ID232: Computational Analysis of Hydrogen diffusion in polycrystalline nickel and irregular polygonal micro and nano grain size effects.

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MultiHy

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BACKGROUND

MOTIVATION

MICROSTRUCTURAL MODEL

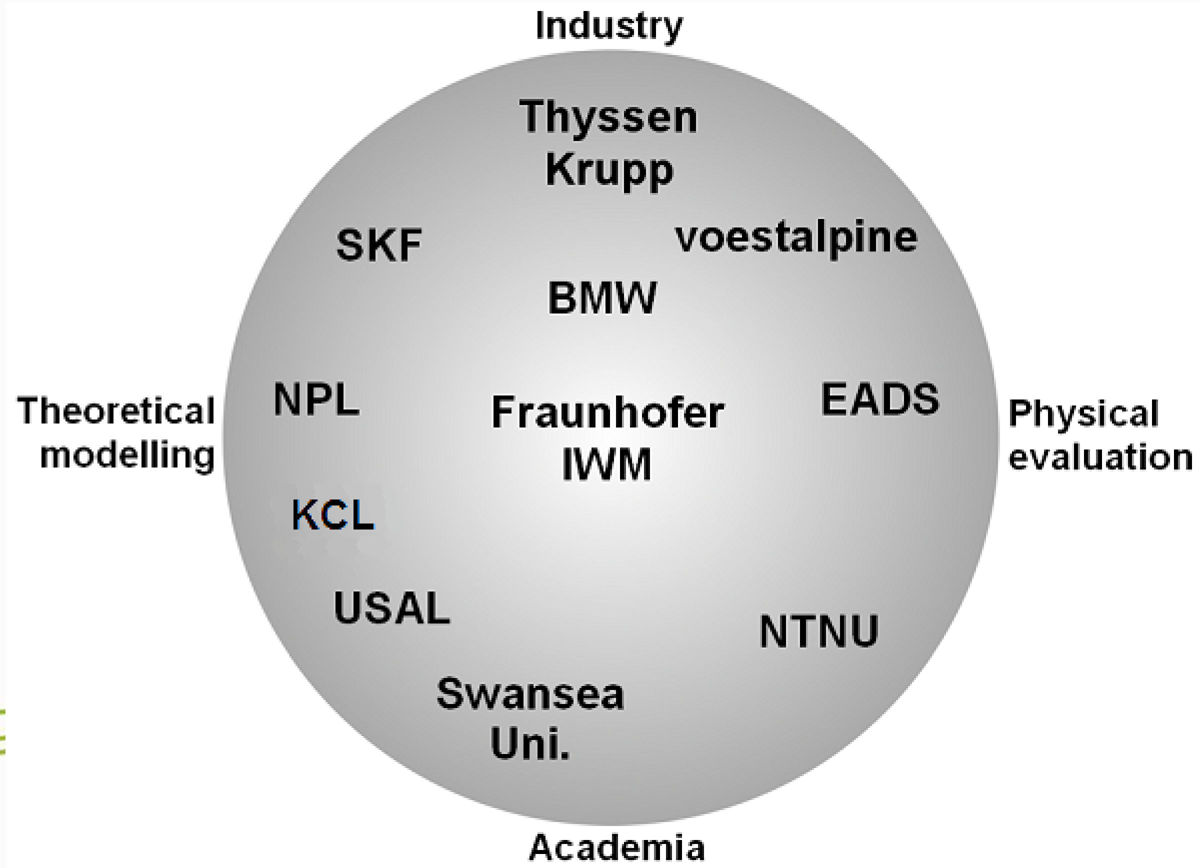
RESULTS

BACKGROUND

Multiscale Modelling of Hydrogen Embrittlement

AIM:

- Develop a Model to predict the HE at design stage : Reliable and industrially applicable
- Modelling framework: Atomistic – Continuum (Meso)- Component(Macro)

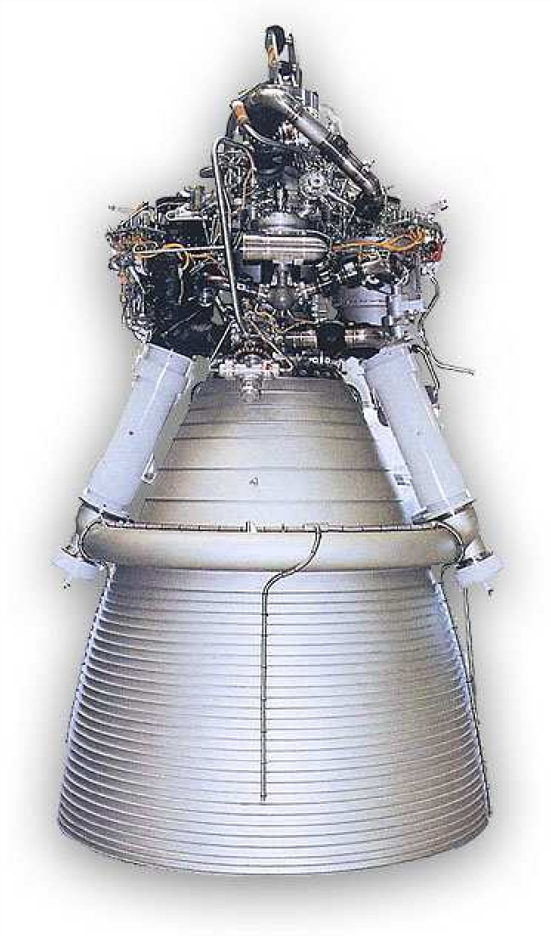


MultiHy Case Studies

- Within MultiHy there are three case studies within the fields of
  - Space
  - Automotive
  - Renewable energy
- Swansea's role involves component modelling of the first case.

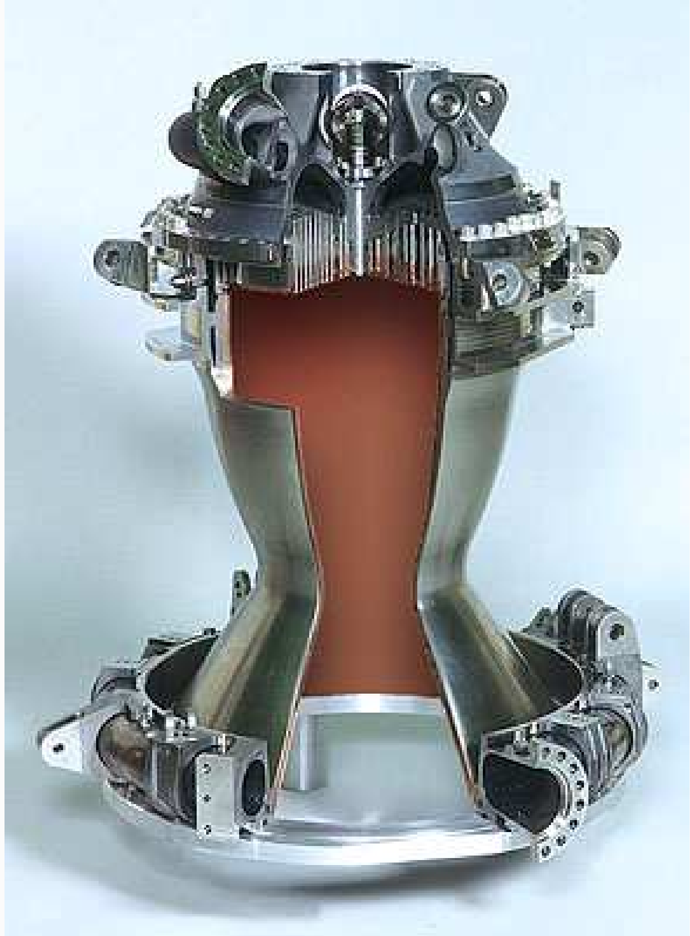
MultiHy - Case Study 1

- Ariane 5 combustion chamber
  - o Astrium/EADS
- Material of interest
  - o Pulse plated Nickel
- Cracks have been observed.
  - o Initiation associated with a welding process
- Cracks propagate to the surface along grain interfaces



MultiHy - Case Study 1

- Plating process has been changed
  - o Cracks currently not a problem
- EADS/Astrium want to improve the process again
- Need to be confident that the old problems will not reoccur

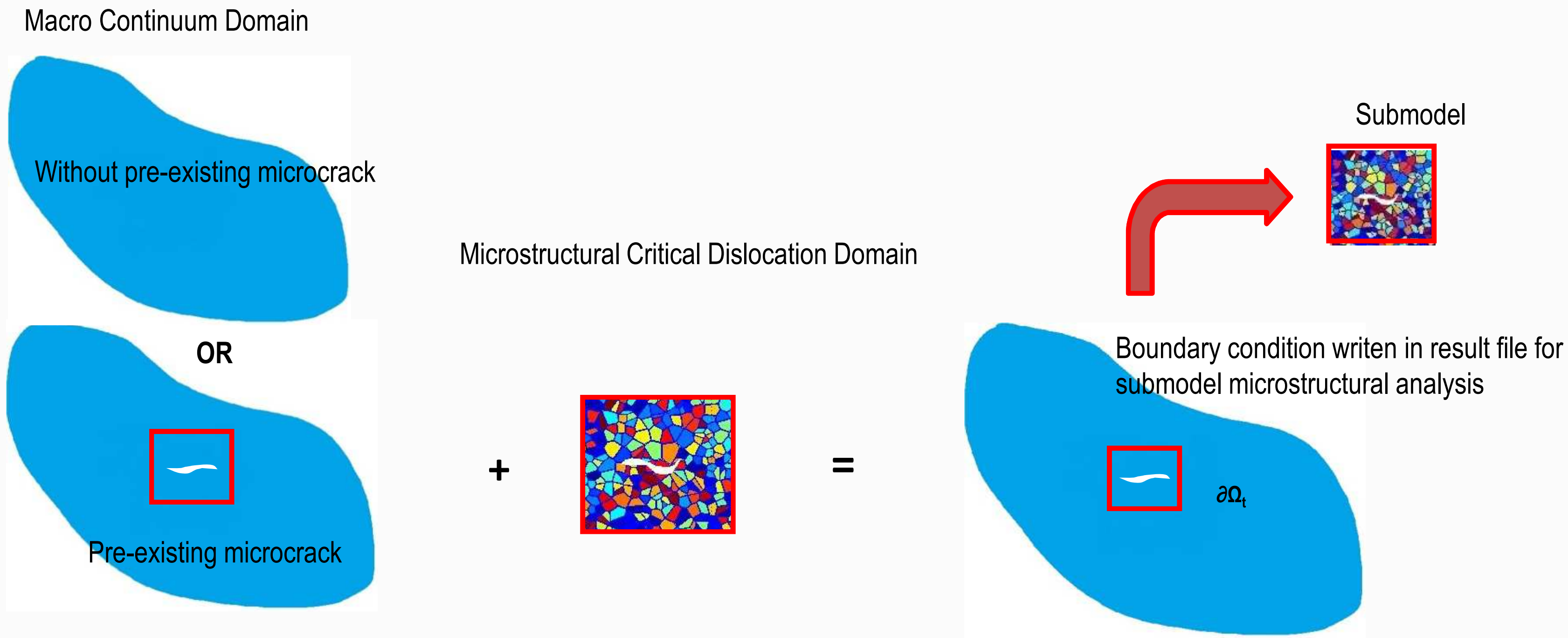


MOTIVATION

Hydrogen Embrittlement

- It is believed hydrogen diffusion plays a major role in the crack formation.
  - How to model the component?
- Homogeneous macro scale model is:
  - Comparatively computationally efficient
  - Certainly will suffice for most of the component
- Heterogeneous micro scale model will enhance
  - Accuracy where changes are rapid
  - Both spatially and temporally

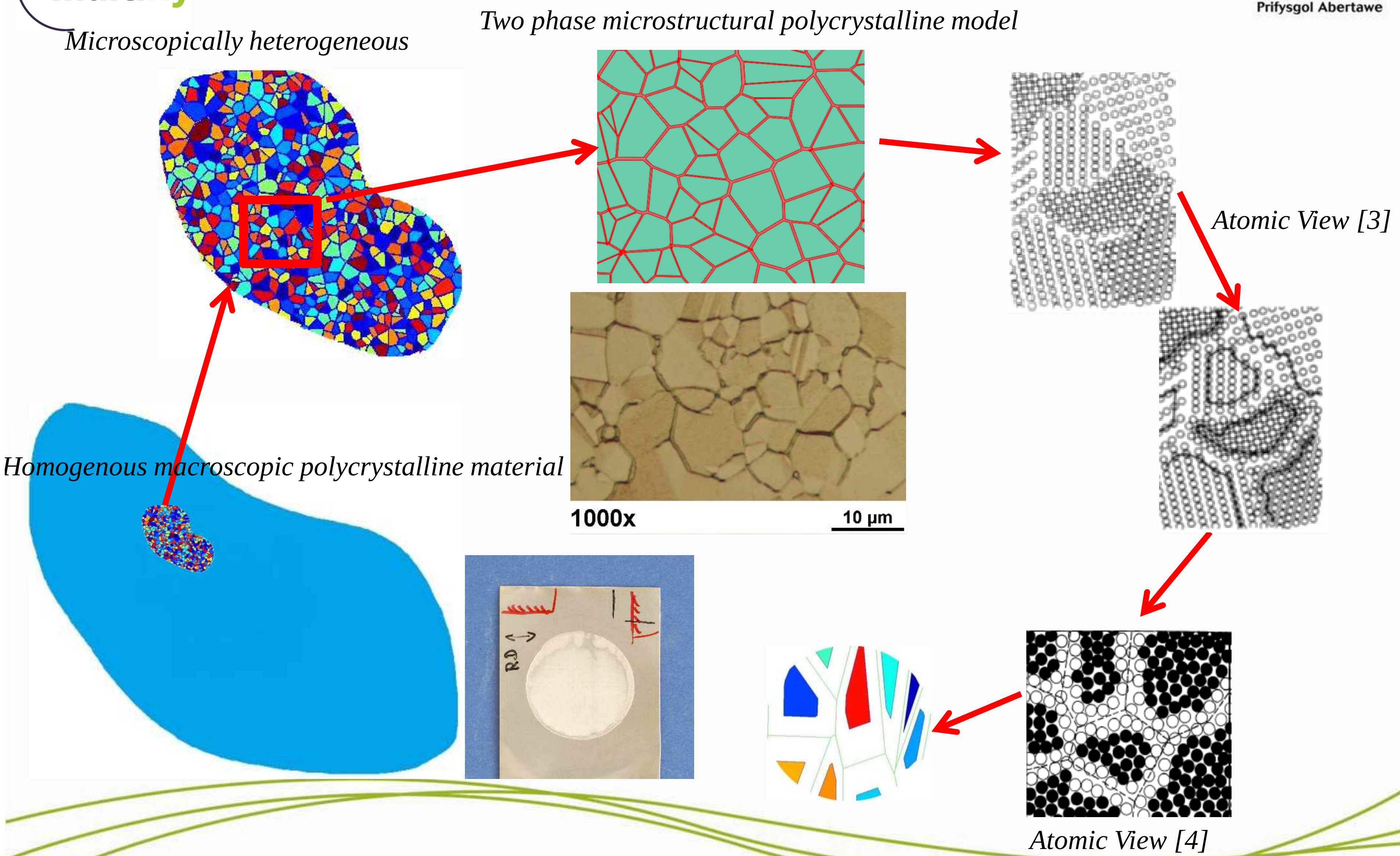
Multi Scale Model



- Initially analysis the macro continuum model without mesoscale model and find the critical sites
- Extract the boundary condition of the submodel by writing in the result file of Macro model.
- This boundary conditions result file of macro model is take as input for the mesoscale submodel of the critical site as separate analysis
- In this way we can reduce the analysis time.

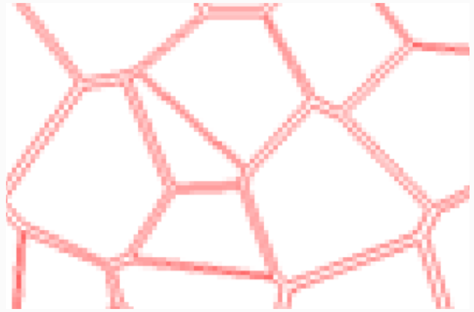
MICROSTRUCTURAL MODEL

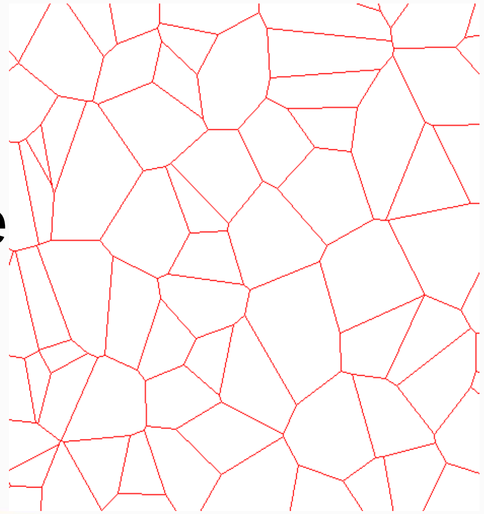
Multiphase Microstructural Model

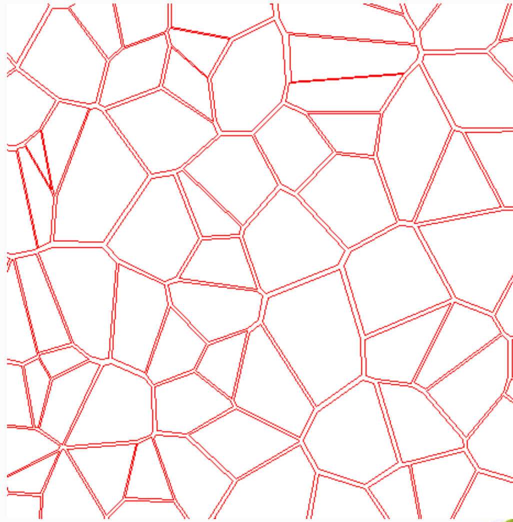


Microstructural Model

- Synthatic Microstructural Model (SMM) is developed
  - o Modified Voronoi Model (Double line)
- SMM consists of two phases
  - o Intergranular phase
    - – Grain
    - – Pores
  - o Intragranular Phase
    - – Grain boundary
    - – Dislocations

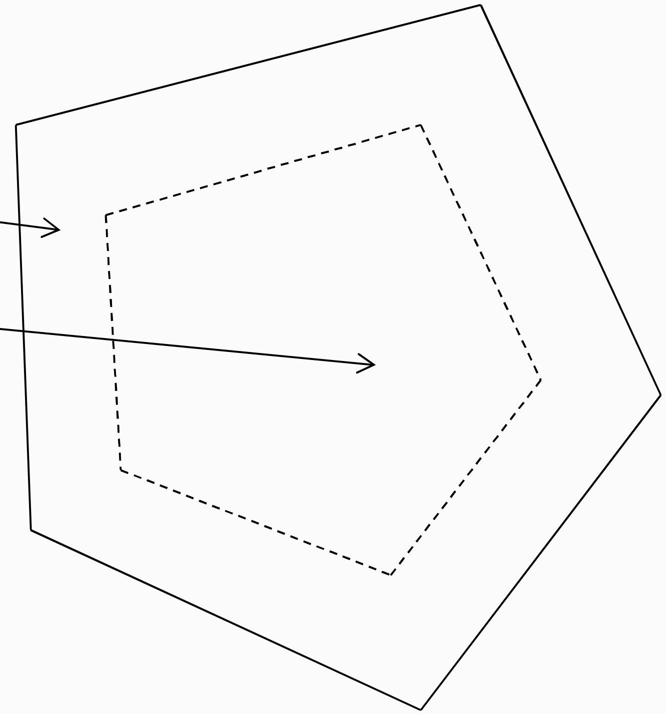






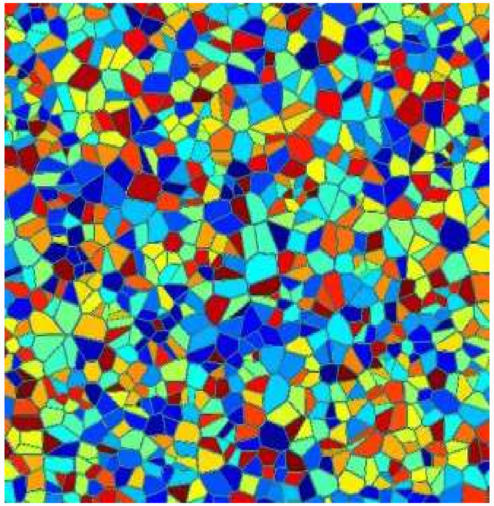
Microscale grain model

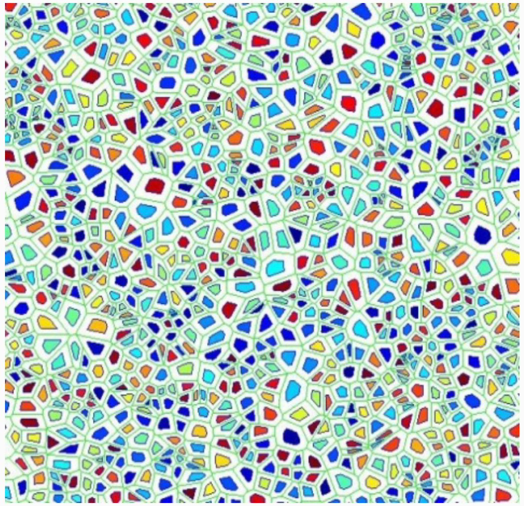
- Two phase microstructural model
  - o with intergranular
  - o and intragranular regions.
- Differential H transport along intragranular and intergranular regions.
  - o **D_{intra}~ 70 D_{inter} [1,2]**



Multiphase Microstructural model

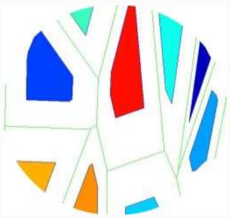
10 μm

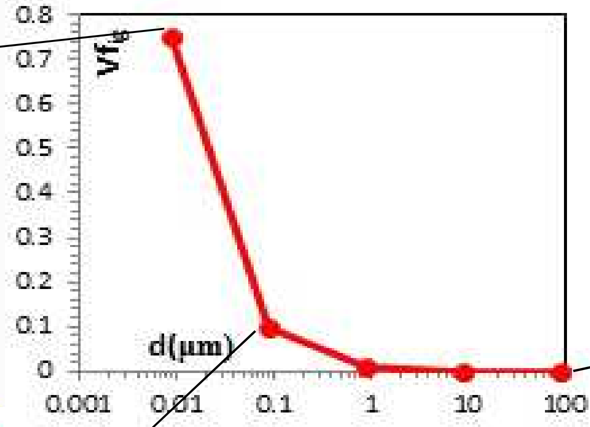


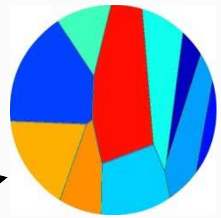


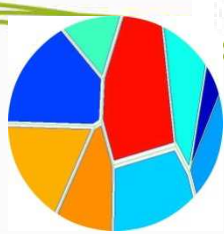
10 nm

- *Close view of microstructure : relative fraction of intergranular and intragranular phase*
- *Decrease in grain size from micro to nano scale increases the intergranular relative fraction*









RESULTS

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Microstructural model for hydrogen diffusion calculation

Effects of microstructure on the diffusion of hydrogen in polycrystalline material .

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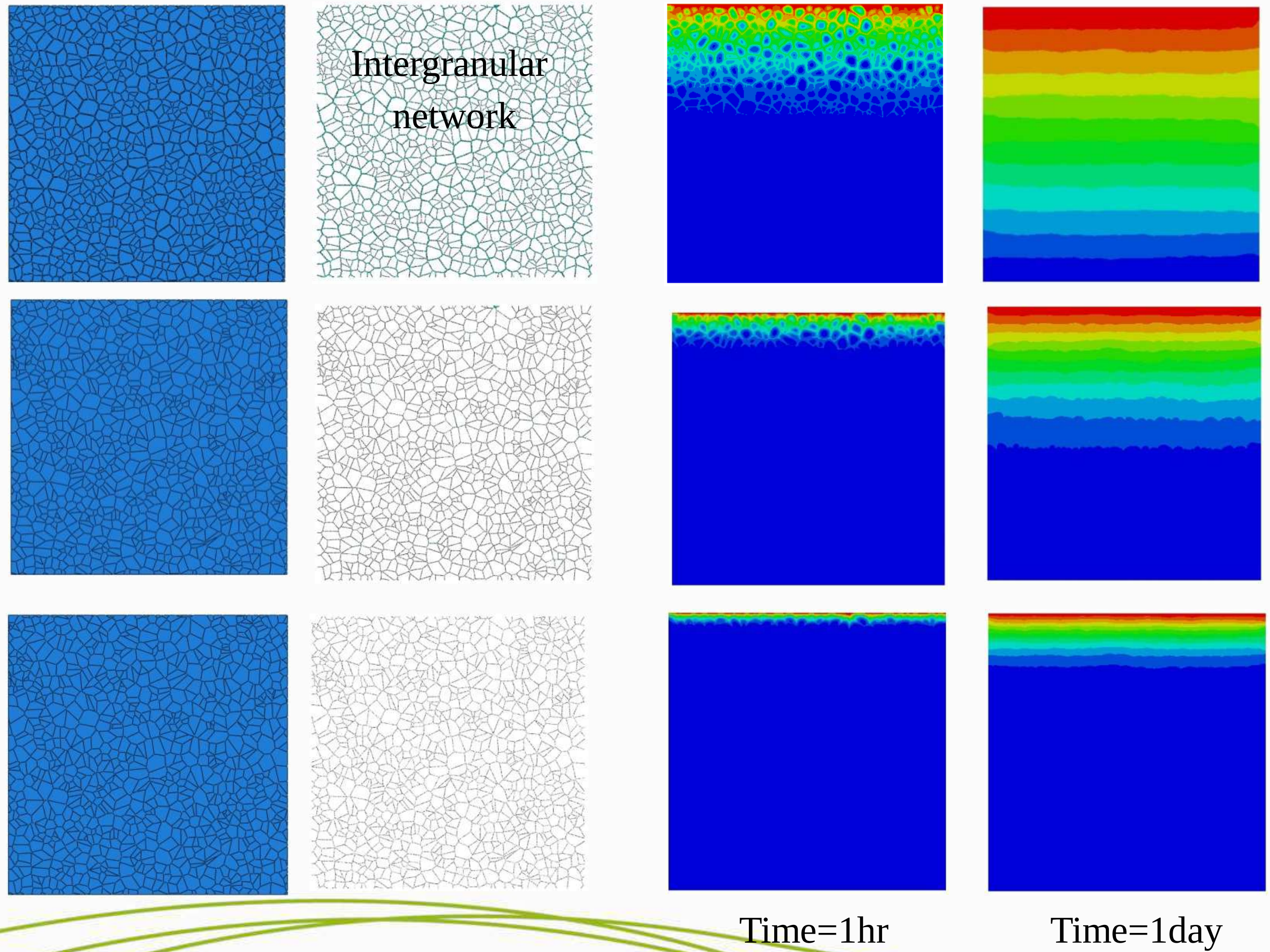

- *Polycrystalline material with different micro scale grain size.*
- *Increase in intergranular relative fraction, increases the diffusion of hydrogen*
- The hydrogen diffusion is delayed in the bigger grain size and accelerated in smaller grain size polycrystalline Material.

Microstructural model for hydrogen diffusion calculation

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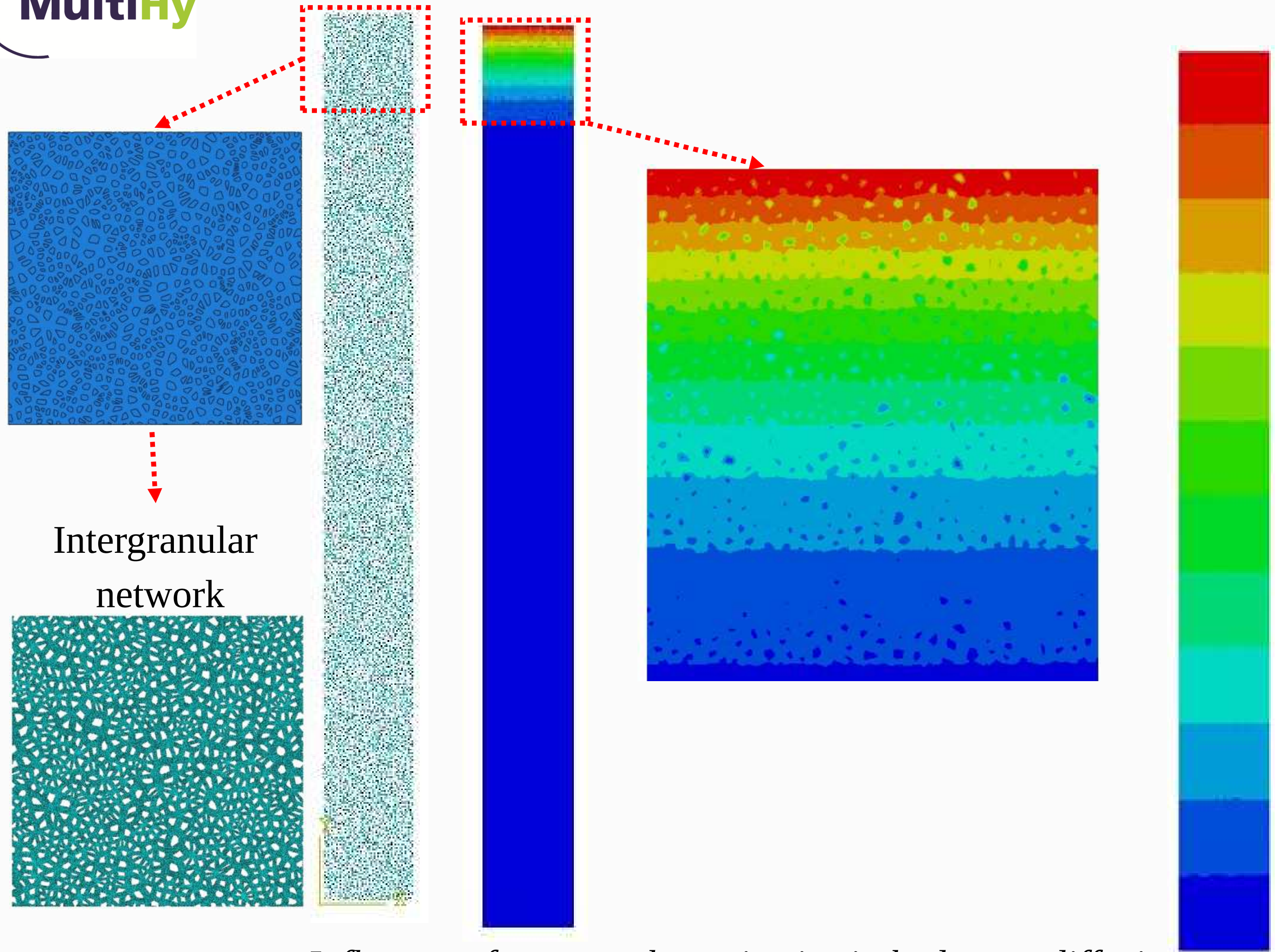
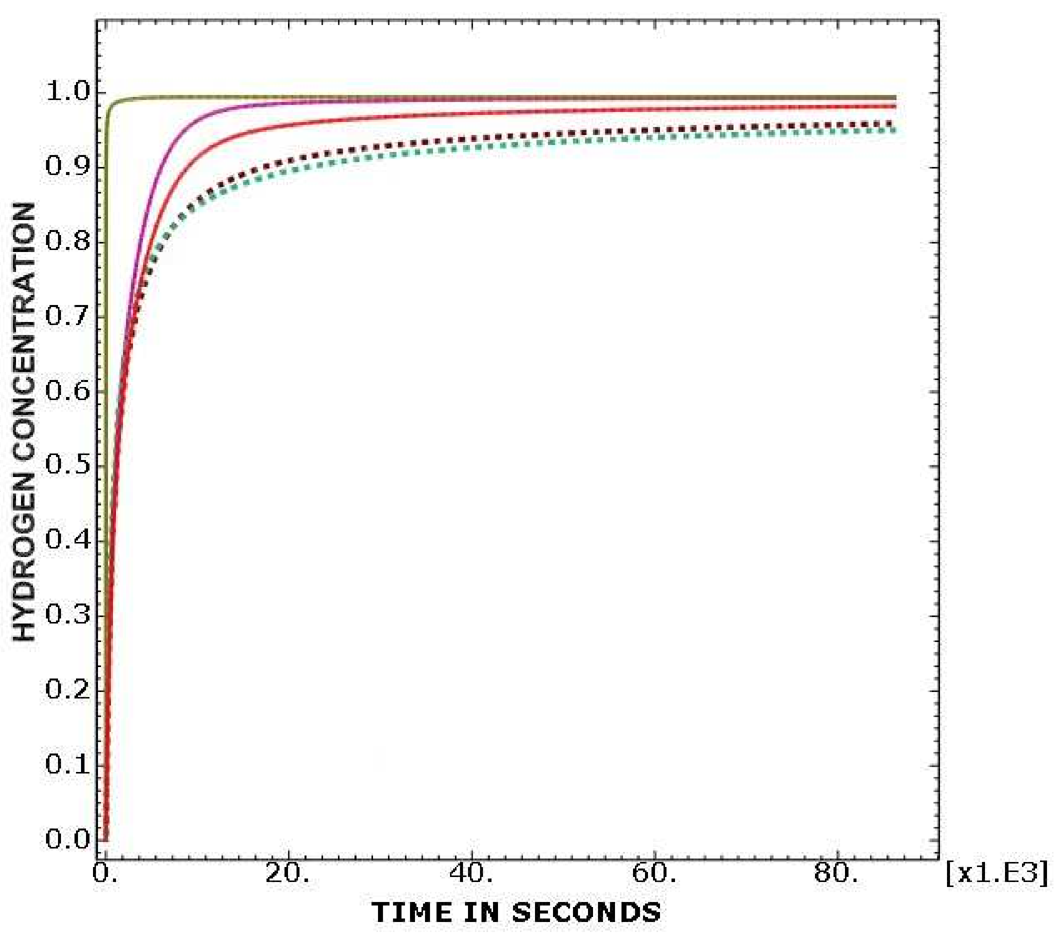


Influence of nano scale grain size in hydrogen diffusion

- *Polycrystalline material with average grain size of nano scale.*
- *Increase in intergranular relative fraction, increases the diffusion of hydrogen*
- The hydrogen diffusion is delayed in micro scale grain size and accelerated in nano scale grain size polycrystalline Material.

Microstructural model for hydrogen diffusion calculation



The hydrogen attains the steady state early in the following cases

- higher relative fraction of intergranular region,
- Smaller grain size polycrystalline material.

Nano scale grain size polycrystalline Nickel attain steady state much earlier than the Micro scale grain size polycrystalline nickel.

Hydrogen diffusion for different relative fraction of intergranular and grain size

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Microstructural model for hydrogen diffusion calculation

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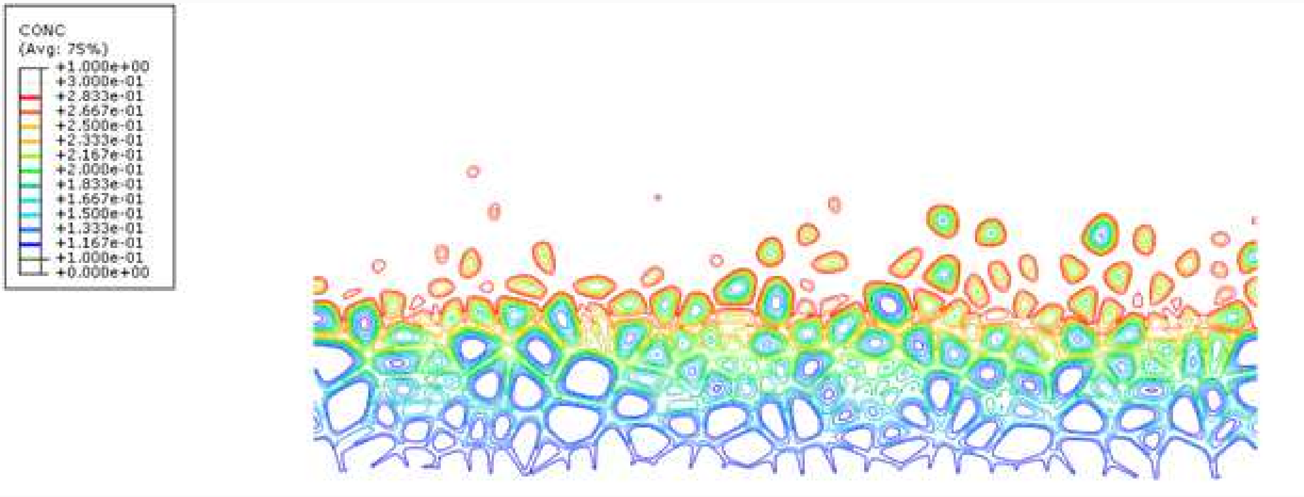
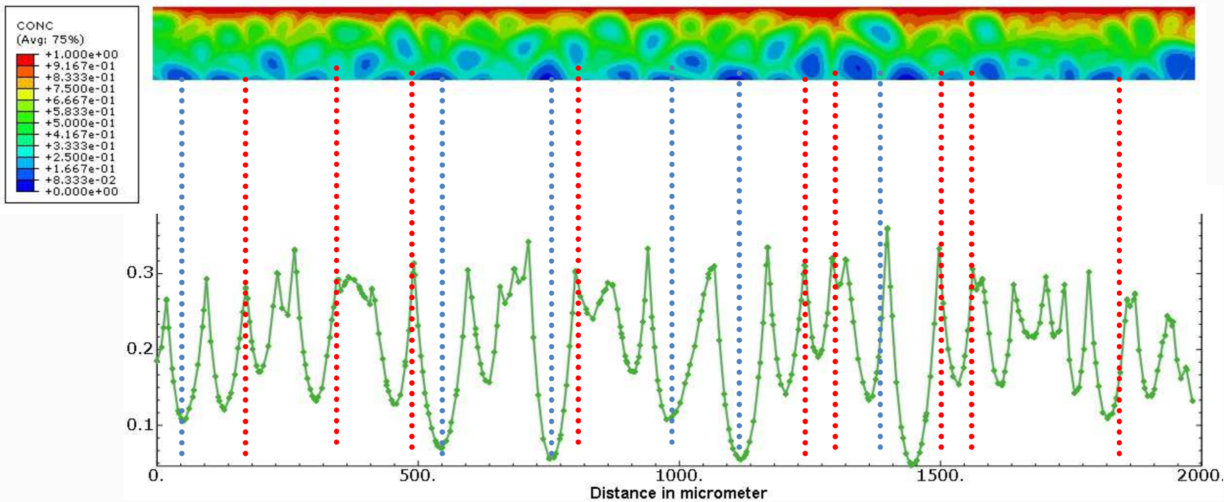
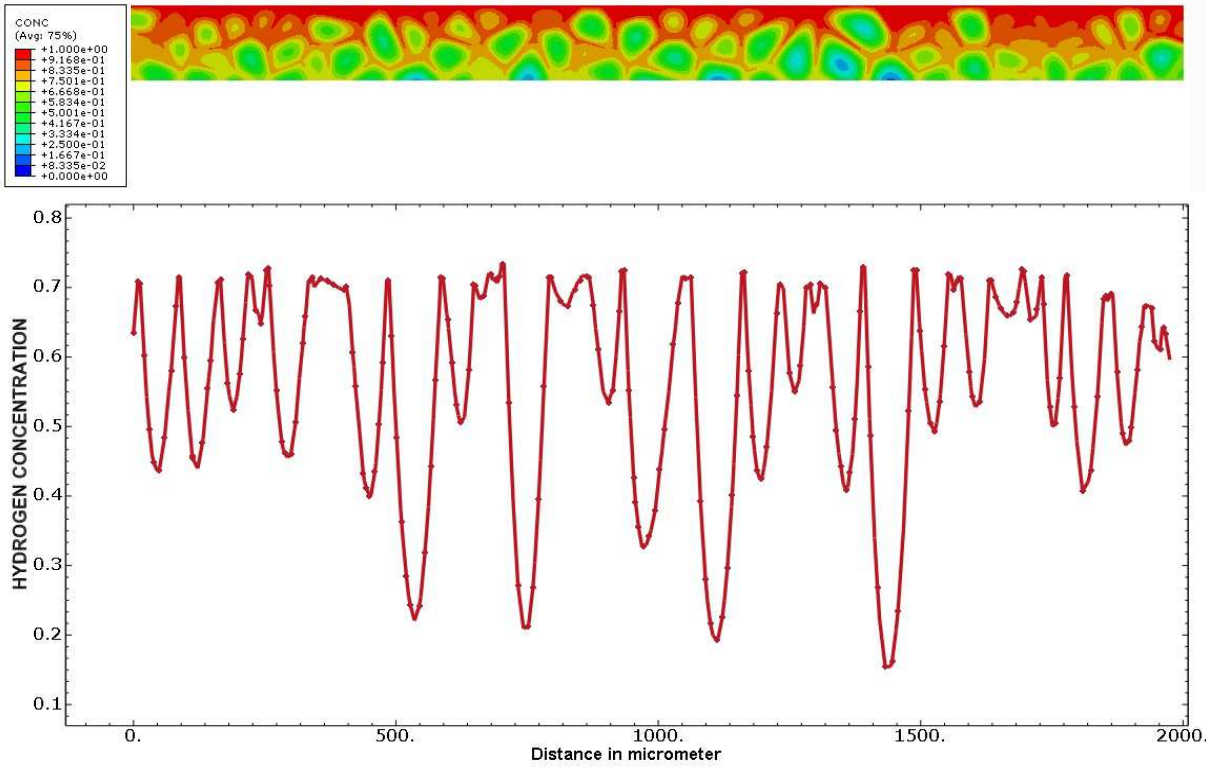




Inhomogeneous behaviour of hydrogen transport and accumulation in polycrystalline material between intergranular region and grain region with smaller grain size.

Microstructural model for hydrogen diffusion calculation



Inhomogeneous behaviour of hydrogen diffusion and accumulation in polycrystalline material between intergranular region and grain region with bigger grain size.

Future Focus

- Real microstructure from Microscopy and its orientation from EBSD

- Couple and Implement the developed micro scale effects with the macro scale model.

- Investigate the phenomena that affect hydrogen diffusion in nickel
  - Trap sites (Already developed the model and validated it)
  - stress, Plastic strain
  - Grain orientation
  - Segregation of hydrogen along GB
  - Pores and cluster

Acknowledgement

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Thank You

for listening

References

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2. Hongtao Wang, Wei Yang etc., Enhances diffusivity by triple junction networks, Scripta Materialia, 52, 69 (2005).