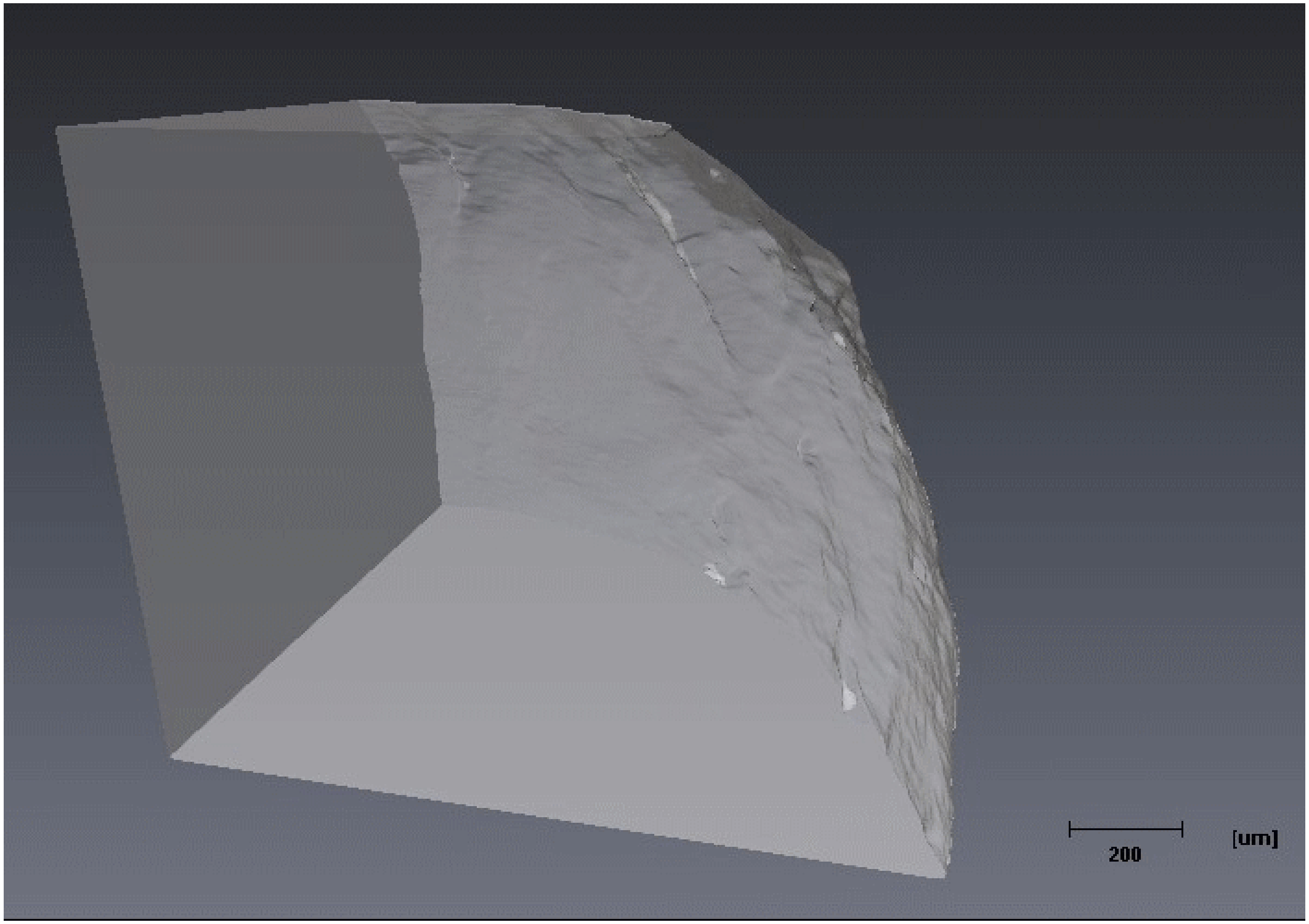


However, the synchrotron observations helped answer other questions:
1. when/where do the intermetallics nucleate, and
2. do pores nucleate on intermetallics



Cooled at 3° C/min

Do pores nucleate on intermetallics?



Cooled at 3° C/min

Conclusions

In situ observation shows us the kinetics of microstructural formation, clarifying dominate mechanisms and causality

Nurture can matter as much as Nature

We need to look out for the rebels when during the Materials Genome Initiative

Acknowledgements

- Ford, Tata Steel, GE
- Diamond Light Source & I12 Team
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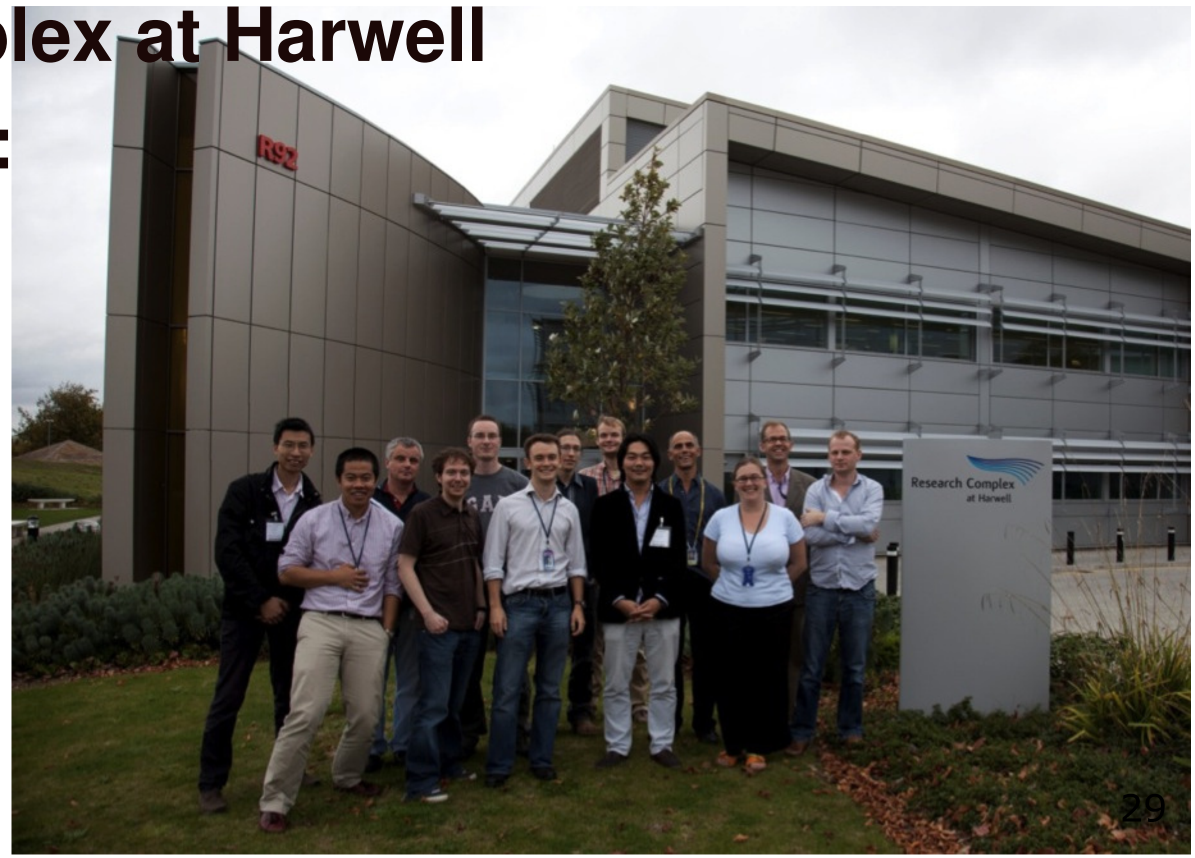
- Research Complex at Harwell
- The MXIF Team:
  - UoM
  - RCaH
  - Diamond
  - Imperial College



Questions?