JMC 1 JOURNÉES de la MATIÈRE CONDENSÉE du 24 au 27 Août 2021

Minicolloque n° CPR25
« Nano-Matériaux Magnétiques : effet de la nanostructuratlon sur le control des propriétés macroscopiques »

Effect of microstructure on the diffusion property of polycrystals

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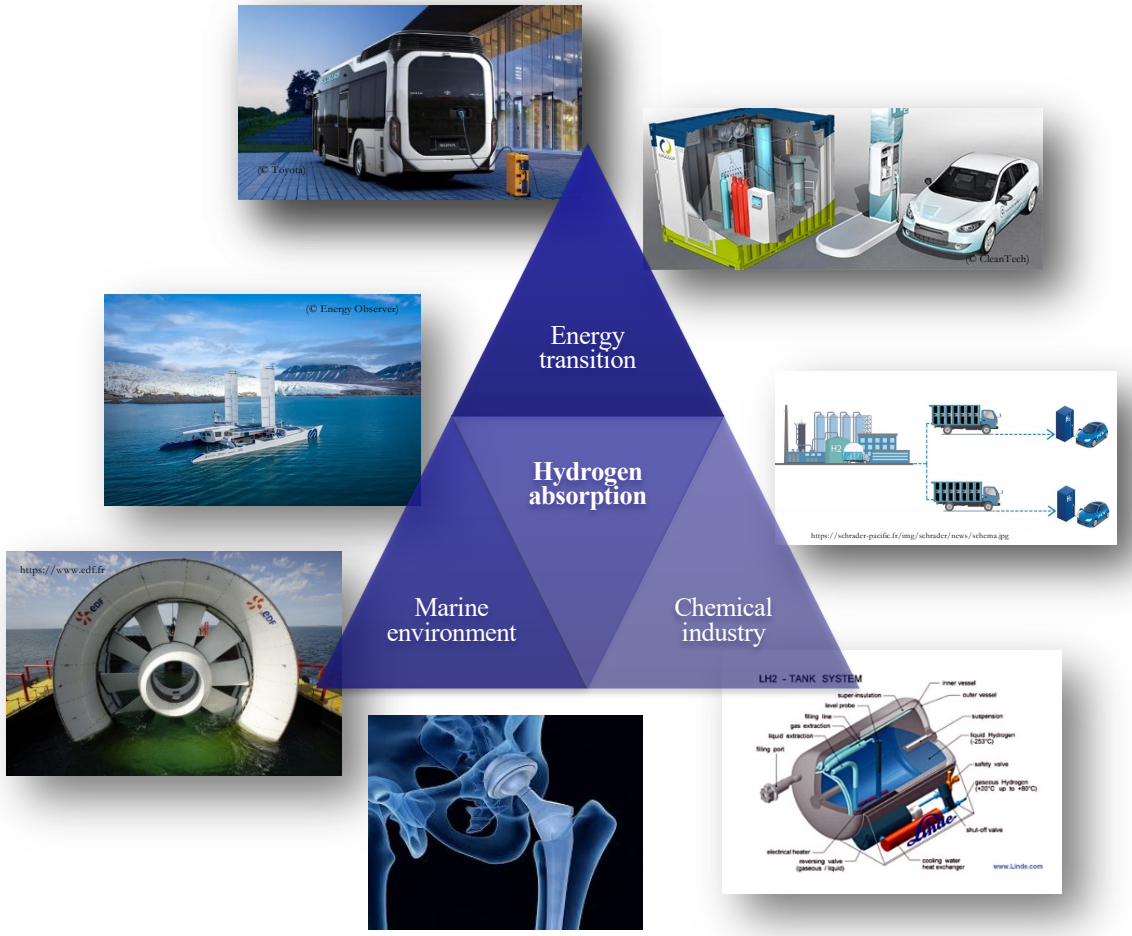
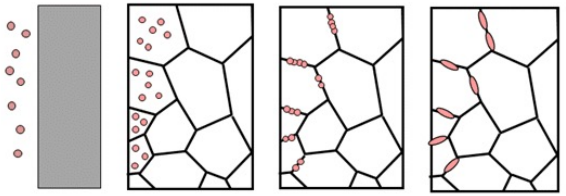
Context

Hydrogen a large set of industry and societal applications



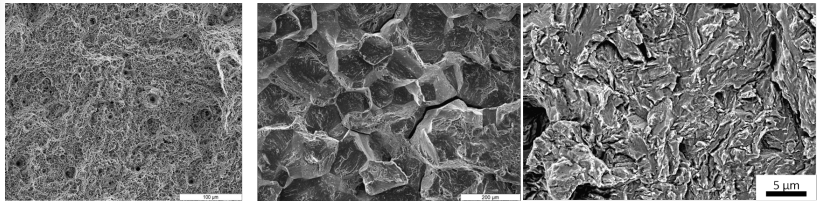
Consequence of Hydrogen absorption:

→ Inherent modifications of material properties



https://www.imetllc.com/training-article/hydrogen-embrittlement-steel/

Without H	With H	With H
Ductile	*Intergranular*	*Quasi-cleavage*



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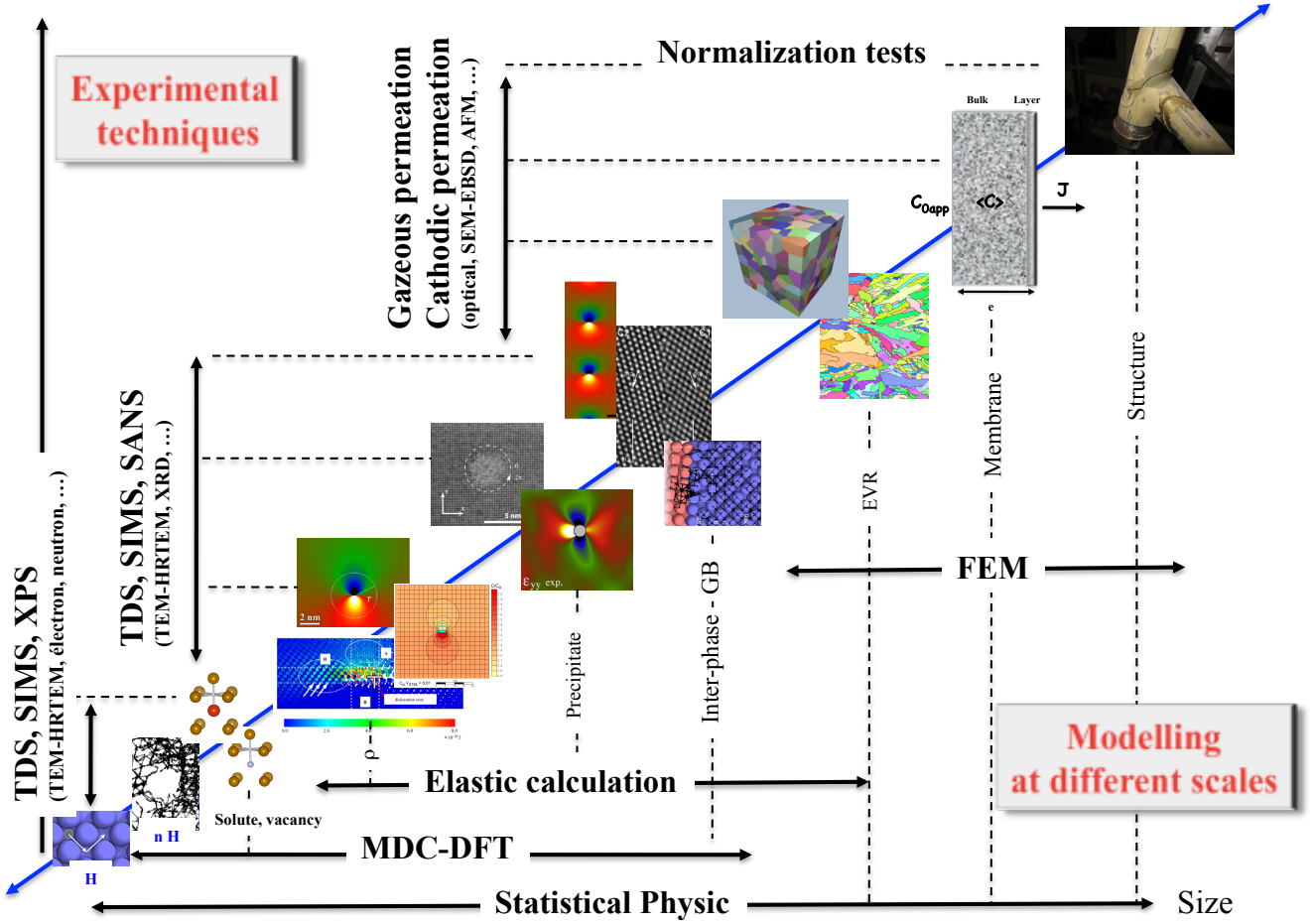
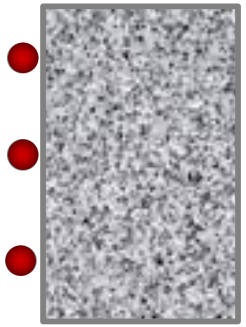
Hydrogen/metallurgy: Multi-scales analyses



Feaugas et al. A3TS, 2010

Context

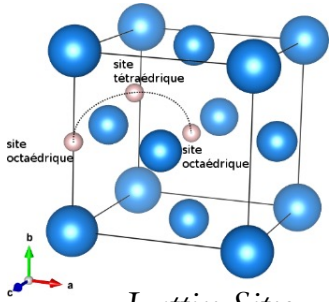
Hydrogen states *vs* microstructural defects



Lattice Diffusion

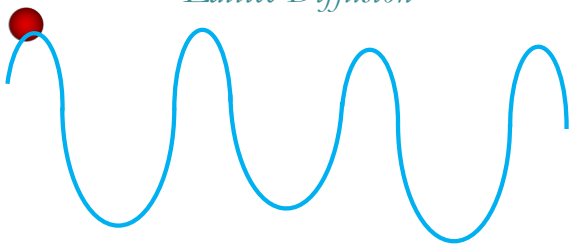
Trapping

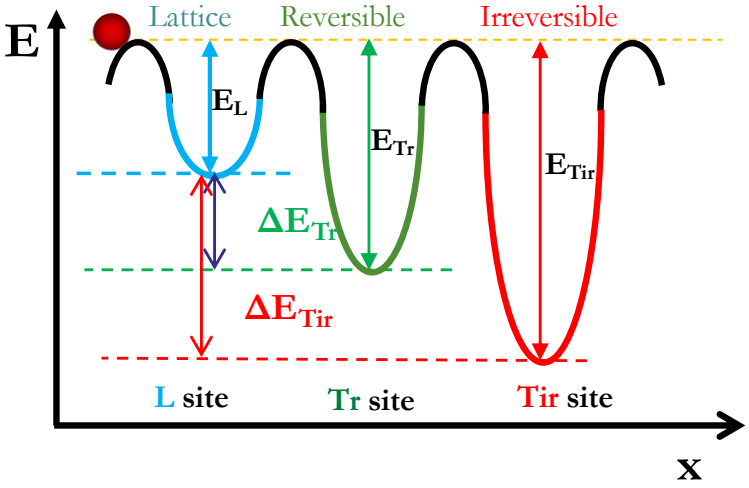
Diffusion Short cut



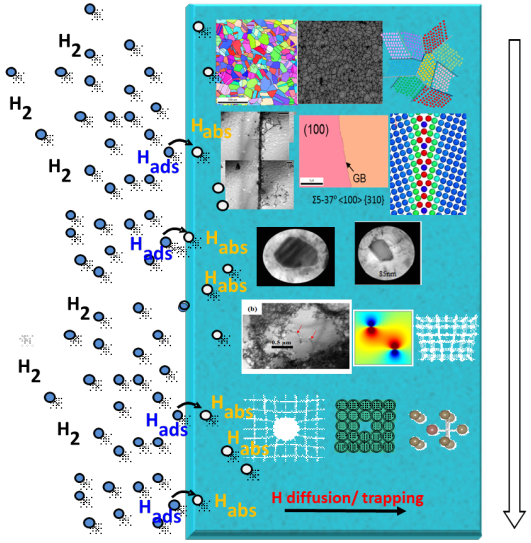
Lattice Sites

Lattice Diffusion





Defects at different scales



Polycrystal

Grain boundaries

Precipitates

Dislocations

Vacancy / Solutes

- diffusible (Lattice or diffusion short circuit)
- trapped Revesibly (elastic fields, edge dslocations, precipitates)
- trapped irreversibly (vacancies, dislocation cores)

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Context

Modelling: generalized Fick transport equation

n traps, density $N_{T,i}$, binding energy $E_{T,I}$

→ H concentration $C_{T,i}=N_{T,i}\theta_{T,i}$

H in interstitial, density N_L

→ H concentration $C_L=N_L\theta_L$

Total H concentration:

$$C = C_L + \sum_i C_{T,i}$$

Transport equation:

$$\boldsymbol{\varphi} = -D_L \boldsymbol{\nabla} C_L - \frac{V_H D_L}{RT} C_L \boldsymbol{\nabla} P_H \quad \Rightarrow \frac{\partial C_L}{\partial t} + \sum_i \frac{\partial C_{T,i}}{\partial t} = -\boldsymbol{\nabla}.\boldsymbol{\varphi}$$

McNabb & Foster, Transactions of the Metallurgical Society of AIME, 227(3), 618–627, 1963
Krom et al, Journal of the Mechanics and Physics of Solids, 47(4), 971–992, 1989

Trapping equation:

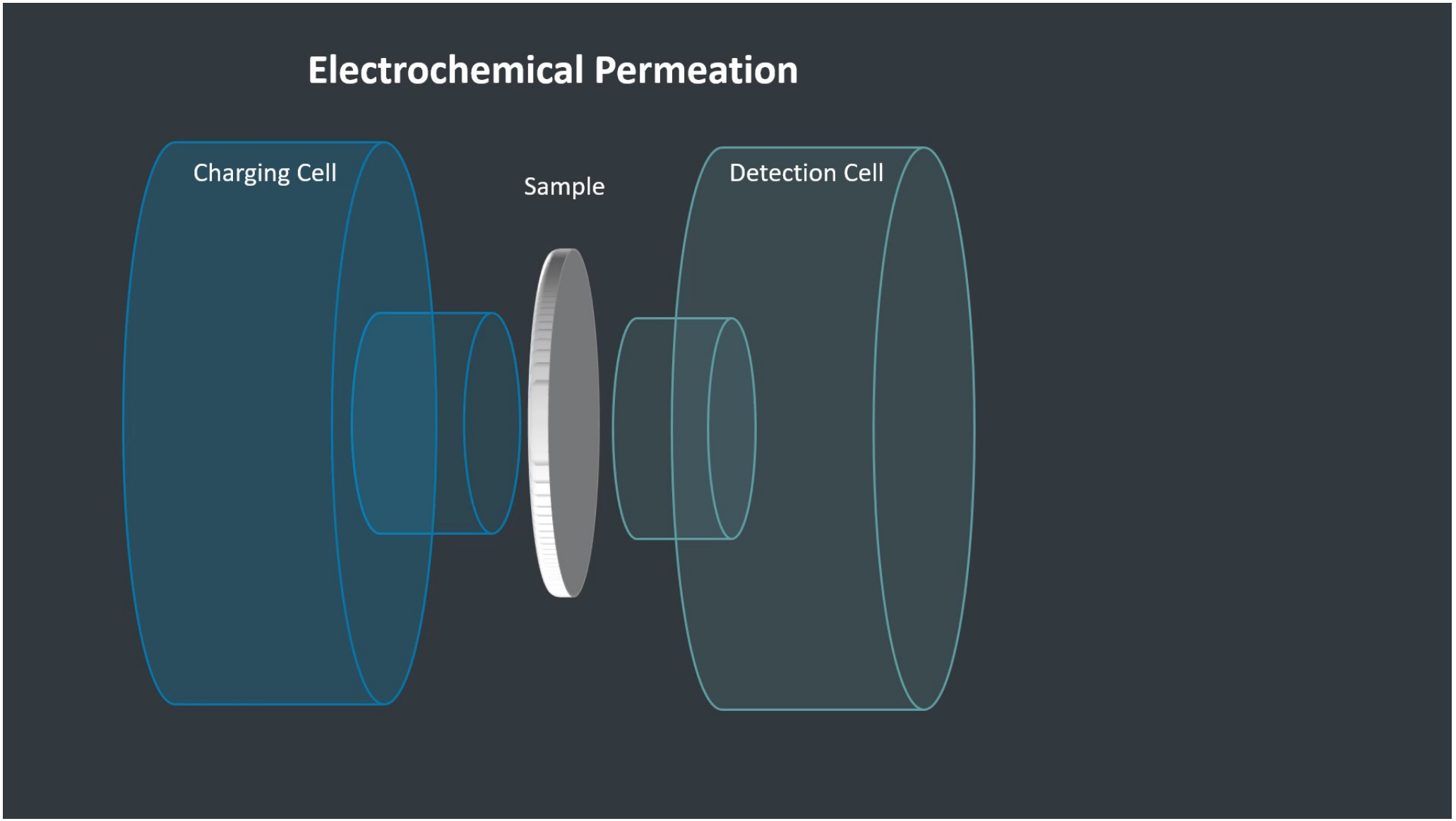
$$\frac{\partial \theta_{T,i}}{\partial t} = k_i \theta_L \left(1 - \theta_{T,i}\right) - p_i \theta_{T,i} \Rightarrow K_{T,i} \theta_L = \frac{\theta_{T,i}}{1 - \theta_{T,i}}$$

Oriani, Acta Metallurgica 18(1), 147–15, 1970

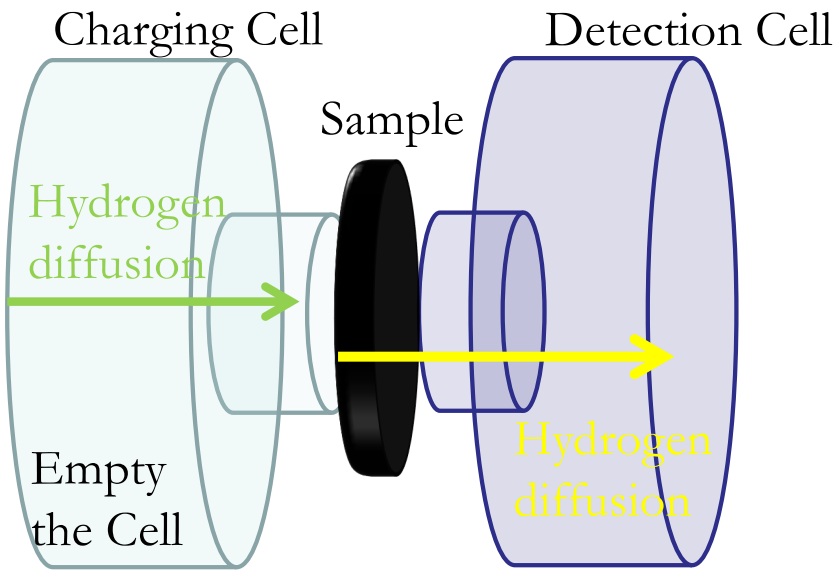
Apparent H diffusion coefficient

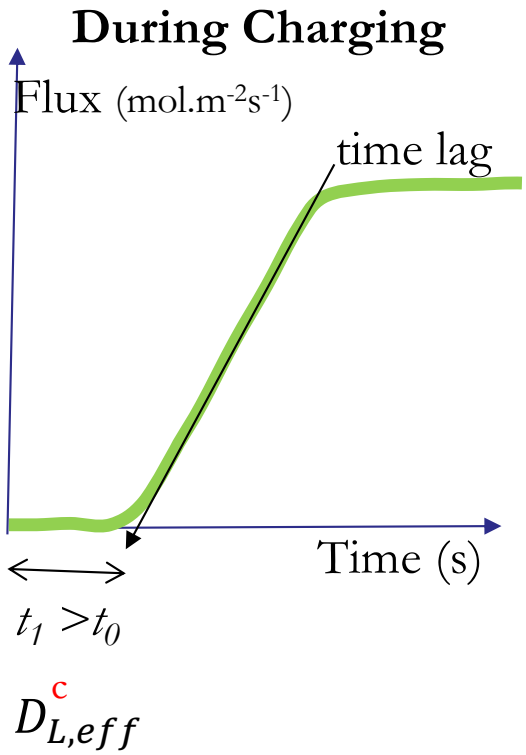
$$D_{L,eff} = \frac{D_L}{1 + \sum_i \frac{C_{T,i}\left(1 - \theta_{T,i}\right)}{C_L}}$$

Context

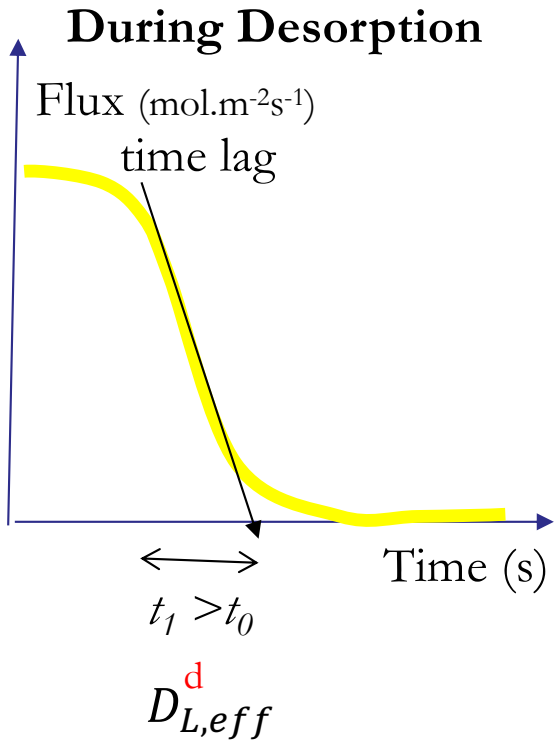

Electrochemical Permeation
Charging Cell
Sample
Detection Cell

Context





$D^{c}_{L,eff}$

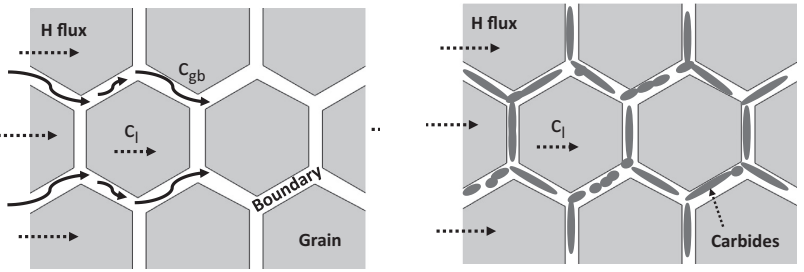


$D^{d}_{L,eff}$

Affected by

- Trap distribution / kind
- Stress heterogeneity & temporal evolution
- Microstructure (texture, boundaries…)

From short-circuit ……. to barriers



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Outline

1. Influence of the microstructure heterogeneities: Focus on Grain Boundaries connectivities

2. Influence on plastic strain

3. Summary

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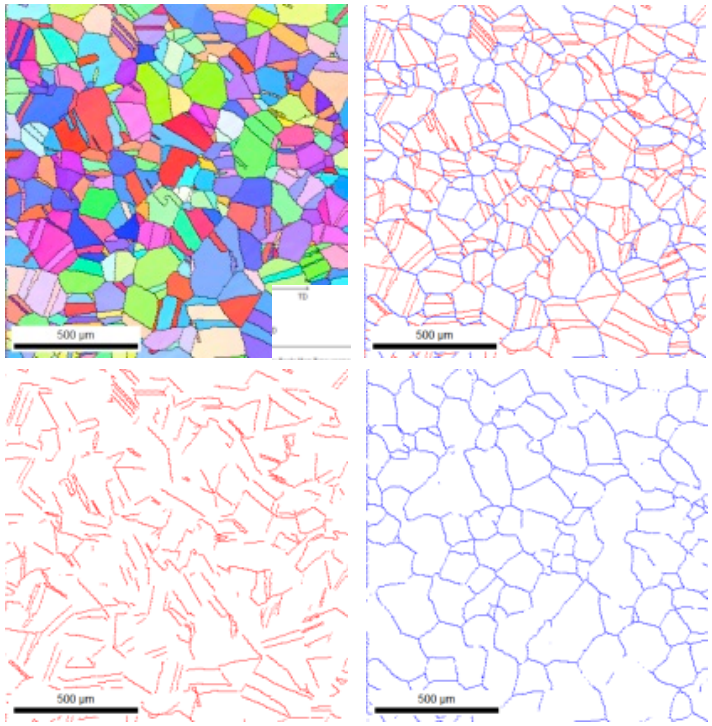
Focus on Grain Boundaries

Impact of the type of Grain Boundary on diffusion

Polycrystalline nickel

Grain size from 50 nm to 168 µm



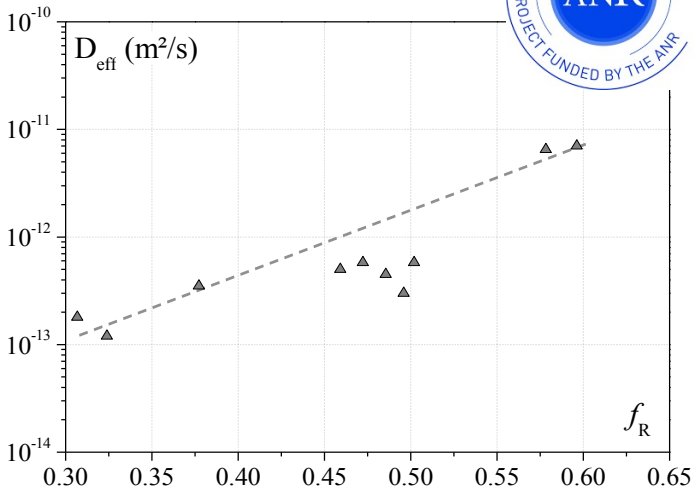
Special GBs ($\sum < 29$)

Random GBs ($\sum > 29$)

Random GBs

Acceleration of H diffusion

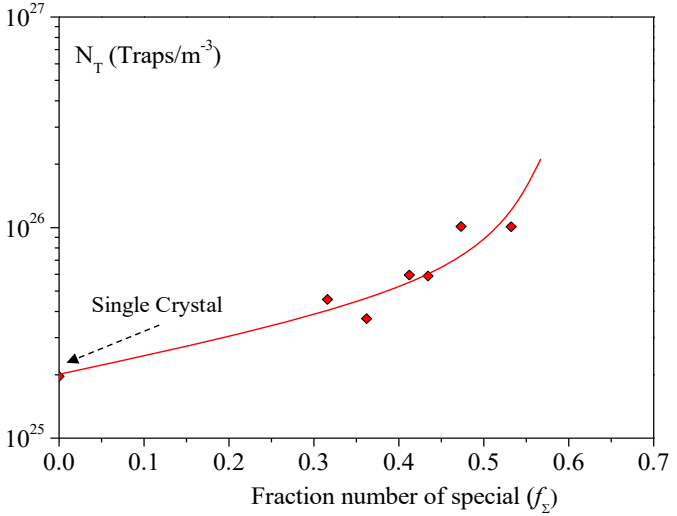
Short-circuit diffusion along the Random GBs



Special GBs

Increasing of traps density

Special GBs are preferential zones for H trapping ?



A. Oudriss, et al., Acta Materialia 2012

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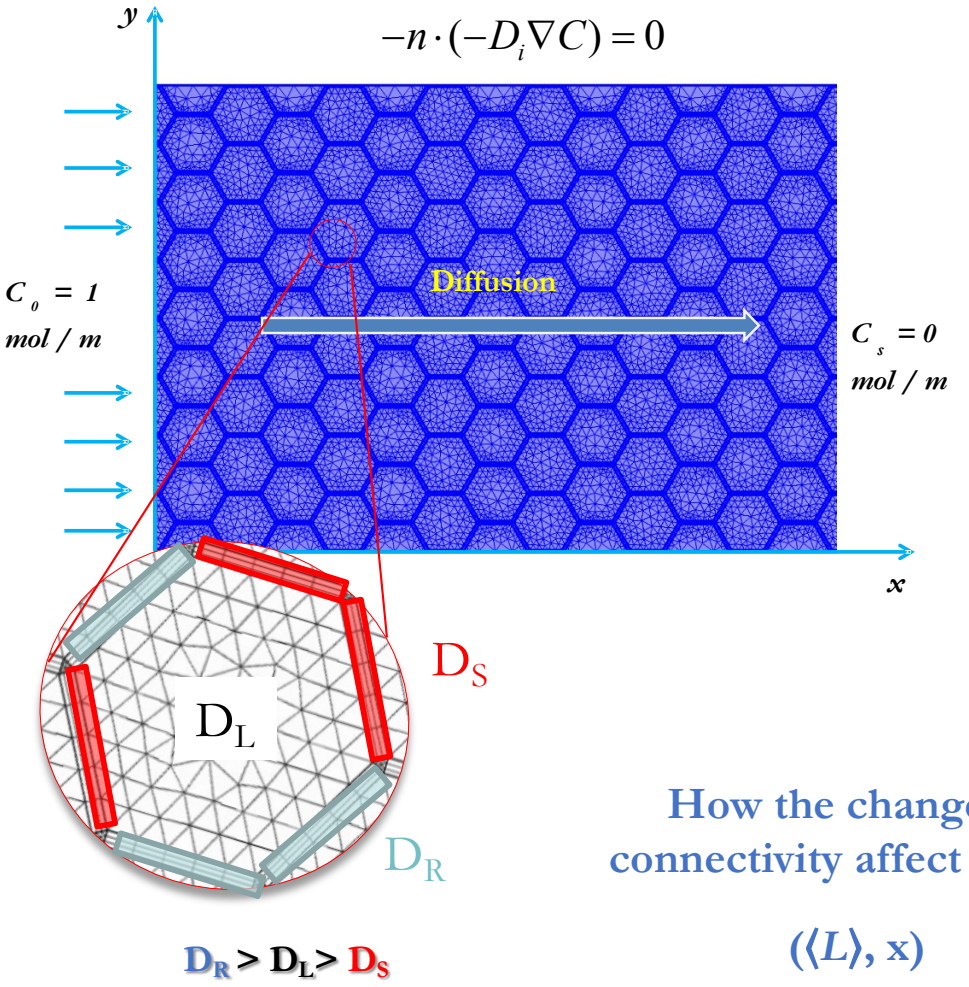
Focus on Grain Boundaries

Effect of the volume fraction of RGB

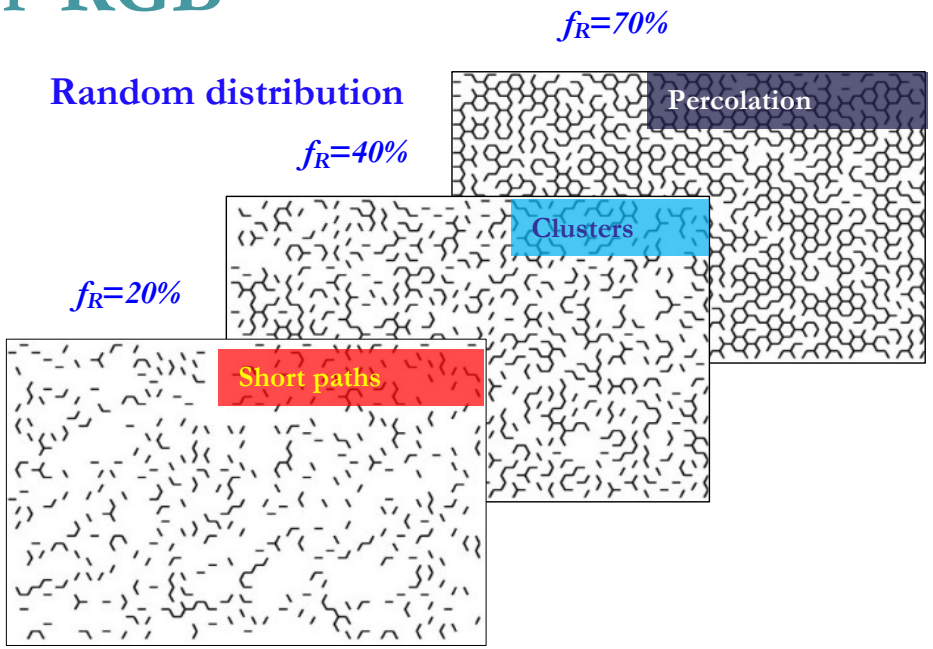
FE modeling of permeation test in 2-D (no trapping)

$$-n\cdot(-D_i\nabla C)=0$$



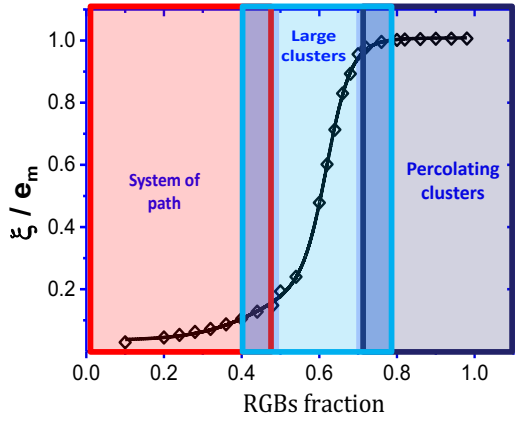
$D_R > D_L > D_S$

Random distribution



How the changes in the GB network connectivity affect the effective diffusivity?

$(\langle L\rangle, x) \xrightarrow{?} D_{eff}$



Osman Hoch et al. Computational Materials Science, 2015

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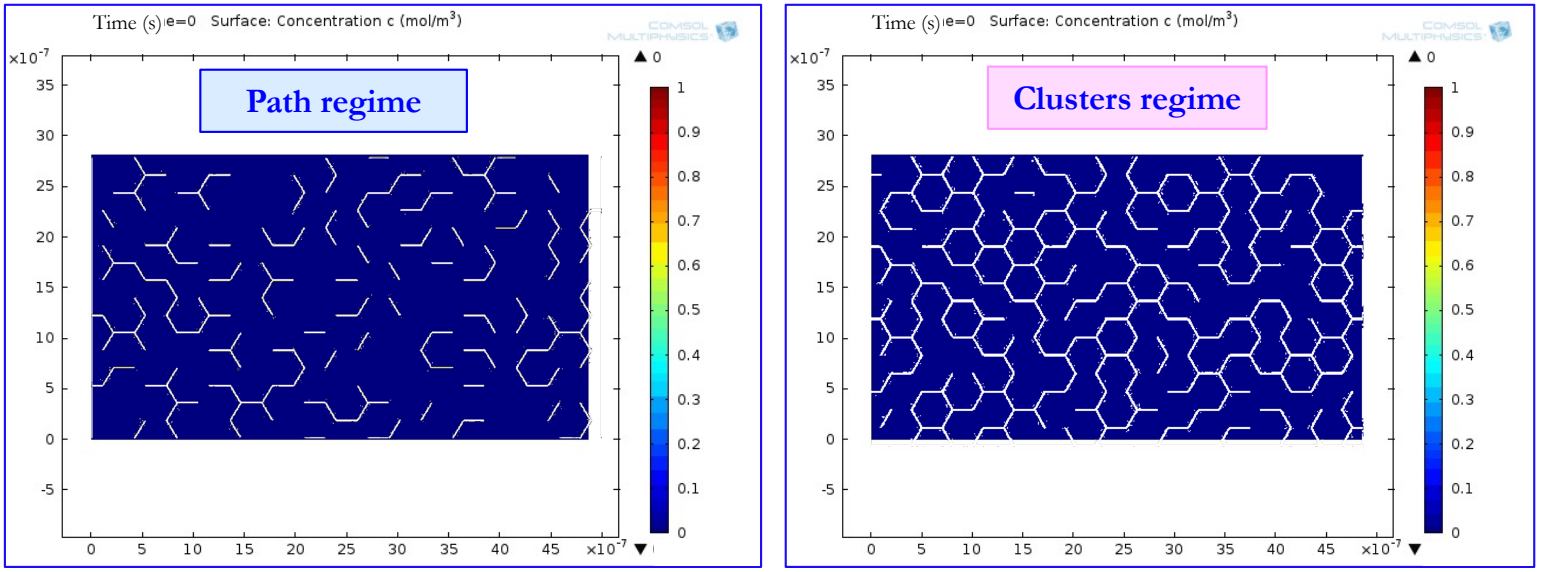
Effect of the volume fraction of RGB

Evolution of diffusion front



Clusters regime:

- More important acceleration of the H diffusion
- Heterogeneous front

Transition scale: implications of the connectivity effects

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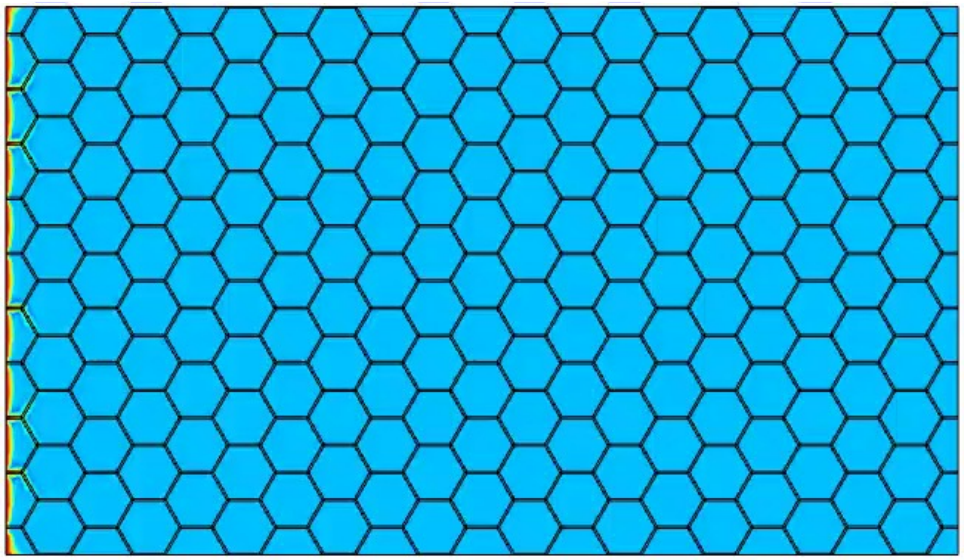
Focus on Grain Boundaries

Effect of the connectivity

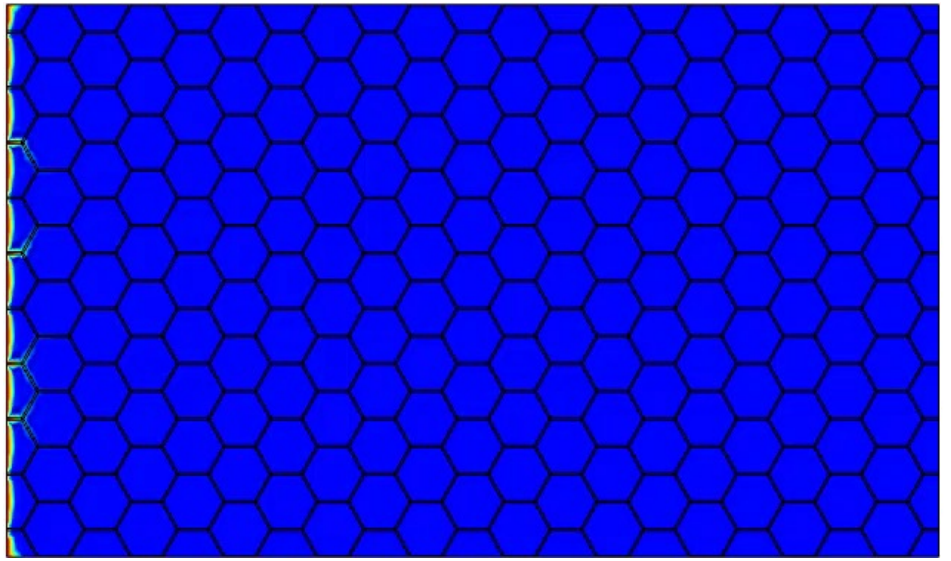
Same fraction of RGB, and TJ.

Random attribution



$$D_{eff} = 2.9e^{-13} \mathrm{m}^2/\mathrm{s}$$

Constrained attribution

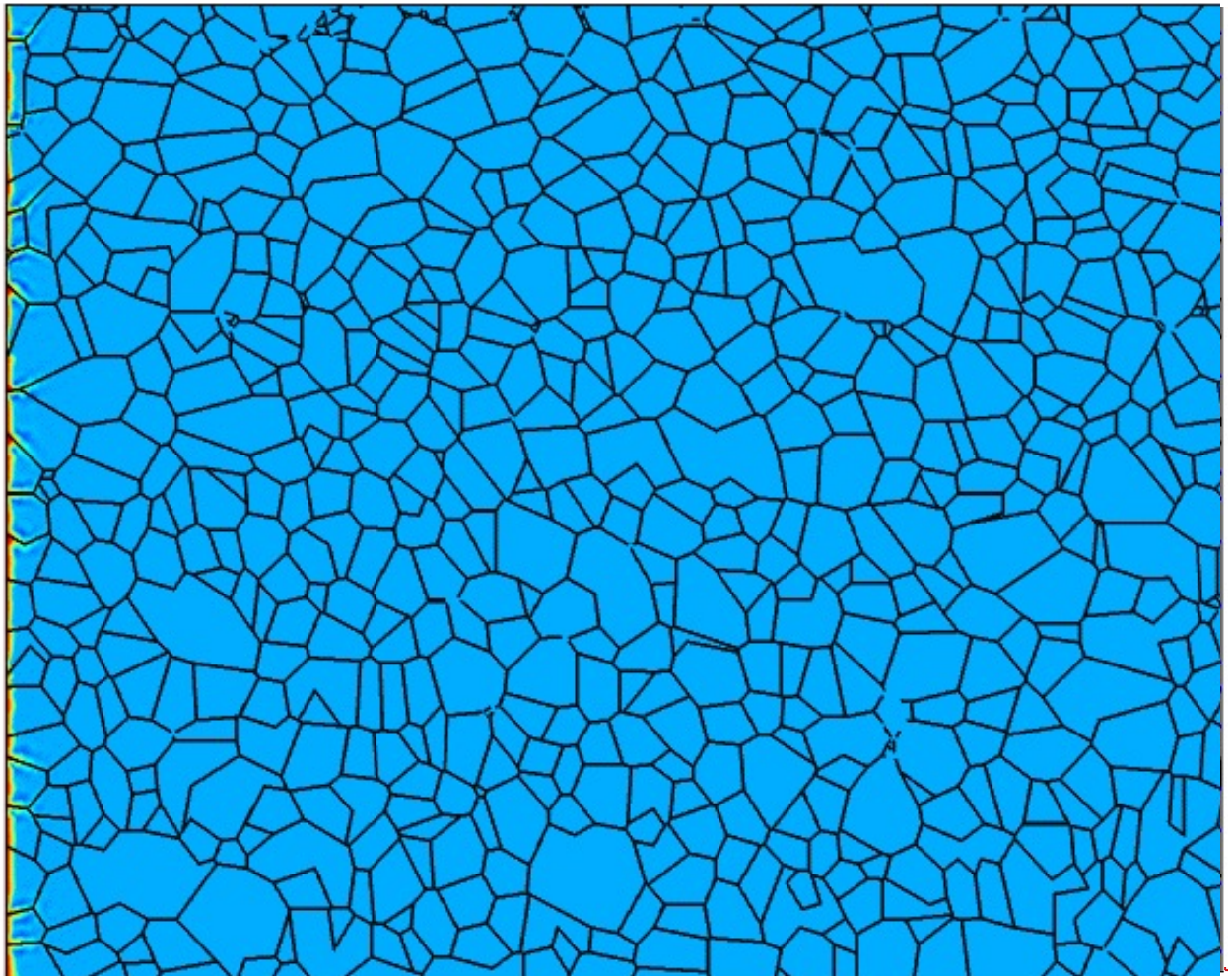


$$D_{eff} = 9.34e^{-13}\ \mathrm{m}^2/\mathrm{s}$$

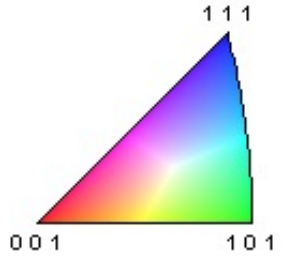
El Sayed Ph.D in progress

Focus on Grain Boundaries

Effect of GBs & their connectivity: real microstructure



Diffusion of hydrogen and study of the real microstructure to compare with the experimental results



Osman Hoch Ph.D
A. Ventura PhD
El Sayed Ph.D in progress

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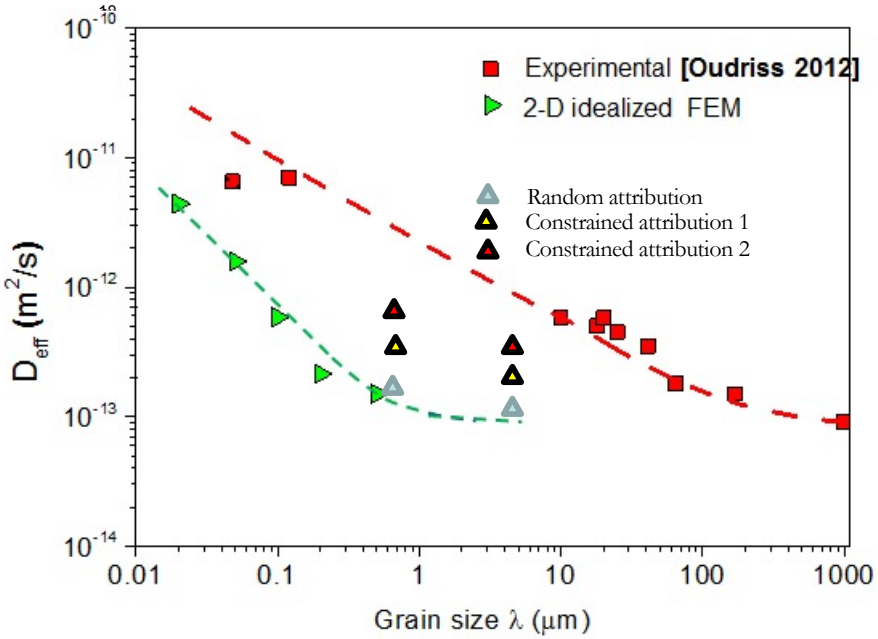
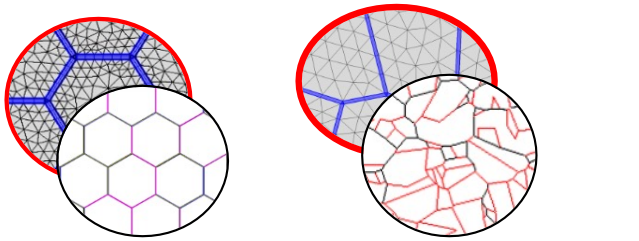
Focus on Grain Boundaries

Effect of GBs & their connectivity: comparison





Modèle Ideal FEM EBSD-based FEM

Parameter	Values
D_L	10^{-13} m²/s*
D_Σ	10^{-16} m²/s
D_R	10^{-10} m²/s *

*[Oudriss 2012]

- The modelling results follow the same trend as the experimental ones.
- Need to develop a large 3-D EBSD/FIB-based FEM, *in progress…*
- Connectivity plays an important role, how AI can optimize the distribution?, *in progress …*
- Identification of the GB behavior, is the GB discrimination in term of CSL and Random accurate?

Osman Hoch Ph.D
El Sayed Ph.D in progress

Outline

1. Influence of the microstructure heterogeneities: Focus on Grain Boundaries

2. Influence on plastic strain

3. Summary

Influence on plastic strain

Effect of plasticity on H transport and trapping

↳ Plastic strain (dislocation: trap)
(Hydrostatic pressure)

$$\frac{\partial C_L}{\partial t} + \frac{\partial C_T}{\partial t} = \nabla.\left(D_L \nabla C_L + \frac{V_H D_L}{RT} C_L \nabla P_H\right)$$

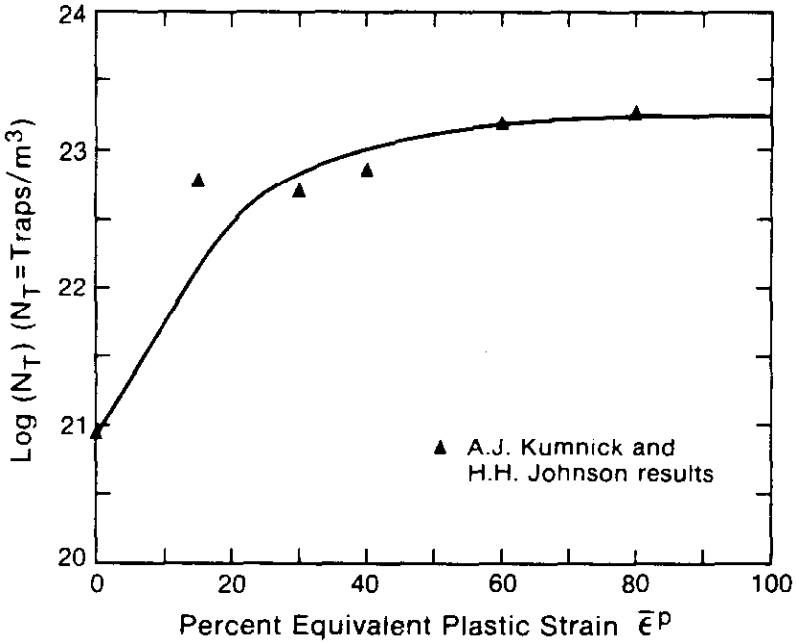
$$\frac{\partial \theta_T}{\partial t} = k\theta_L(1-\theta_T) - p\theta_T$$

$$C_T = N_T(\bar{\varepsilon}_p)\theta_T$$

Polycrystal: slip system and anisotropy

$$\gamma = \sum_{\alpha} \int_0^t \left|\dot{\gamma}^{\alpha}\right| dt$$

Pre-strained α-iron sample
& time lag approach



Sofronis and McMeeking, R. M. Journal of the Mechanics and Physics of Solids, 1989
Kumnick and Johnson Metallurgical Transactions A, 1974

Influence on plastic strain

Effect of plasticity on H transport and trapping

↳ Plastic strain (dislocation: trap)
(Hydrostatic pressure)
Hydrogen dragging by mobile traps

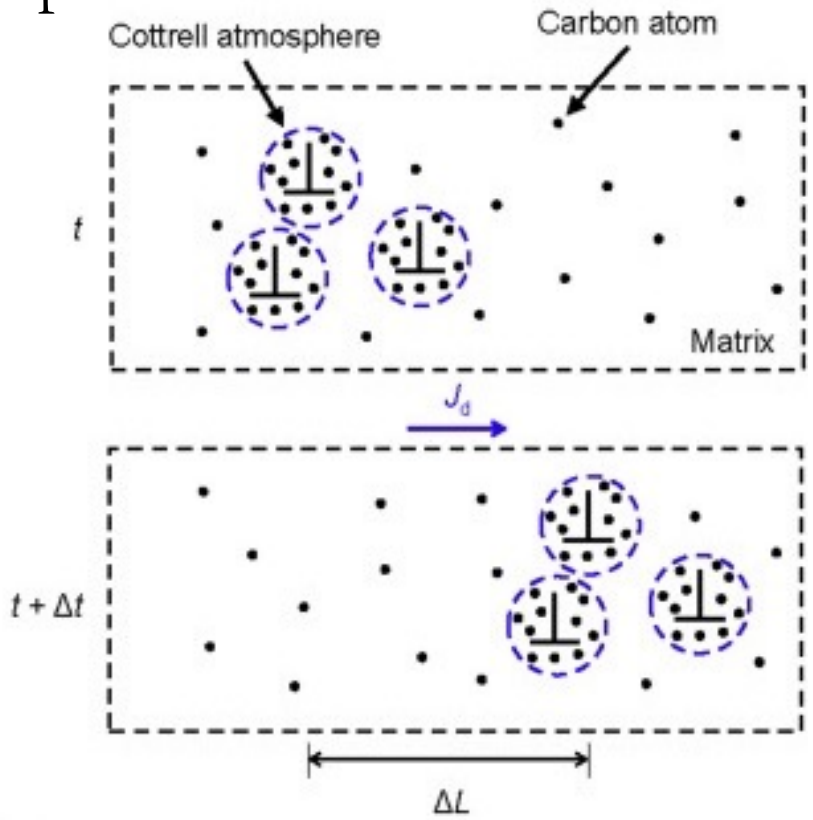
$$\frac{\partial C_L}{\partial t} + \frac{\partial C_T}{\partial t} = \boldsymbol{\nabla}.\left(D_L \boldsymbol{\nabla} C_L + \frac{V_H D_L}{RT} C_L \boldsymbol{\nabla} P_H - \boldsymbol{J}_{d,\alpha}\right)$$

$$\boldsymbol{J}_{d,\alpha} = \sum_{\boldsymbol{\alpha}} \theta_{T,\alpha} N_T^{m,\alpha} \boldsymbol{v}_{d,\alpha}$$

$\boldsymbol{v}_{d,\alpha}$ // slip direction

$N_T^{m,\alpha} \propto \dot{\gamma}^{\alpha}$

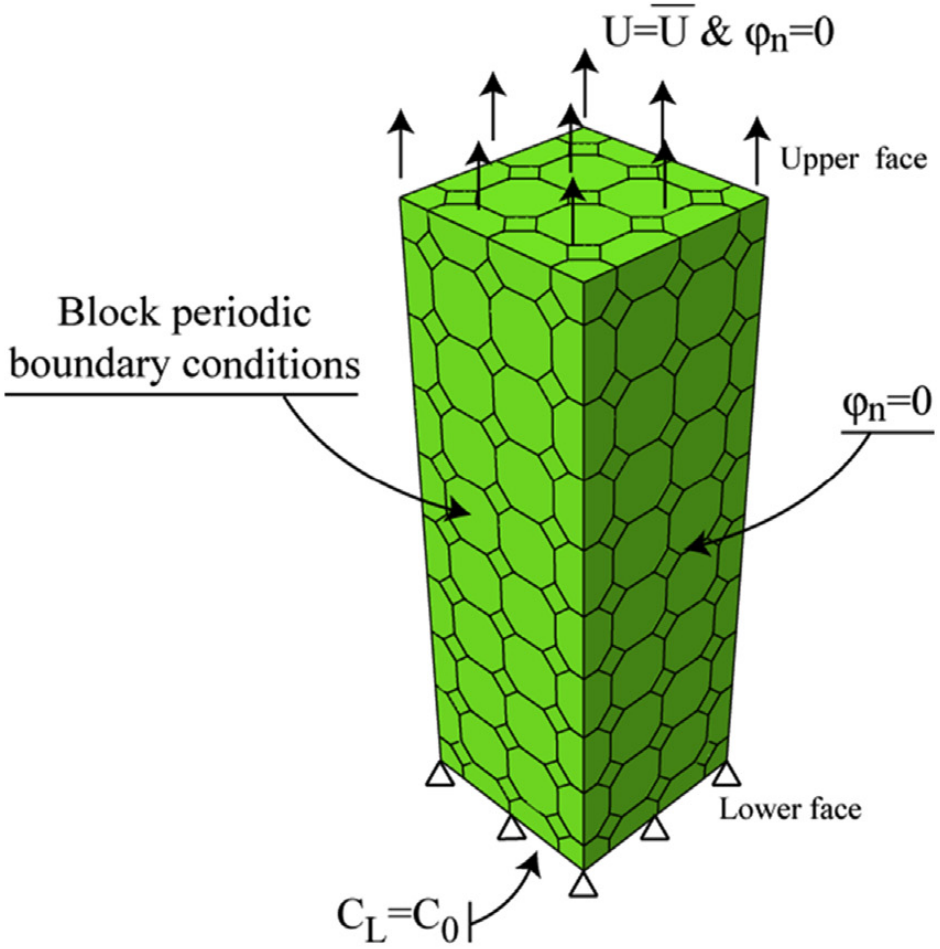
Charles et al. In: Mechanics and Physics of Solids at Micro-and Nano-Scales, 2019.



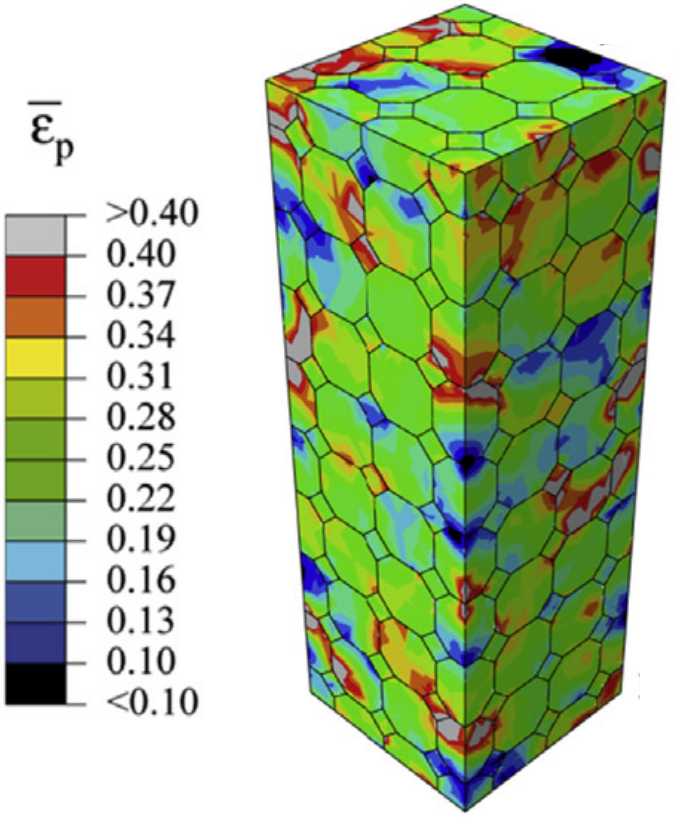
Fu et al. *Acta Materialia, 2018*

Influence on plastic strain

Pre-strained regular polycrystal (isotropic texture)



(20%)



α-iron & 12 slip systems

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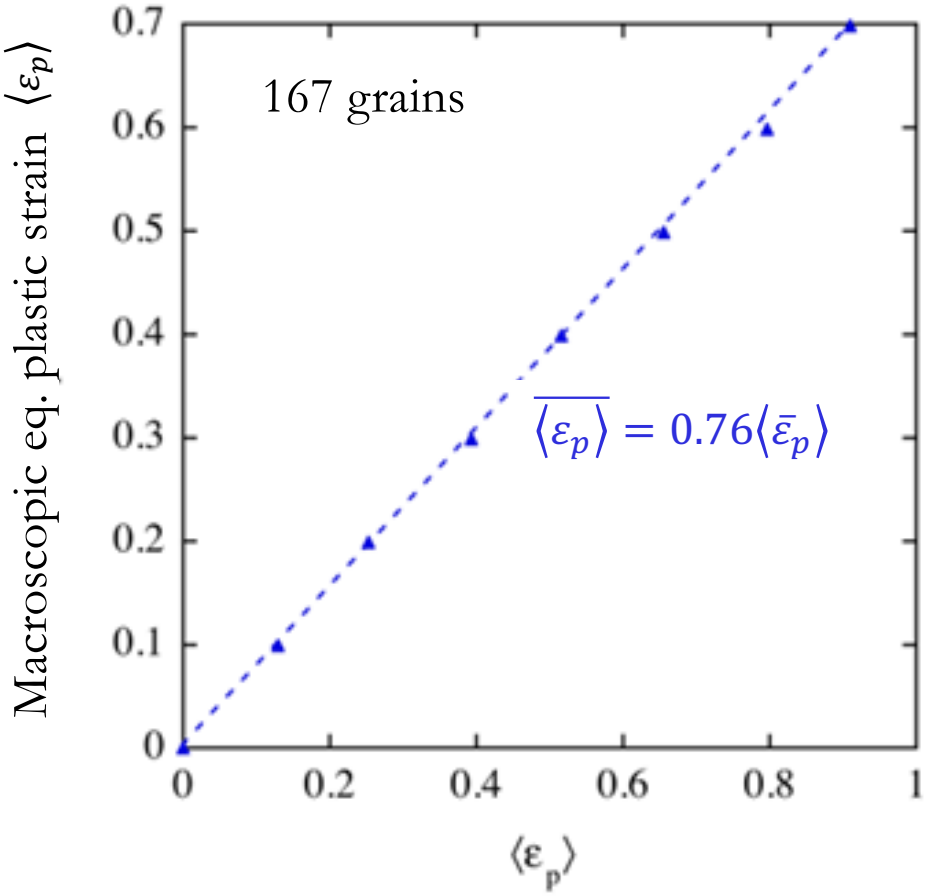
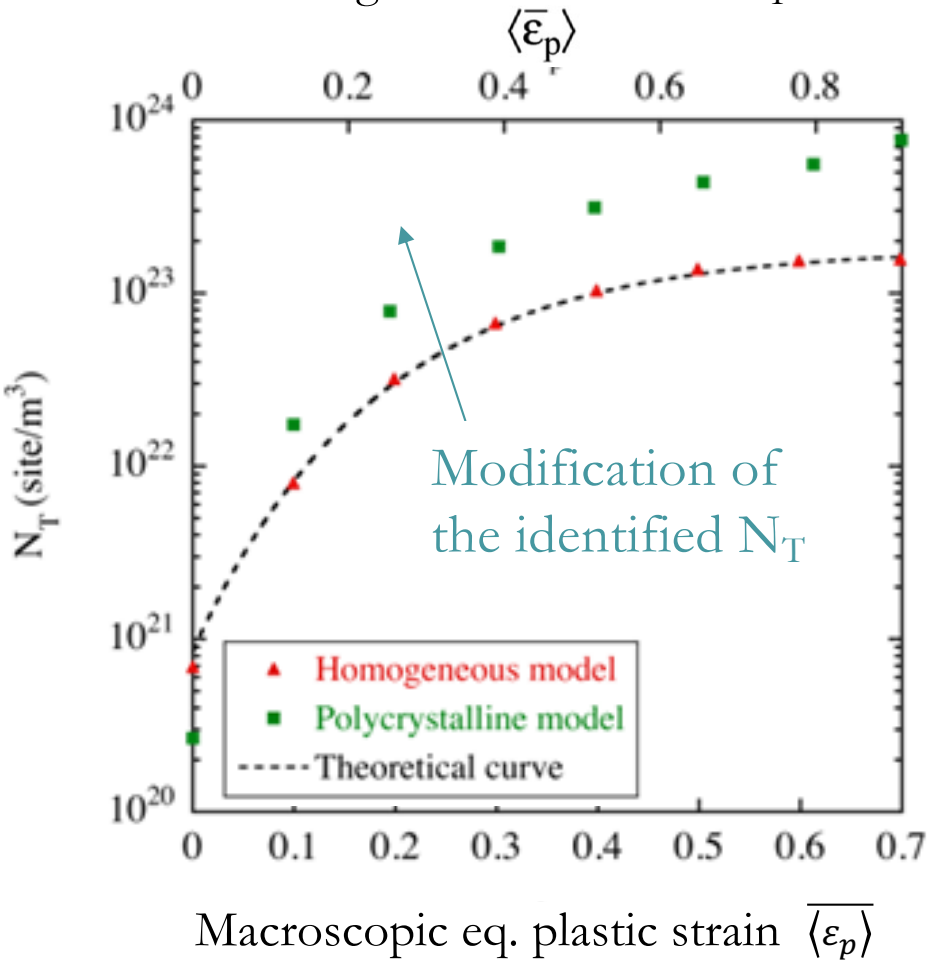
Influence on plastic strain

Effect of plastic strain heterogeneity



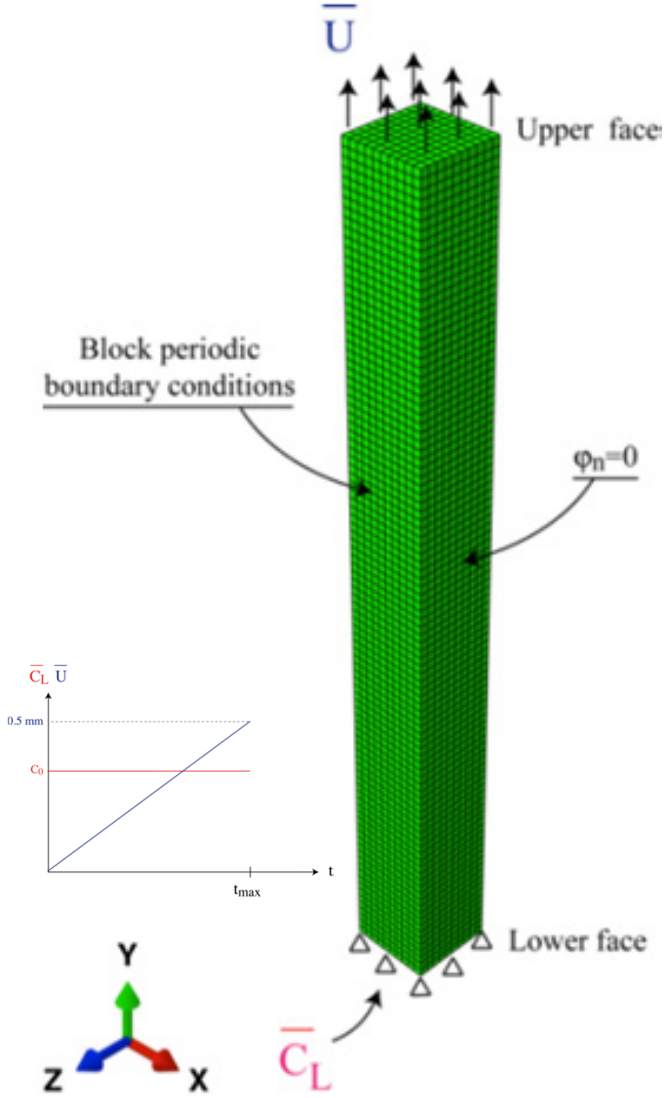
Time lag identification of N_T



Charles et al. In: Mechanics and Physics of Solids at Micro-and Nano-Scales, 2019.

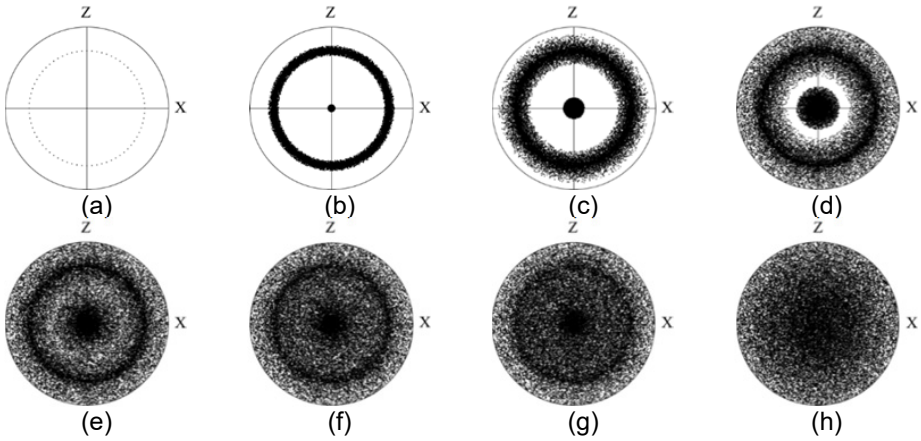
Influence on plastic strain

Effect of trapped H dragging by mobile traps



Upper face concentration

⟨111⟩ pole figure

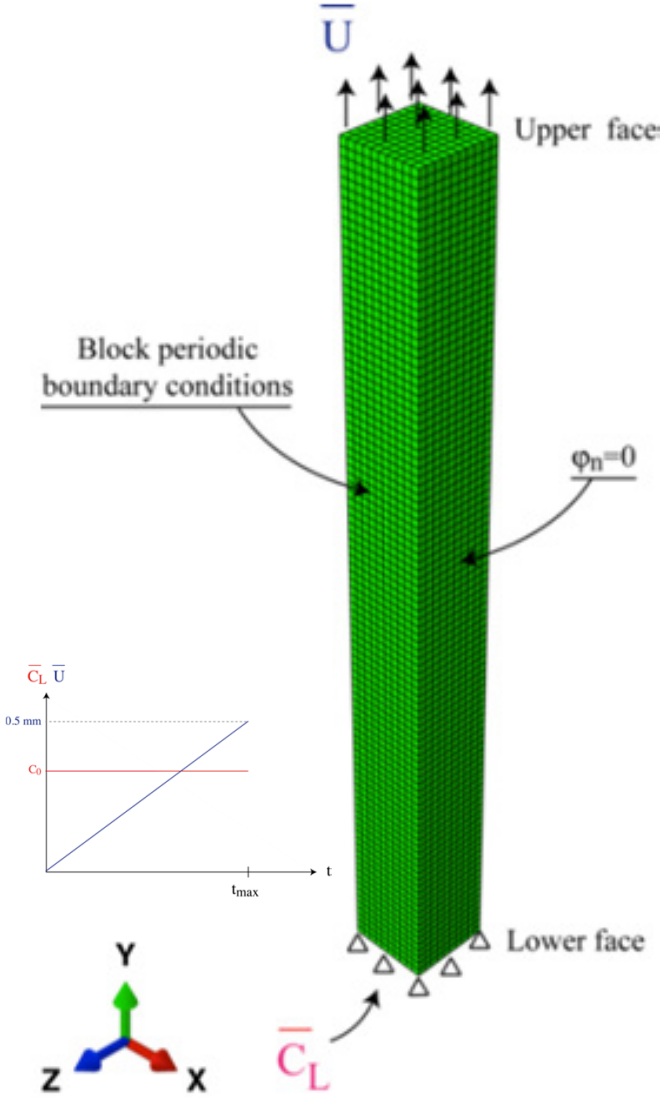


Isotropic texture

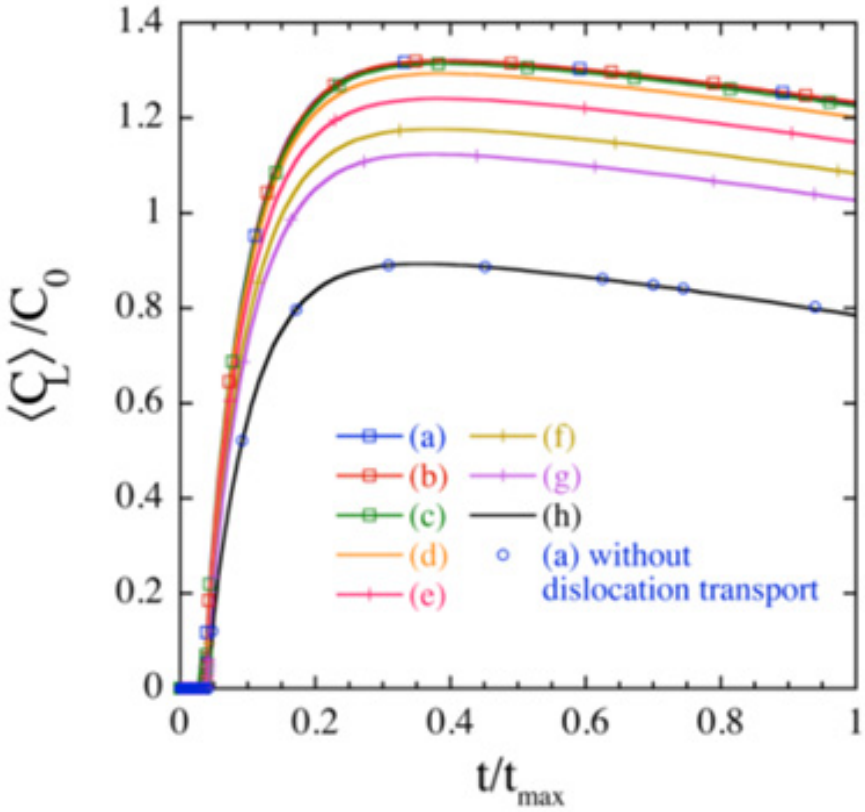
Charles et al. In: Mechanics and Physics of Solids at Micro-and Nano-Scales, 2019.

Influence on plastic strain

Effect of trapped H dragging by mobile traps



Strain rate: 10^{-6} s^{-1}



$$J_{d,\alpha} \rightarrow 100\text{x}\, J_{d,\alpha}$$

Charles et al. In: Mechanics and Physics of Solids at Micro-and Nano-Scales, 2019.

Summary

- Strong correlation with local material feature
  - Grain boundary connectivity
  - Metallurgy

- Influence of texture and mechanical fields

- Global experimental measurement of $D_{L,eff}$

→ Toward model systems (single grains, boundaries…) and local modelling (DFT, FE, DD….)

« Model-experiment dialogue »