Stress Driven Bubble Growth: Influence of Stress Gradient on Bubble Migration

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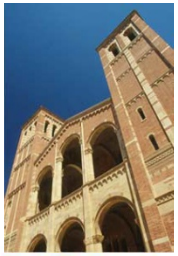

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OUTLINE

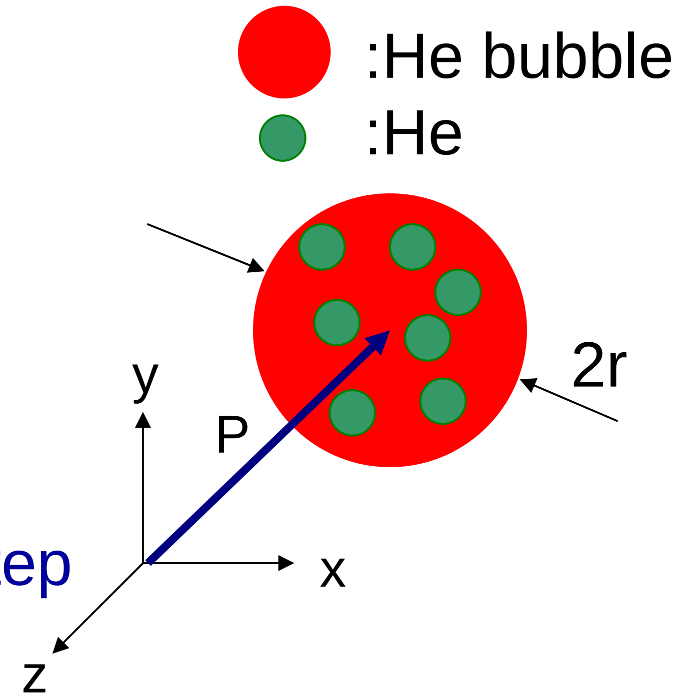
1. Formulation of He-Bubble Growth in stress gradient using Event Kinetic Monte Carlo (EKMC)

2. Single Bubble in a stress gradient

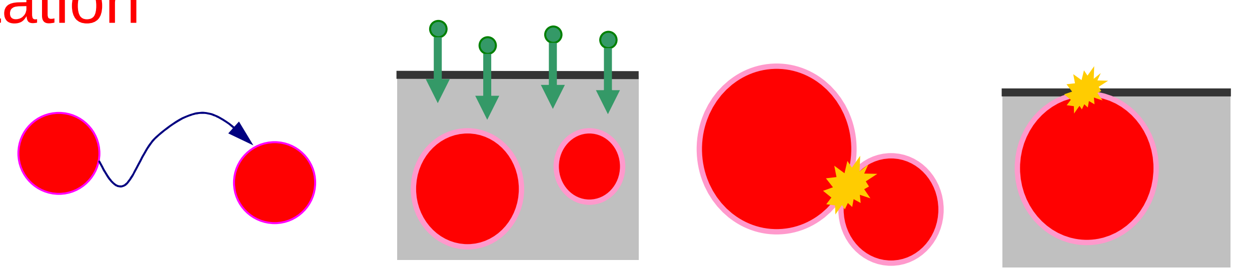
3. Collection of Bubbles in a stress gradient

Event Kinetic Monte Carlo

- Helium bubbles are treated as particles
  - Position vector
  - Number of helium atoms
  - Radius (Diameter)



- An event can take place at each time step
  - Diffusion
  - Helium Implantation
  - Coalescence
  - Surface pore formation

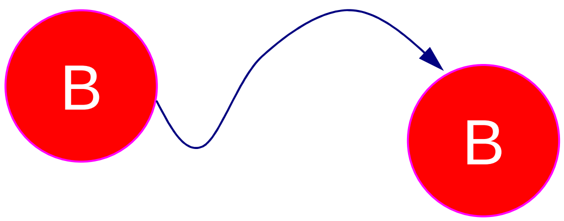


Diffusion Implantation Coalescence Pore form.

Event (Diffusion Random Walk)

Diffusion of helium bubbles

- The diffusion is in 3-dimensions: random walk model



- Diffusion rate of a helium bubble

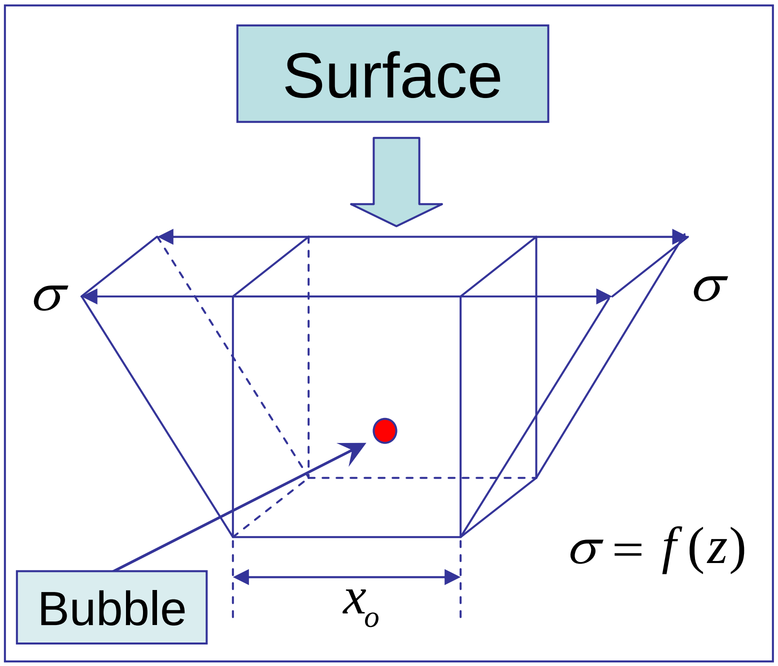
$$D_b = \left(\frac{3\Omega^{4/3}}{2\pi r^4} \right) D_s \qquad \underbrace{D_s = D_0 \exp\left(-\frac{E}{kT} \right)}_{\text{Surface diffusion}}$$

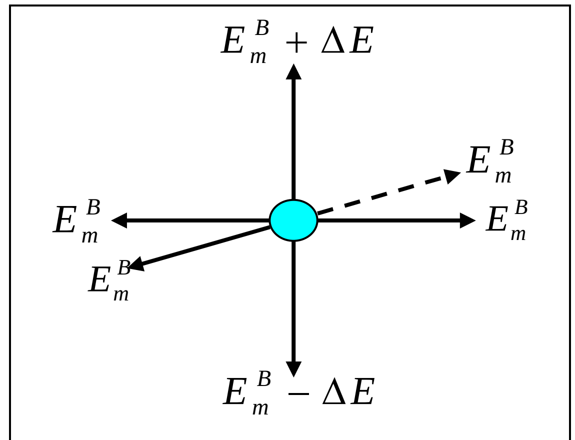
Ω : Atomic volume
r : Radius of helium bubble
D_0 : Diffusion Pre exponential
E : Surface migration energy

J.H. Evans, JNM 334(2004), 40-46

Event (Diffusion in Stress Gradient)

- Stress gradient acts as a driving force on bubble migration:
  Change in total strain energy → Bubble moves up a stress gradient

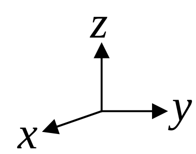




$$\Delta E = \Delta E^{tot}(z) - \Delta E^{tot}(z_0)$$

$$\Delta E_{tot} = -v_p \times \frac{3\delta \cdot \sigma^2}{2E}$$

"Delta-Energy Rule"



v_p: Bubble volume
δ: constant (3.02)
σ: Stress
E: Young's modulus
D_s: Surface Diff.
D_p: Pore Diff.
z: Position after bubble migration
z_0: Starting bubble position

Velocity (V_p) of spherical pore:

$$V_p = B_p F_p$$

B_p: bubble mobility
F_p: driving force

$$B_p = \frac{D_p}{kT} = \frac{3a_o}{2\pi kTr^4} D_s$$

$$F_P = -\frac{\partial \Delta E_{tot}}{\partial z} = -v_p \times 3\delta \times \sigma/E \times \partial\sigma/\partial z$$

*Leiden & Nichols (1971)

With Stress

$V_p \propto 1/r$

No Stress

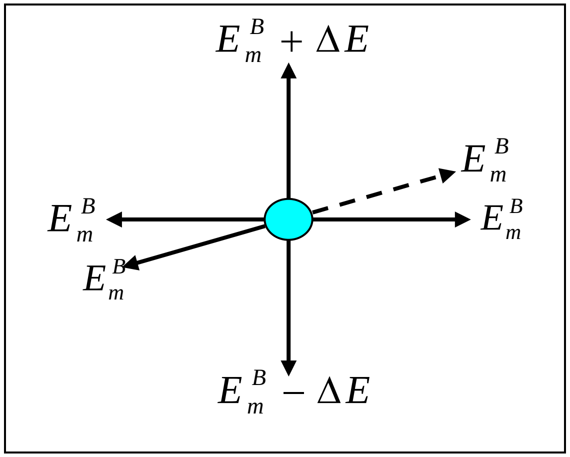
$V_p \propto 1/r^4$

Event (Diffusion in Stress Gradient)

- Helium bubble migration in matrix

$$D_b = \left(\frac{3\Omega^{4/3}}{2\pi r^4} \right) D_s \qquad D_s = D_0 \exp\left(-\frac{E}{kT} \right)$$

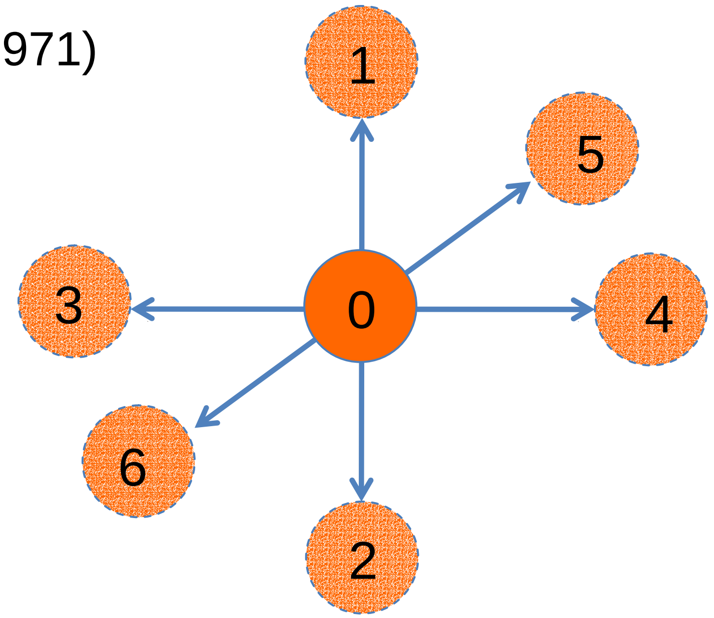
$$E_{bm} = -kT \log\left(\frac{D_b}{D_0^*} \right)$$



- Strain Energy difference

(Leiden, Nichols, 1971)

$$\Delta E_{0\to i} = \frac{4\pi r^3}{3} 3.01 \frac{\sigma_i^2 - \sigma_0^2}{2E} \quad (i=1,6)$$

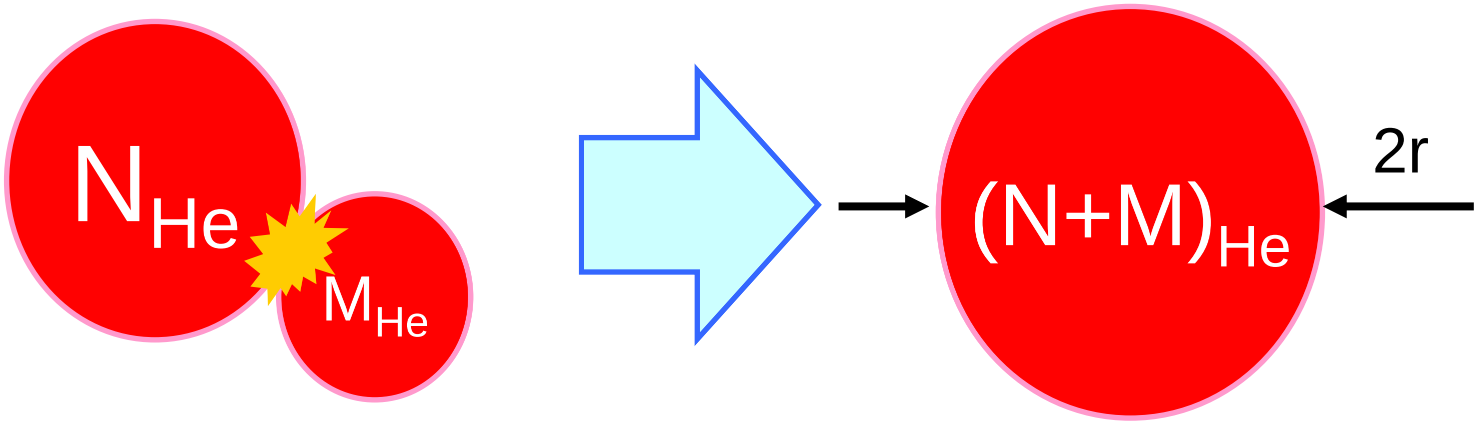


- Diffusion of bubble

$$D_i = D_o^* \exp\left(-\frac{E_{bm} + \Delta E_{0\to i}}{kT} \right)$$

Events (Coalescence)

■ Clustering of two helium bubbles



- Calculation of helium bubble radius

Equation of state: $PV = nkT$

Pressure on the helium bubble surface: $P = \dfrac{2\gamma}{r}$

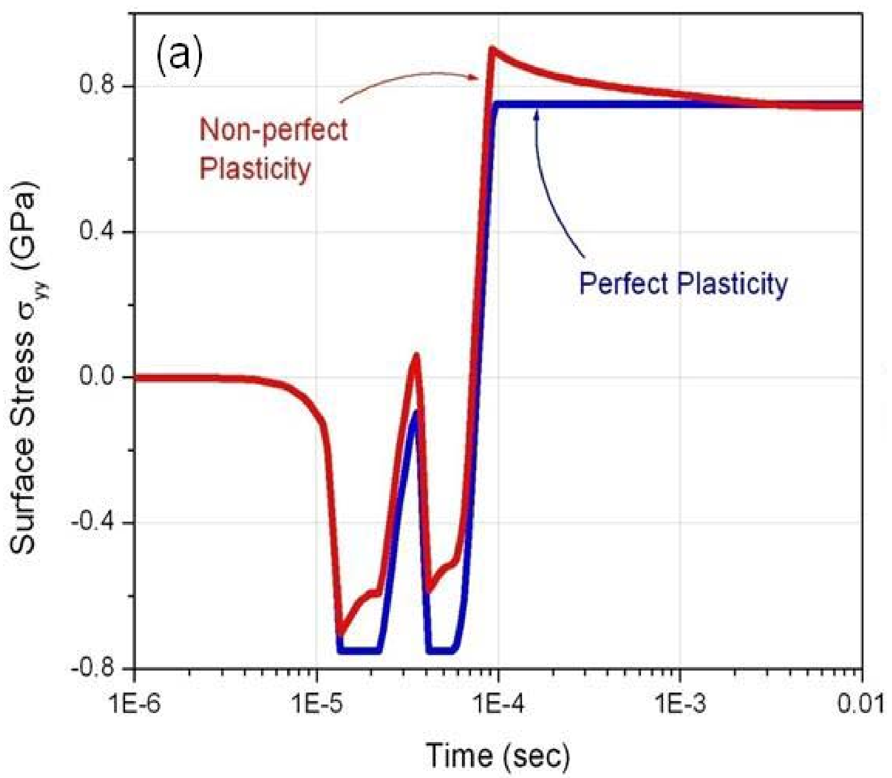
$$\Rightarrow \quad r = \sqrt{\frac{3nkT}{8\pi\gamma}}$$

J.H. Evans, JNM 334(2004), 40-46

Influence of Stress Gradient on Bubble Migration and Coalescence

W-Surface Stress State for HAPL

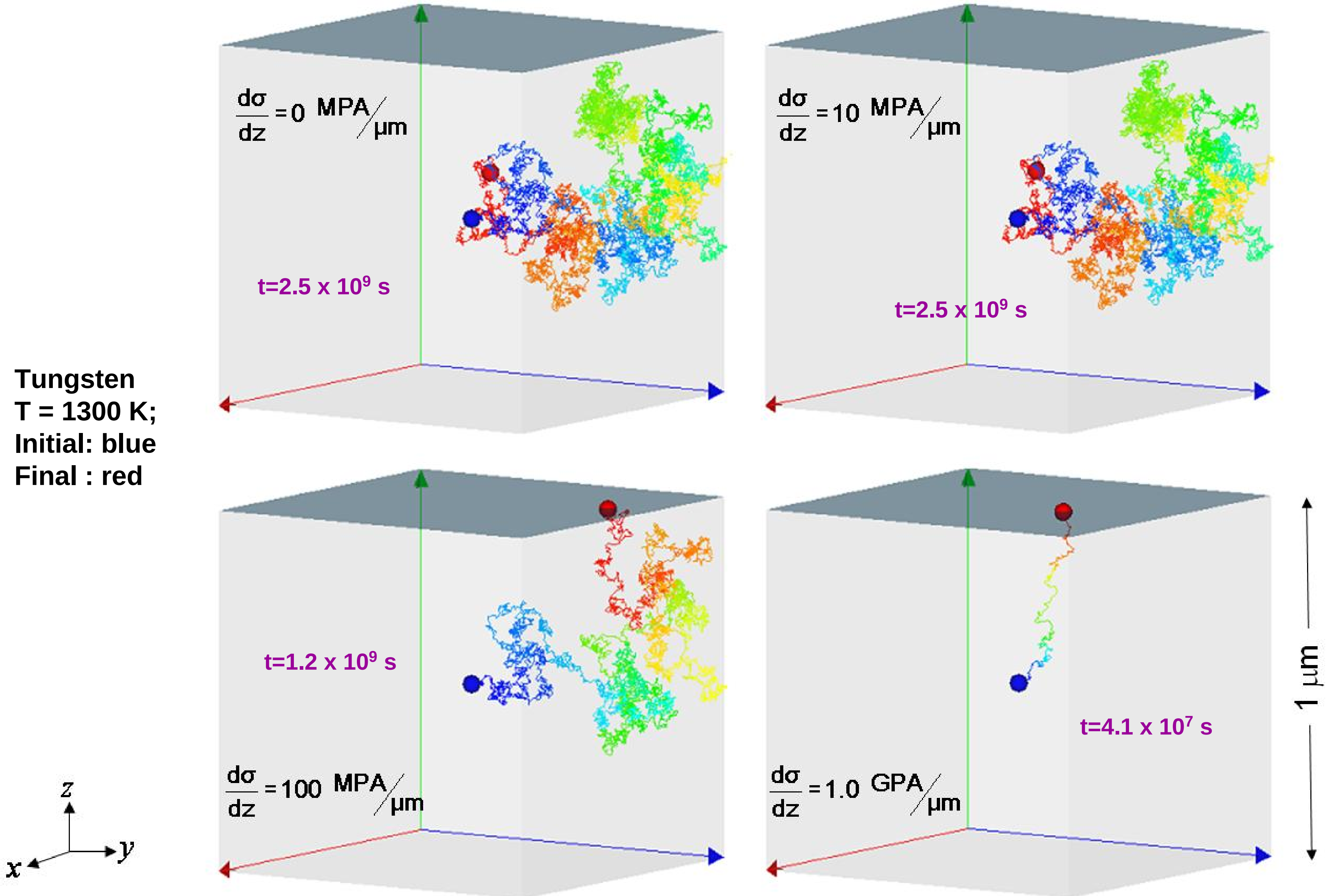
Following the heating/implantation transient the surface remains in a stressed state of about **~0.7 GPa** (UMARCO):



Single Bubble Migration in a Stress Gradient

Stress Gradient Effect on Single 5-nm Bubble

Tungsten
T = 1300 K;
Initial: blue
Final : red



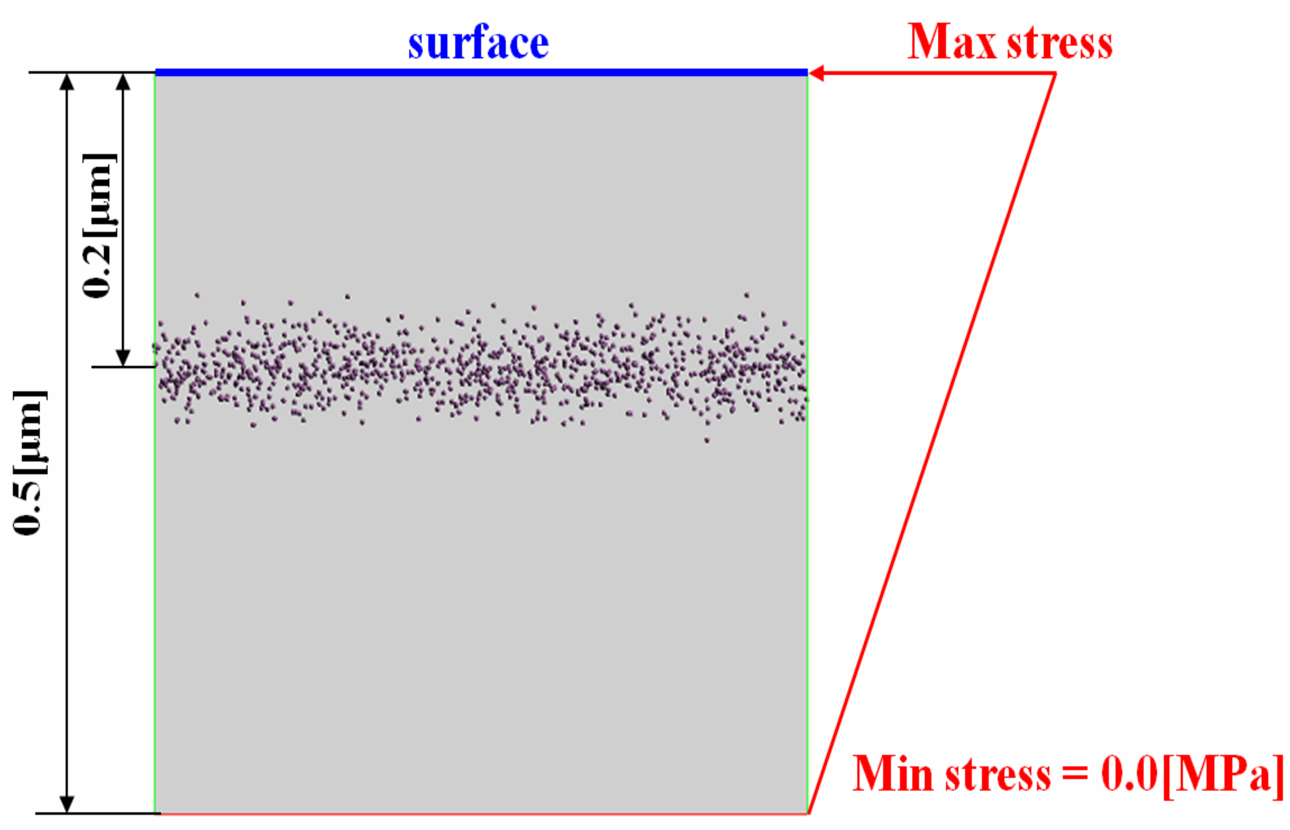
Collection of Bubbles:

Migration PLUS Coalescence in a Stress Gradient

Stress Gradient Effect on Collection of Bubbles

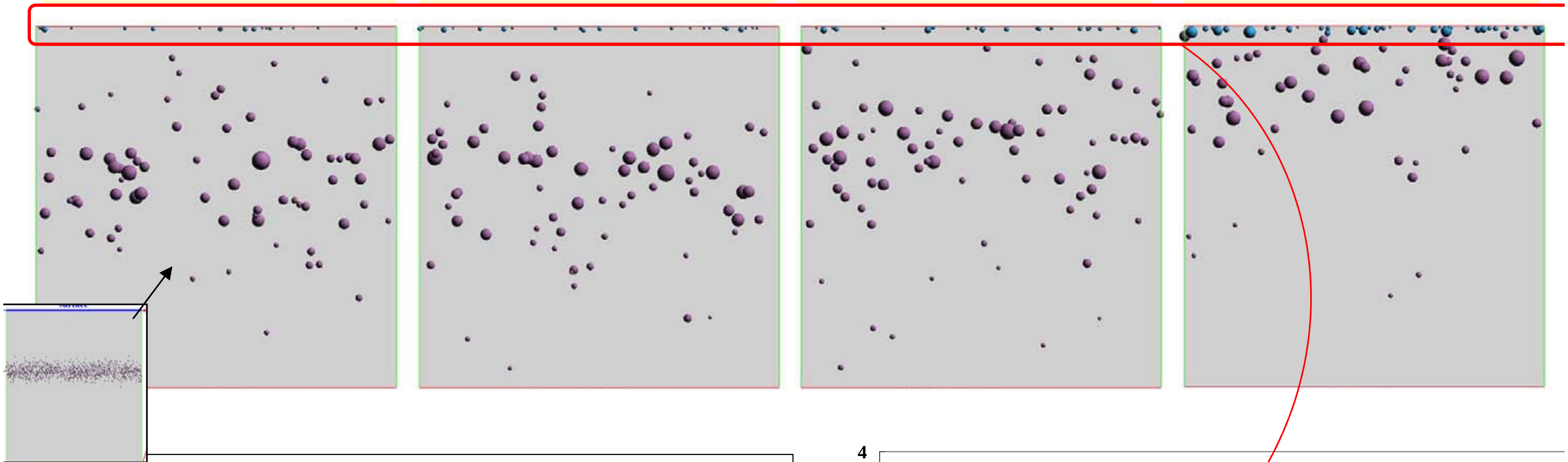
Initial Conditions:

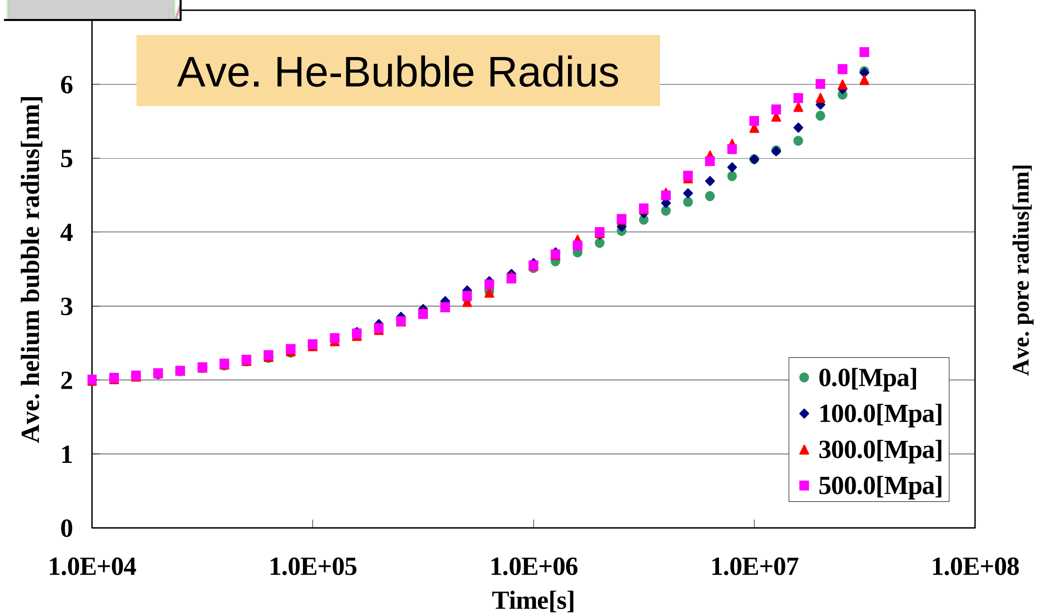
Depth Profile:	0.02 μm – 0.5 μm
Number of Bubbles:	1000
Ave. Bubble Radius:	1.84 nm

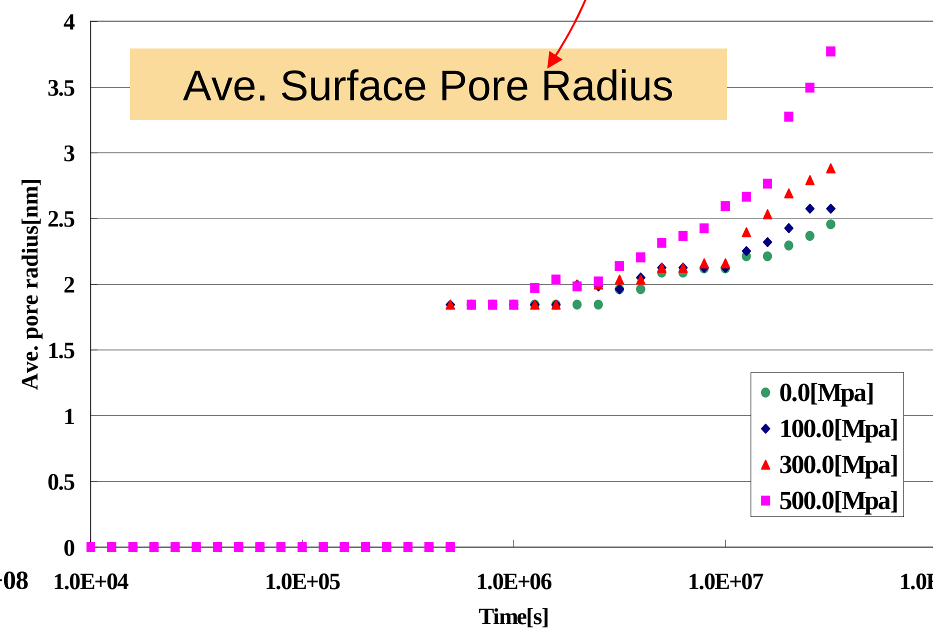


Bubble Distribution at 3×10^{7} s at Given Stress Gradients

dσ/dz = 0 MPa/μm | 200 MPa/μm | 600 MPa/μm | 1000 MPa/μm







Summary & Conclusions

- Influence of stress gradients on He-bubble migration has been incorporated into the McHEROS Code
- Bubble moves up the stress gradient (compressive or tensile)
- Single bubble migration is significantly impacted for stress gradients > 100 MPa/μm
- Collection of Bubble in a stress gradient:
  - Bubbles move up towards the surface as a group
  - Stress gradient does not significantly increase bubble growth
  - Coalescence is not very sensitive to stress gradient
  - Surface pores are slightly larger for large stress gradients
- With a stress gradient bubble velocity is $\propto$ ***1/r***
  Without a stress gradient velocity is $\propto$ ***1/r*** ^{4} *(surf. Diff.):*
- *Stress gradient reduces the relative velocities between small and large bubbles*

Modeling Carbon Diffusion

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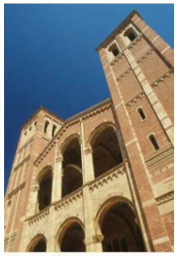

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Carbon Diffusion in Tungsten

- Carbon is implanted between ~0.2 to ~1 μm in W
- Carbon has been shown to diffuse deep after short time anneals (~8 μm at 2000 ^{o}C)
- In HAPL W-surface undergoes rapid temperature transients

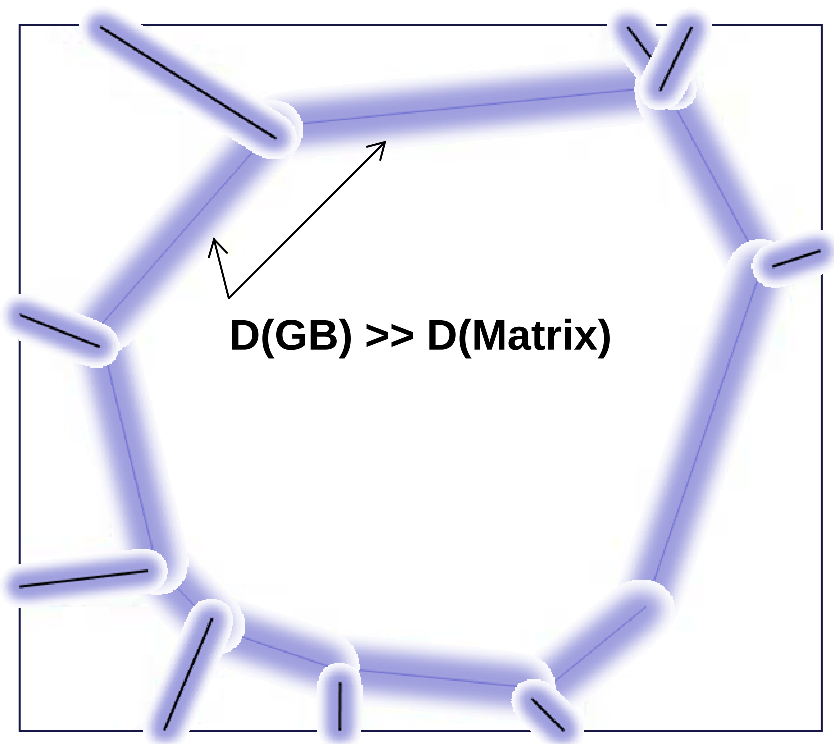
Goal:

– Effect of rapid **temperature transient** on diffusion of C.

– Investigate impact of various (realistic) **grain structures.**

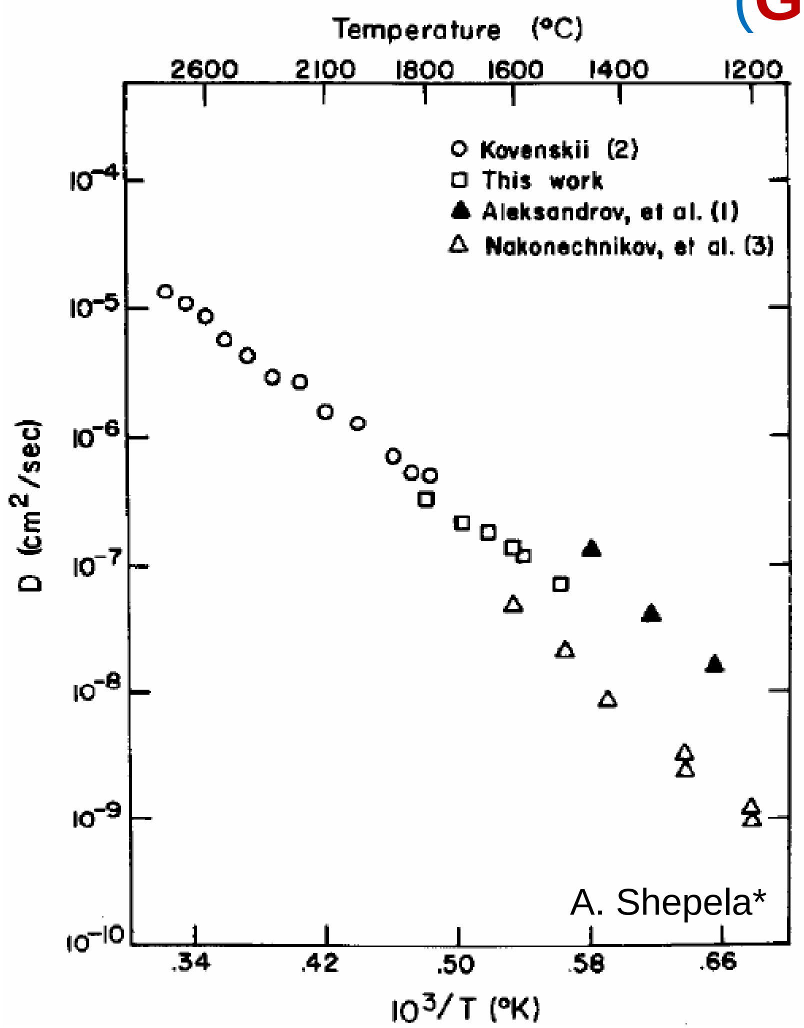
1. Carbon Diffusion Data
2. Grain-Structure Model

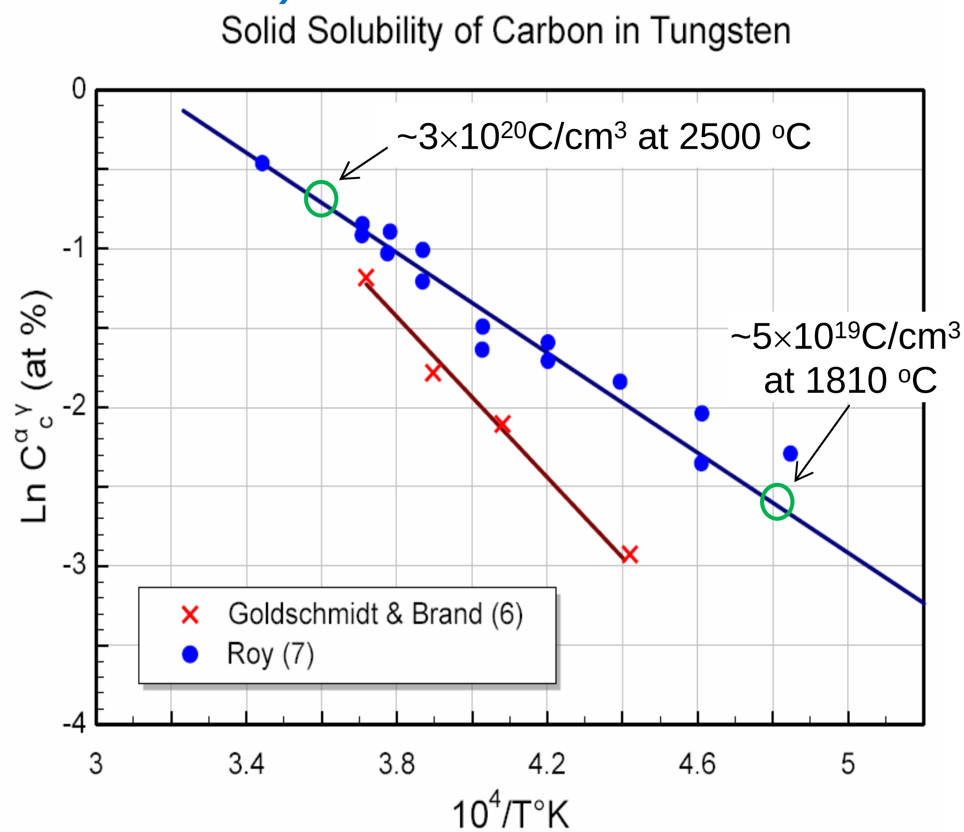
Carbon Diffusion in Grain Boundary region is higher than in Grain Matrix



Carbon Diffusion and Solubility in Single–X W

(Grain Matrix)



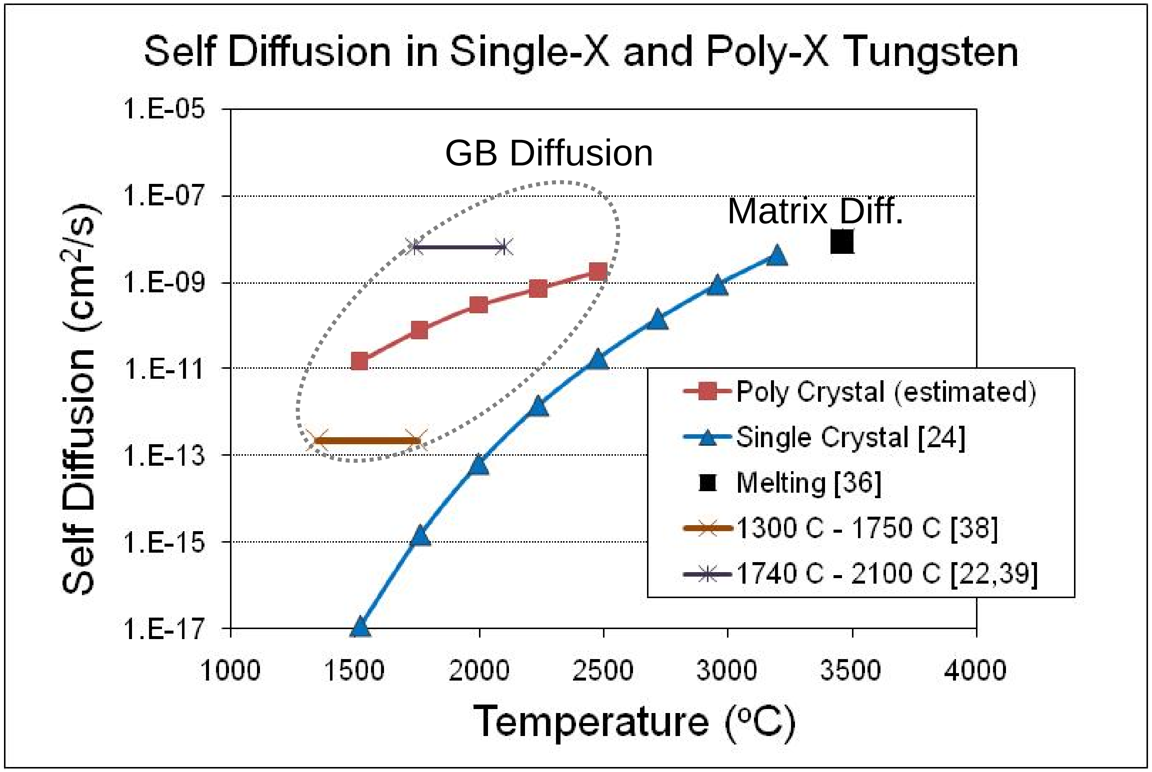


HAPL carbon- implantation ~1×10^{16} cm^{-3} per shot to a depth of ~0.5 μm

$$D\left(C^{14}/W\right) = (3.45 \pm 0.12)10^{-3} exp\left(-\frac{37,800 \pm 140}{RT}\right) \quad cm^2/s$$

*Adam Shepela, J Less Common Met. 26(1972) 33-43

Diffusion in Grain Boundary



- Self-diffusion in POLYCRYSTALLINE tungsten is much higher (T< 2500 ^{o}C)
- Implies that GB self-diffusion is faster by **~10^3 – 10^4** (T < 2000 ^{o}C) and ~ 10^2 (T= 2500 ^{o}C)
- C-diffusion is taken to be a factor of ~ 100 higher in GB region

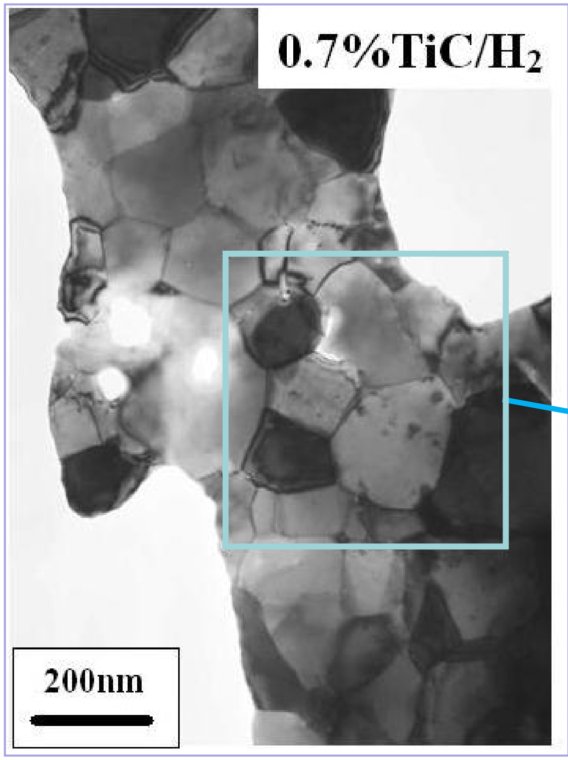
Gmelin Handbook of Inorganic and Organometallic Chemistry, Tungsten Suppl. vol. A 5b, 8th Ed., Springer, Berlin, 1993 (Chapters 7–9)

Carbon Diffusion Models

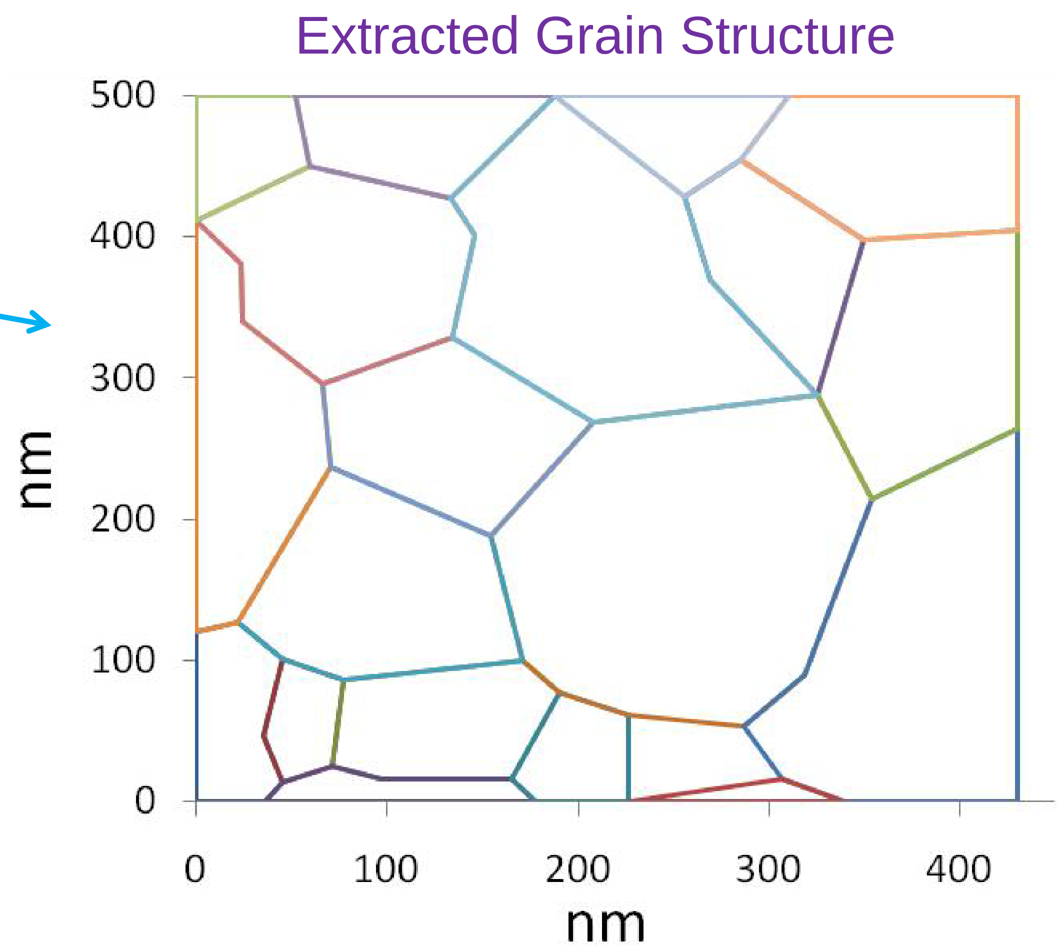
- Model (1):
  - Constant temperature anneal at 2000 ^{o}C with realistic grain structure
- Model (2):
  - Impact of HAPL temperature transient 600 to 2500 ^{o}C in $<10^{-4}$ s
- Model (3):
  - Grain size effect: Fine grain W compared with Single-X W

Grain Structure Model

Ultra-fine Grain (UFG) Tungsten*

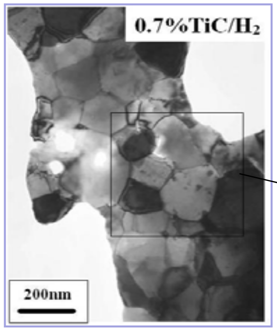


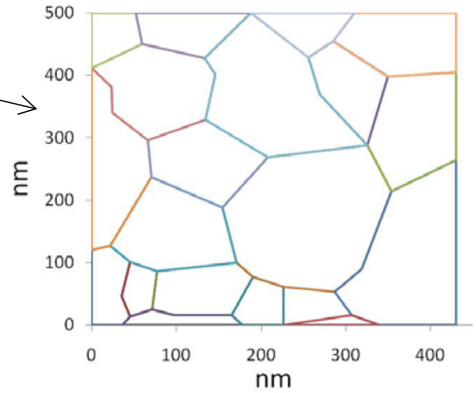
G.S. = 83 nm
R.D. = 99.4 %



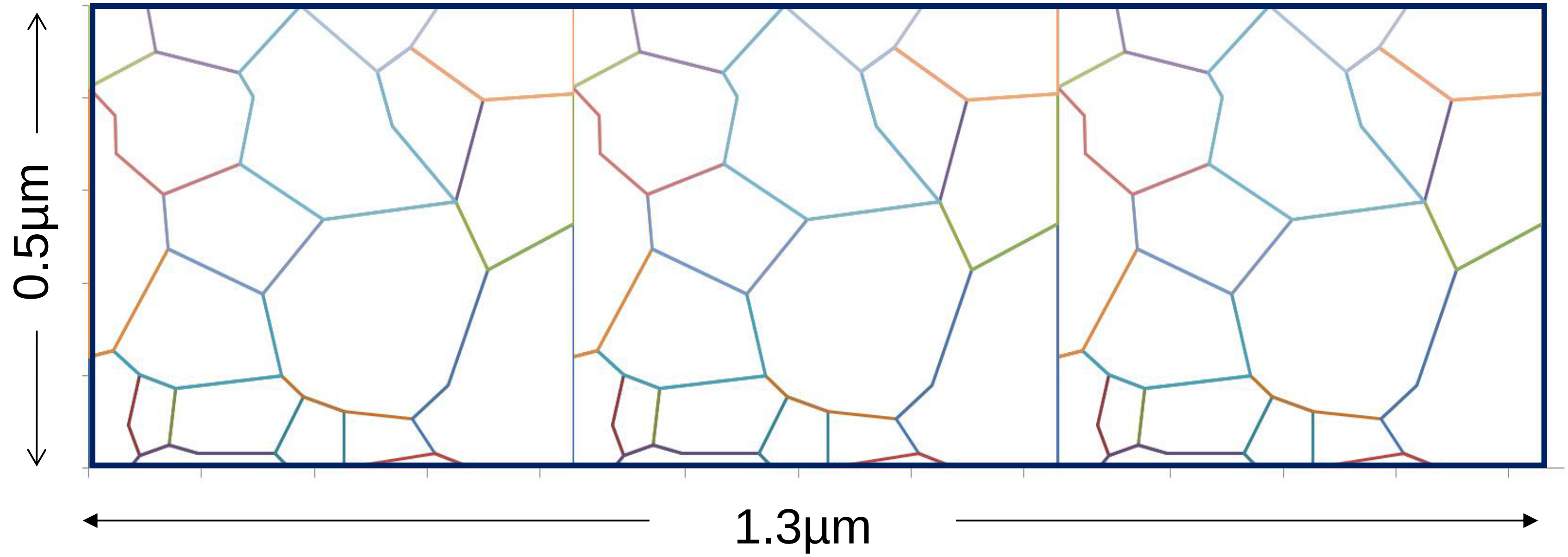
* Y. Ueda et al., 2006 US-J Workshop on Fusin High Power Density components and system and Heat Removal and Plasma-
Materials Interaction for Fusion, Nov. 15-17, 2006, Santa Fe, USA

Tungsten Grain (UFG) Model



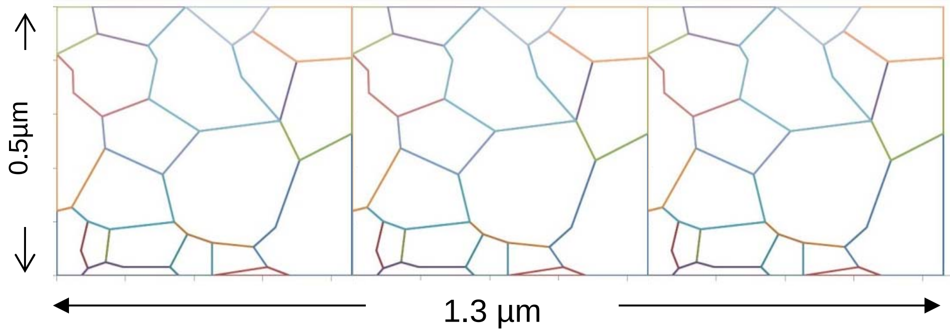


Tungsten Grain Structure Model used for Carbon Diffusion Simulation

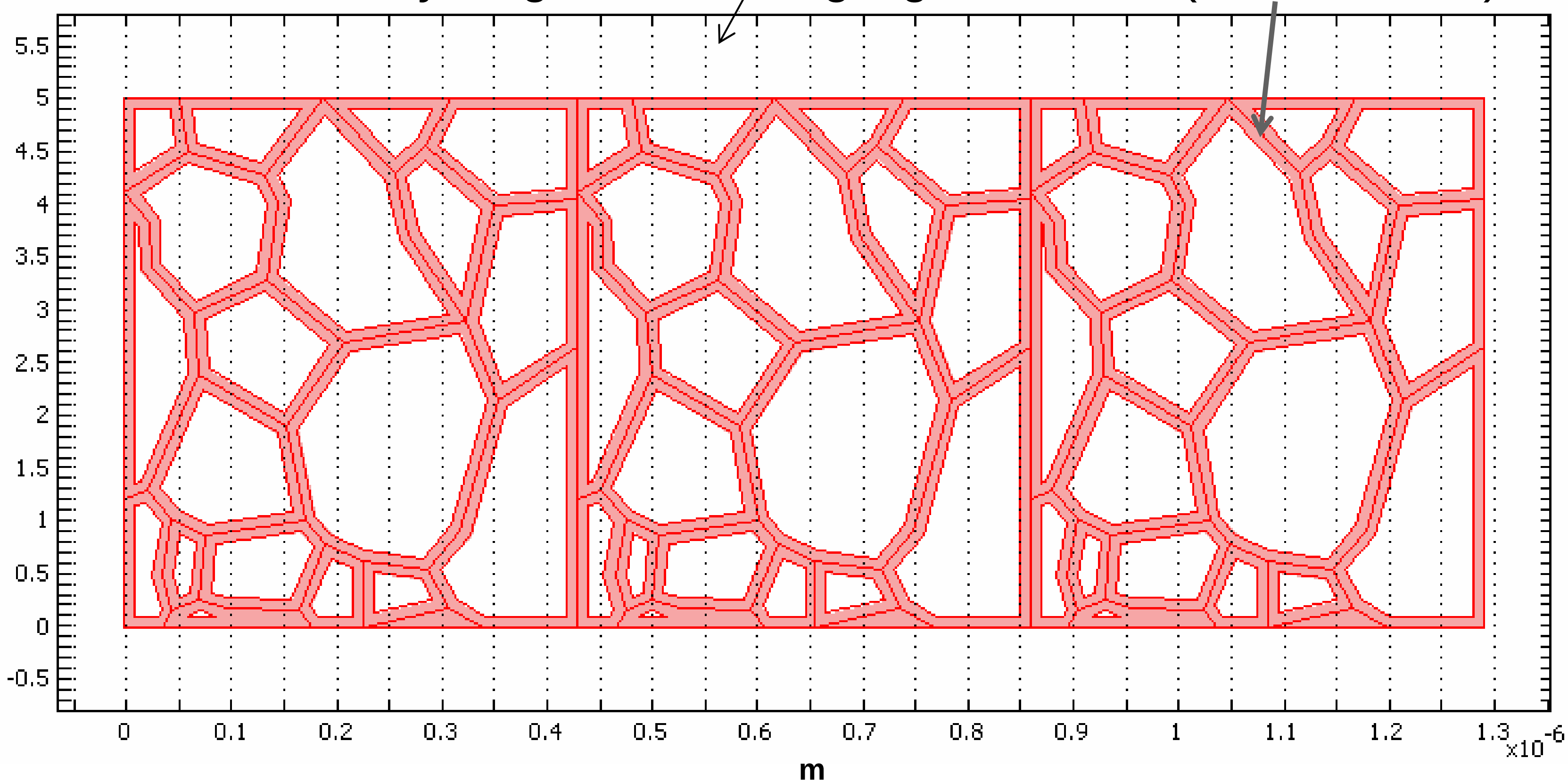


UFG -W with Grain Boundary Region

Tungsten Grain Structure Model used for Carbon Diffusion Simulation



Grain Boundary Regions are highlighted in red (~20 nm wide)



Model (1): C-Diffusion for Anneal at 2000 ^oC

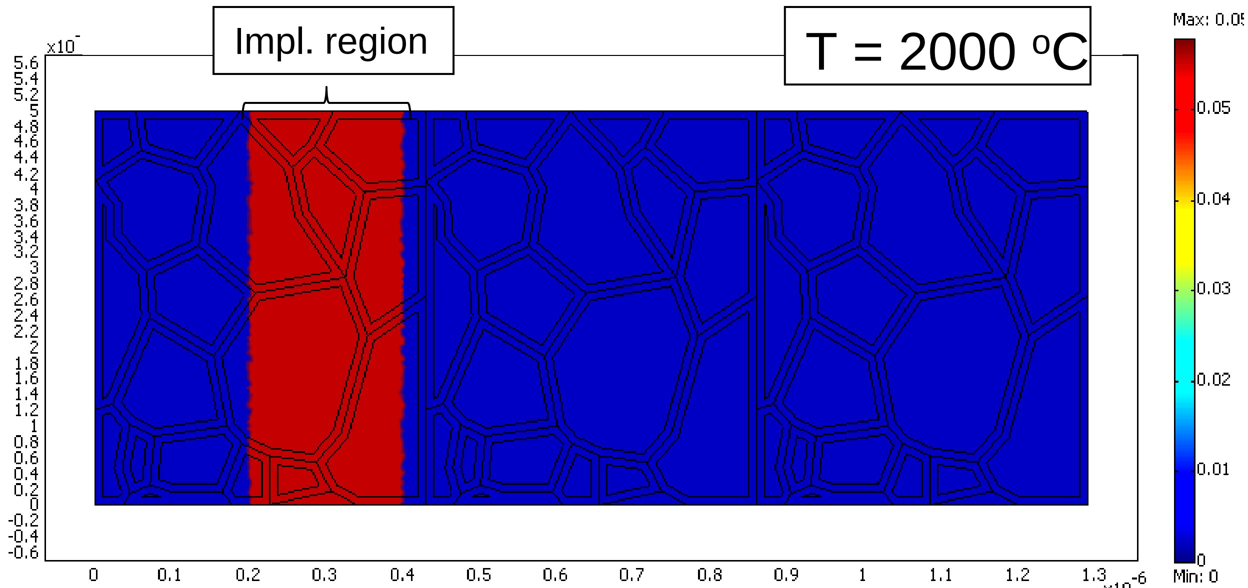
- Model 1 (UFG: fine grain)
  - Fine grains (with enhanced diffusion in 20-nm depth at GB)
  - Model dimensions (1.3 µm × 0.5 µm)
  - Constant diffusion coefficient D = $5.24X10^{10}$ m^2/s in the grains
  - 100 × enhanced diffusion in 20-nm GB region
  - Initial implantation of C (in a region 0.2 µm < X < 0.4µm)
  - **C implantation concentration is constant: <u>3.5×10^{16} cm^{-3}</u>**

- In HAPL maximum Carbon implantation ~1×10^{17} cm^{-3} per shot to a depth of ~0.8 µm

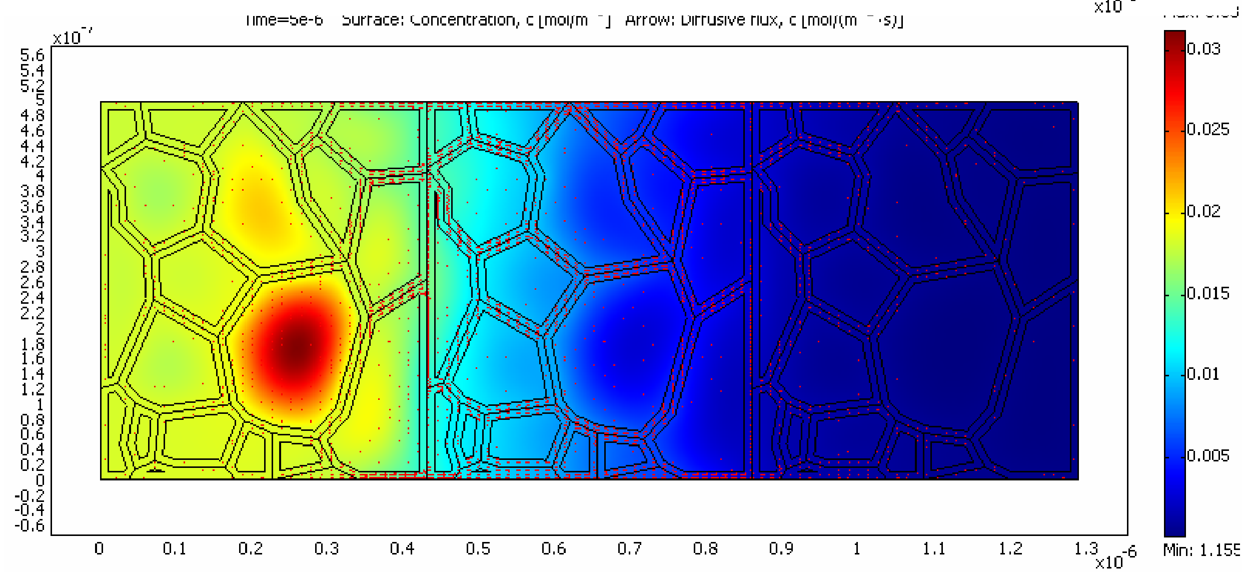
Carbon concentration profile as function of time

Initial C implantation in W (0.2 µm – 0.4 µm): 3.5×10^{16} atoms/cm^3

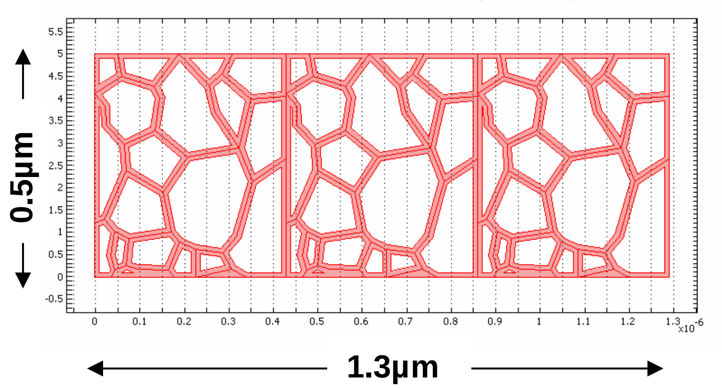
t = 0 s



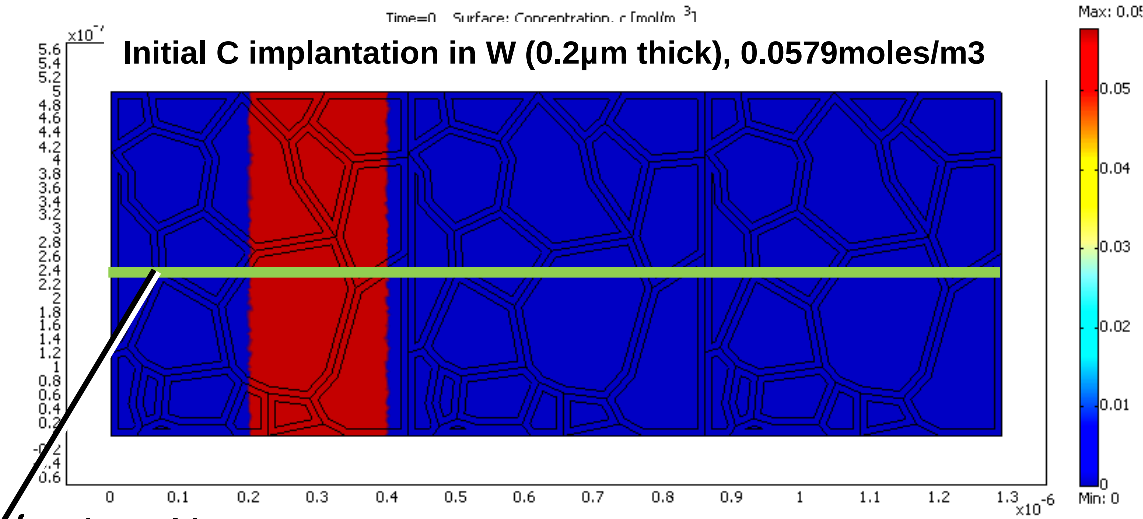
t = 5e-6 s



Grain boundaries are highlighted (20 nm wide)



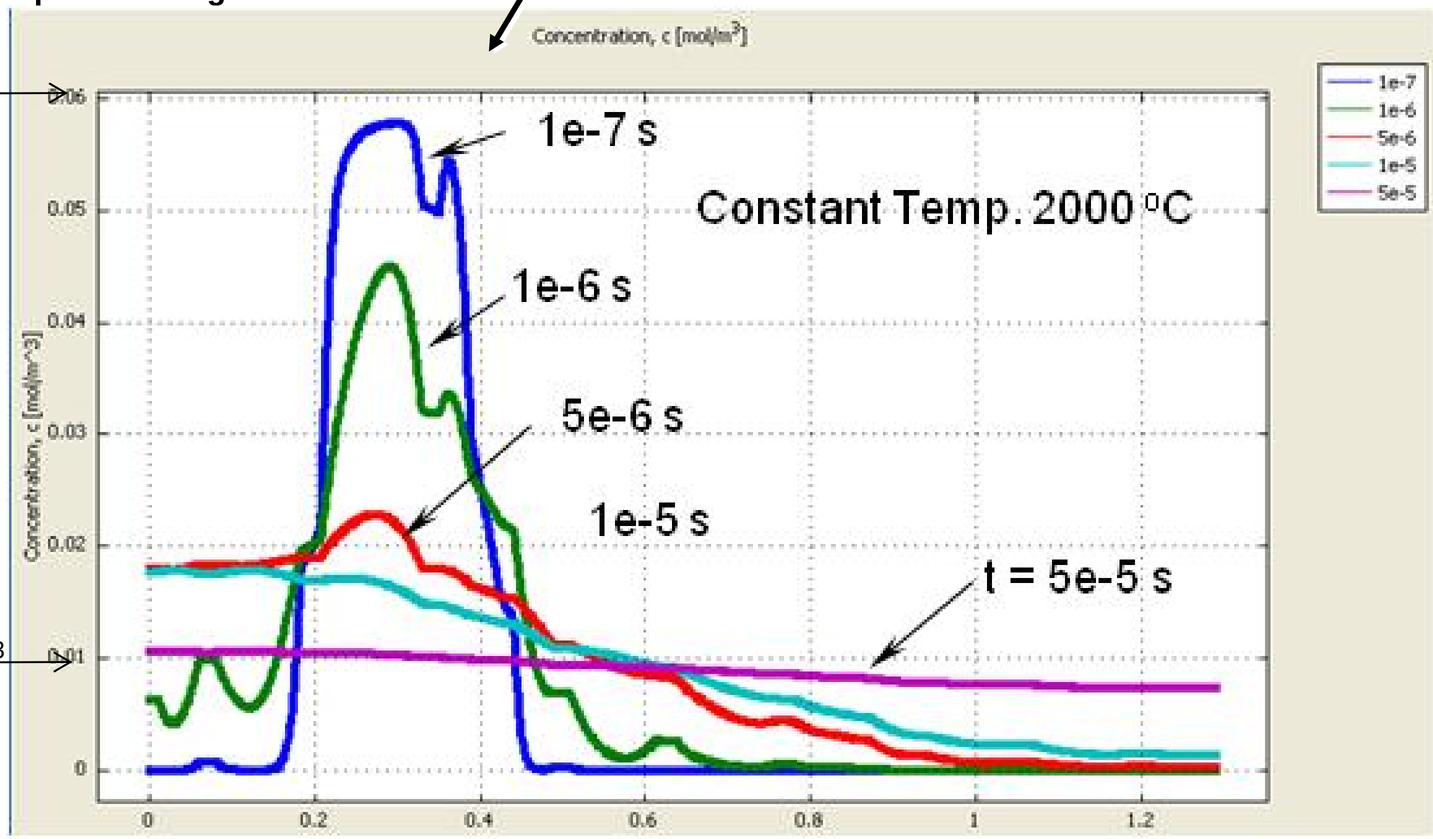
Initial C implantation in W (0.2µm thick), 0.0579moles/m3



Concentration profile along the centerline as a function of time

~4x10^{16} C/cm^3

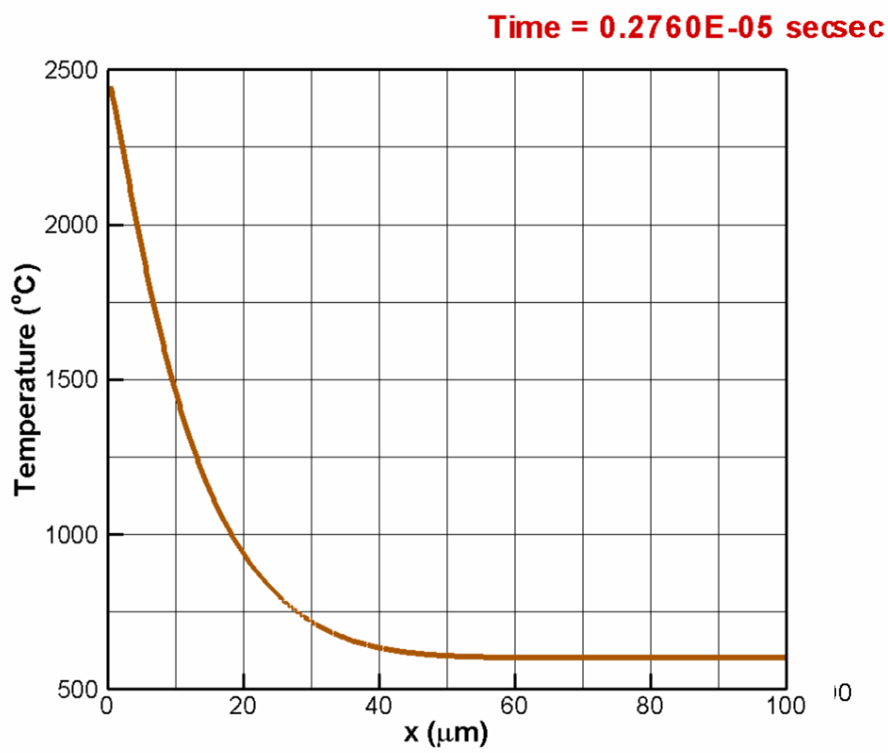
~6x10^{15} C/cm^3



Model (2): Temperature Transient Effect

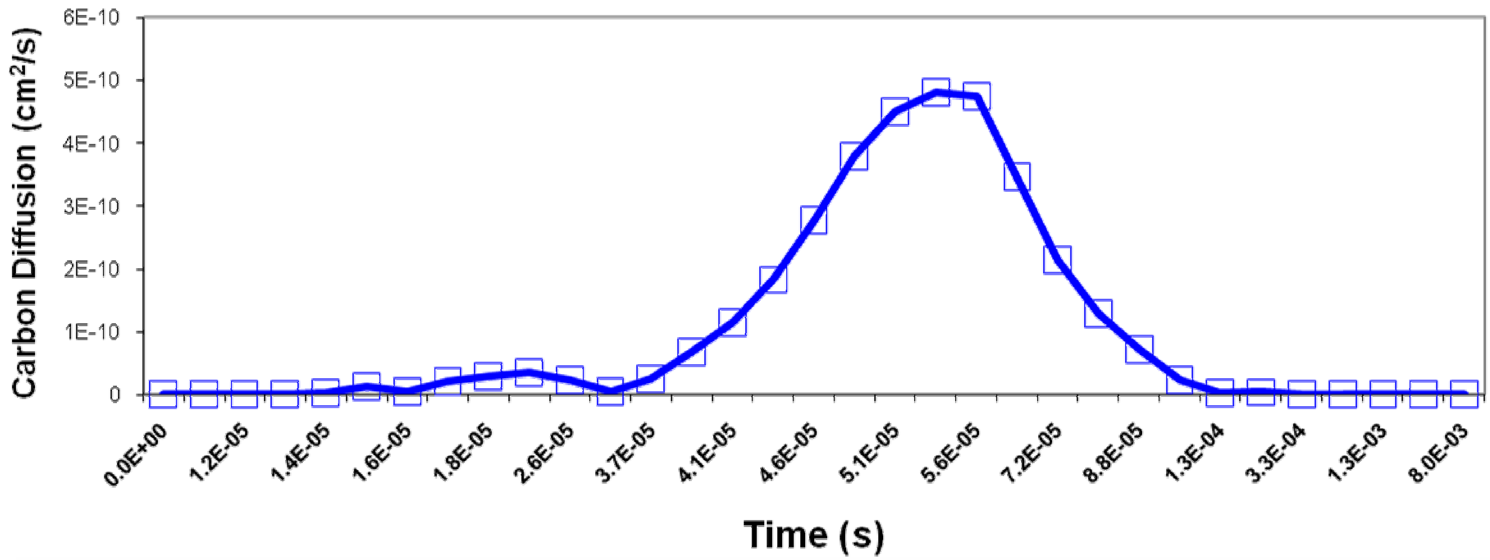
Temperature Transient in HAPL

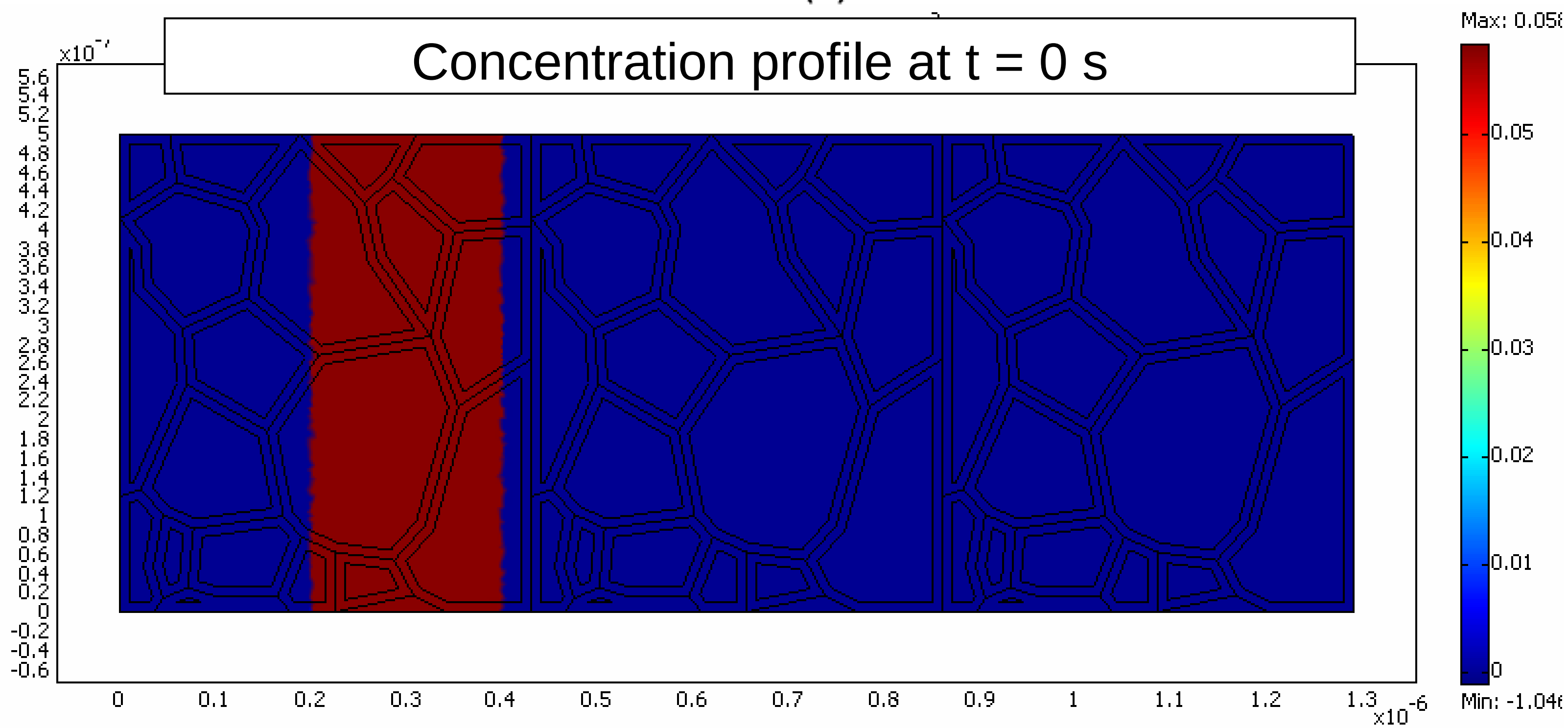
- UMARCO code provides detailed temperature transients as a function of position:

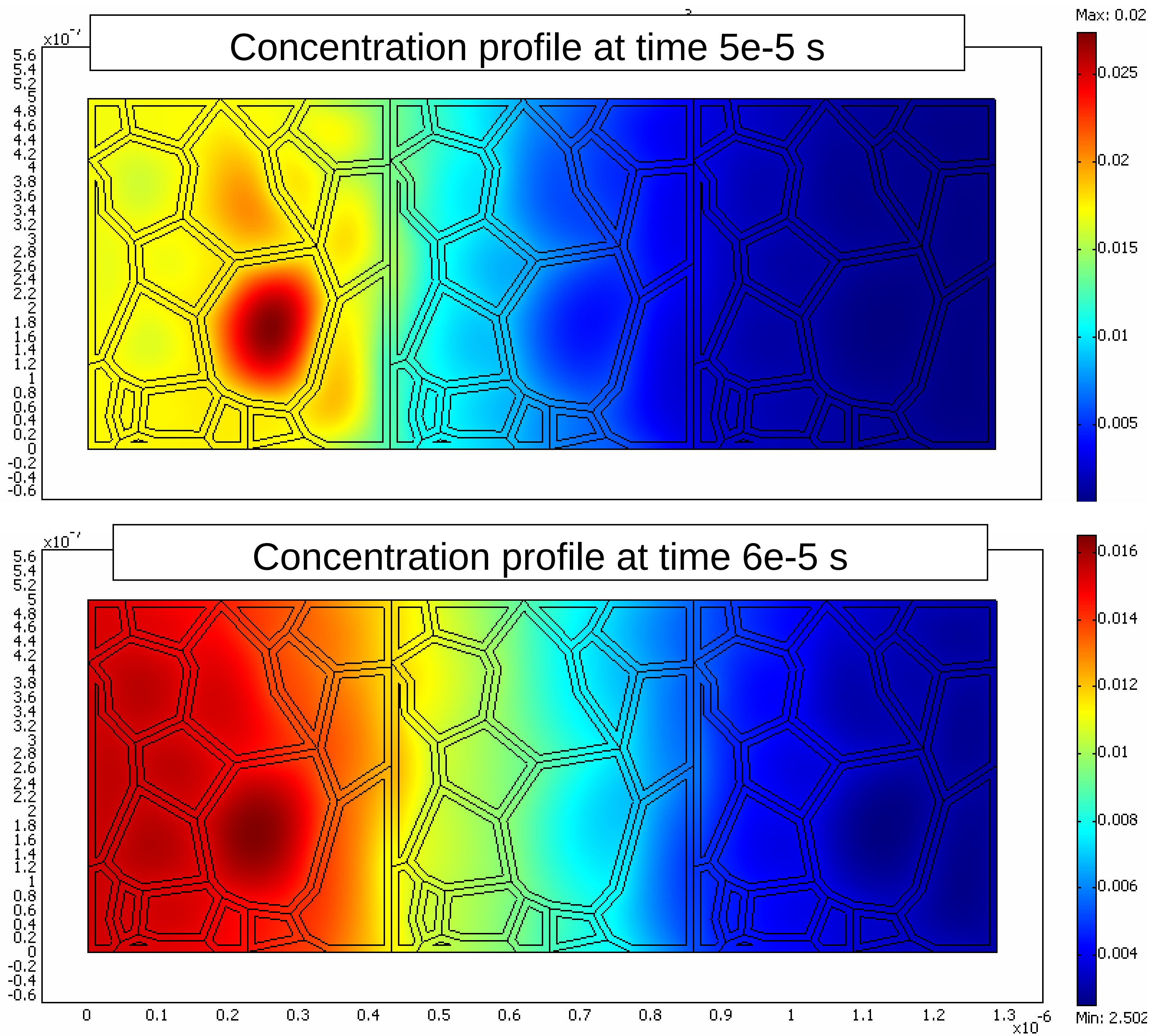


- Couple the transients with the diffusion model

Carbon-Diffusion coefficient variation with time (grain matrix)

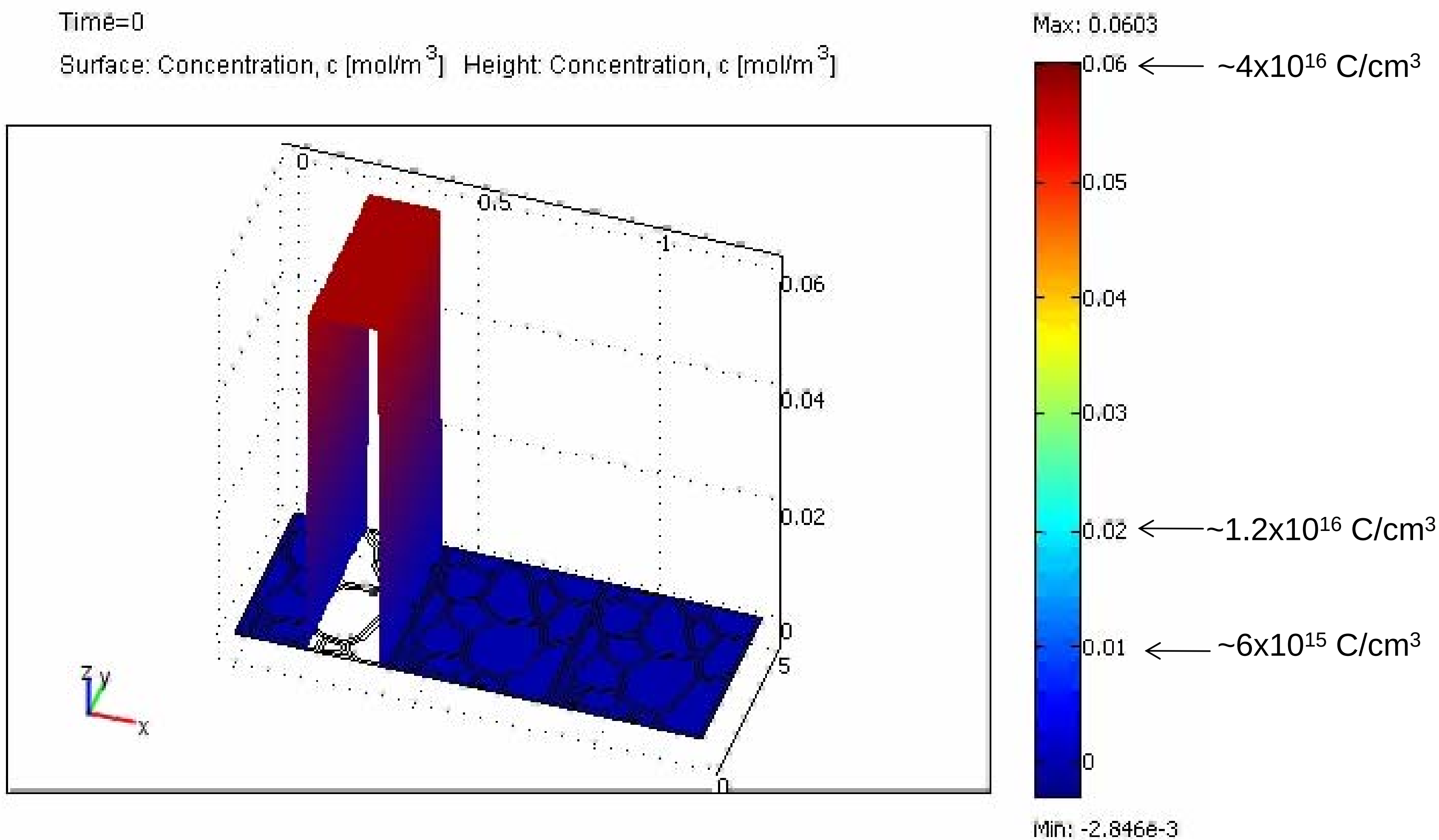





Concentration profile at time 5e-5 s
Max: 0.02
0.025
0.02
0.015
0.01
0.005
Concentration profile at time 6e-5 s
0.016
0.014
0.012
0.01
0.008
0.006
0.004
Min: 2.502
x10^-7
5.6
5.4
5.2
5
4.8
4.6
4.4
4.2
4
3.8
3.6
3.4
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
x10^-6

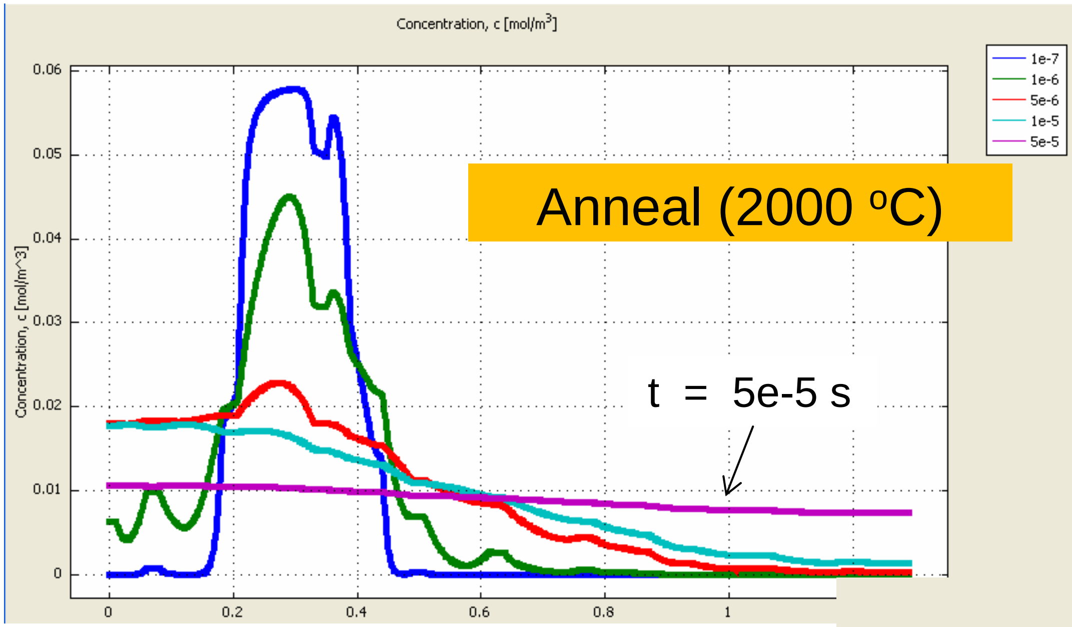
C-Diffusion for HAPL

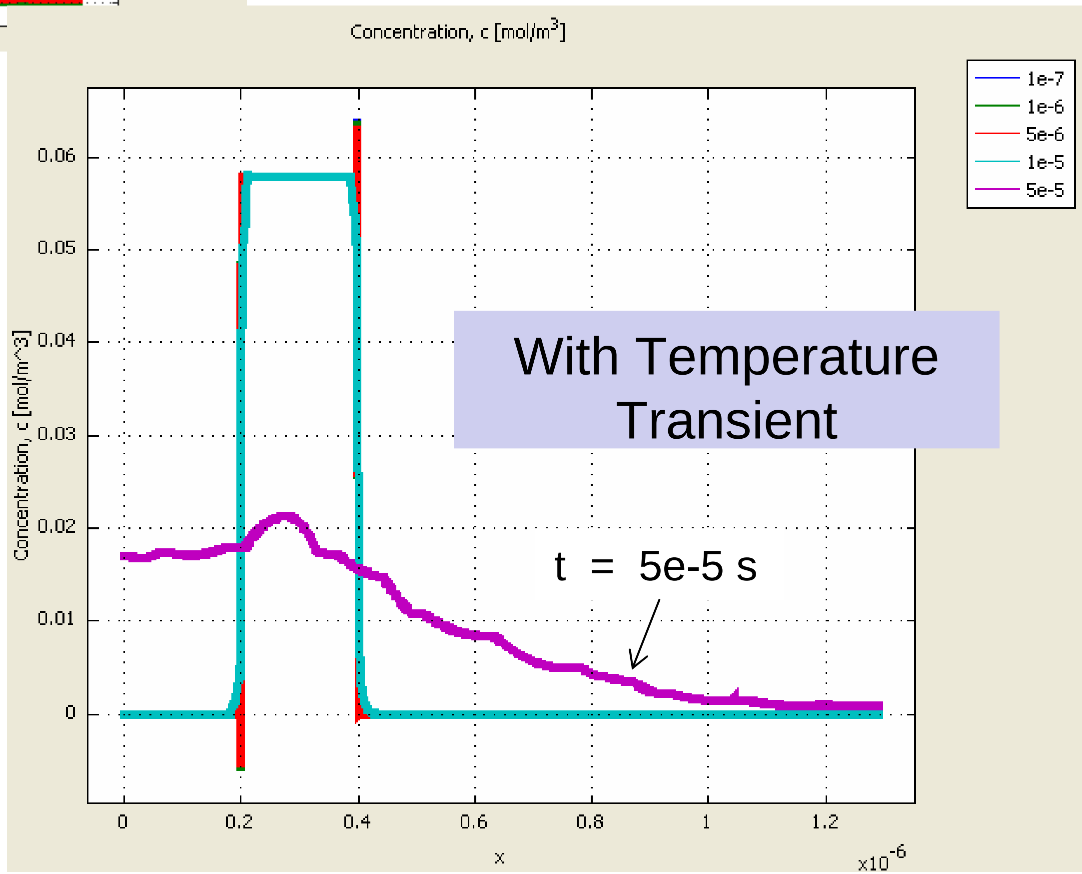
- Animation shows the C-concentration as a function of time for HAPL



Comparison of Concentration Profiles

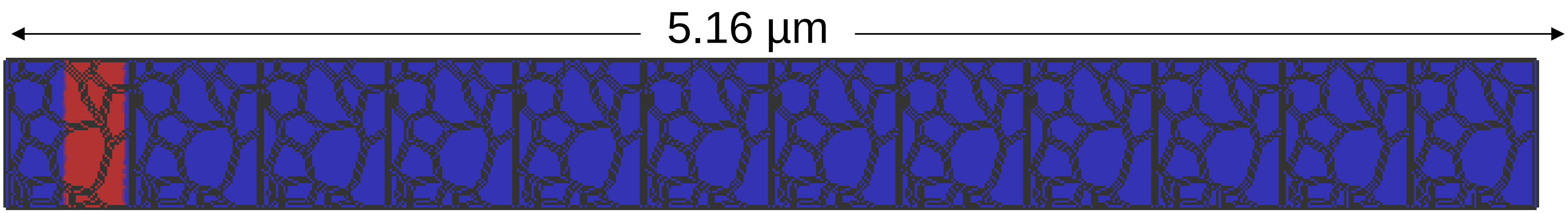
(at the centerline)



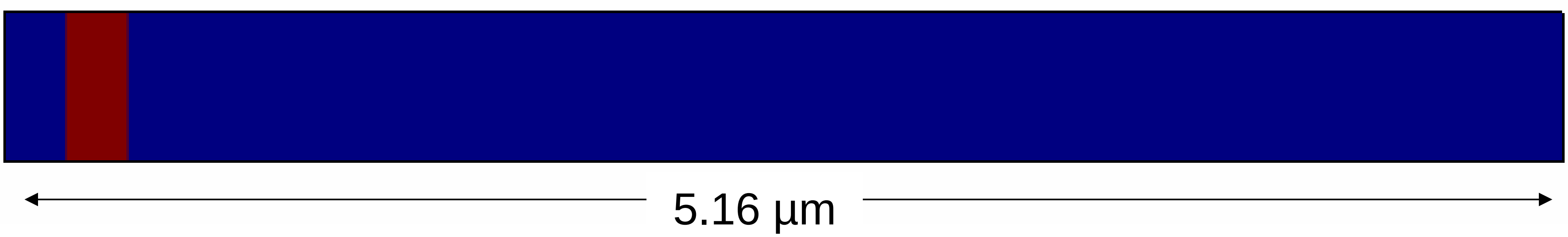


- Annealing "pushes" the Carbon deeper
- Annealing results in a more even distribution
- Rapid Temperature transient results in "pushing" carbon towards the surface

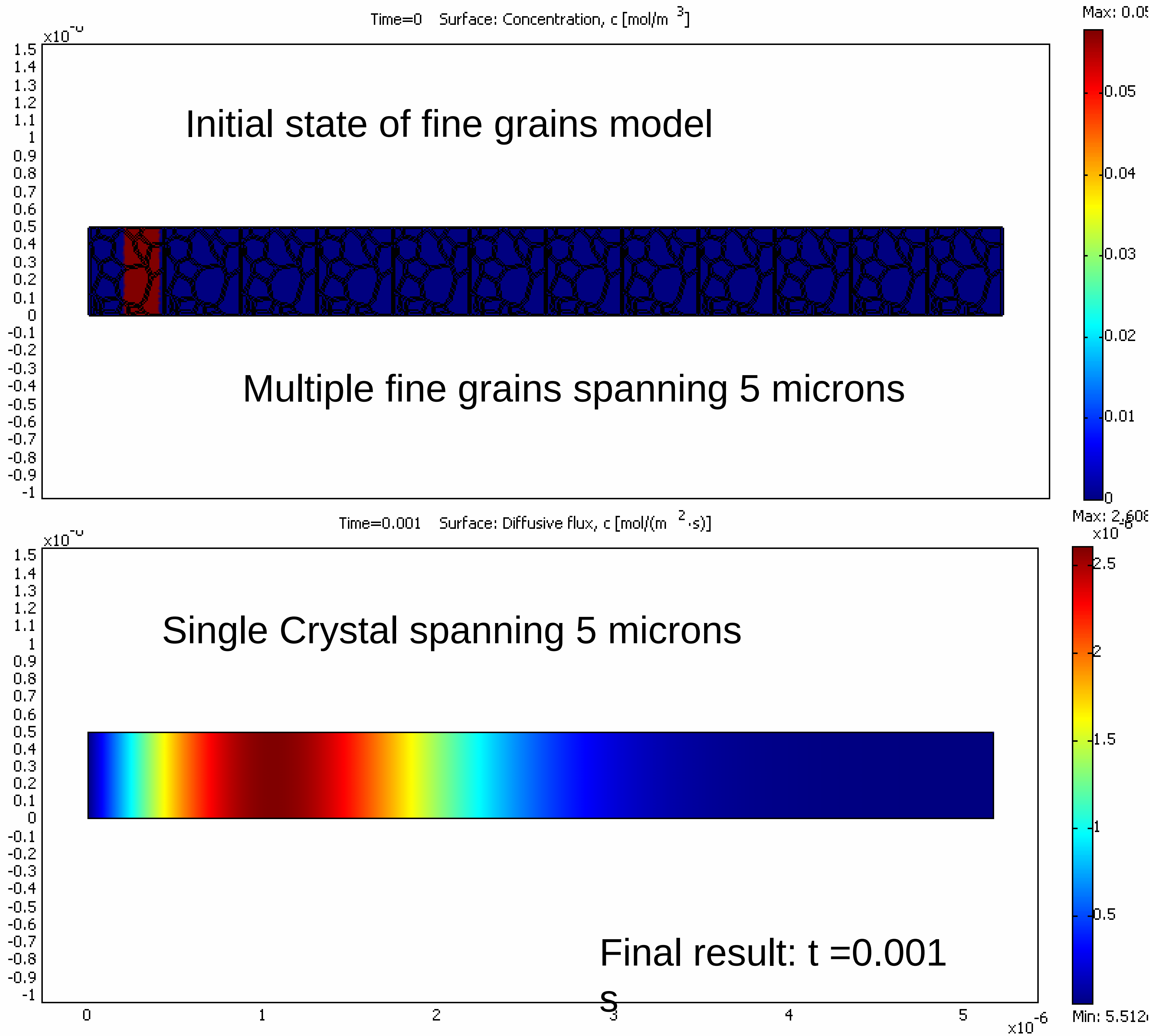
Model (3): Comparison between UFG – and Single –Crystal Tungsten (annealing 2000 ^{o}C)



- **UFG-Tungsten** with 20 nm grain boundary regions:
  D = $5.24X10^{10}$ m^2/s in the grains D = $5.24X10^{12}$ m^2/s in GB region
- The plot shows initial C implantation with the red region ($3.5x10^{16}$ C/cm^3)

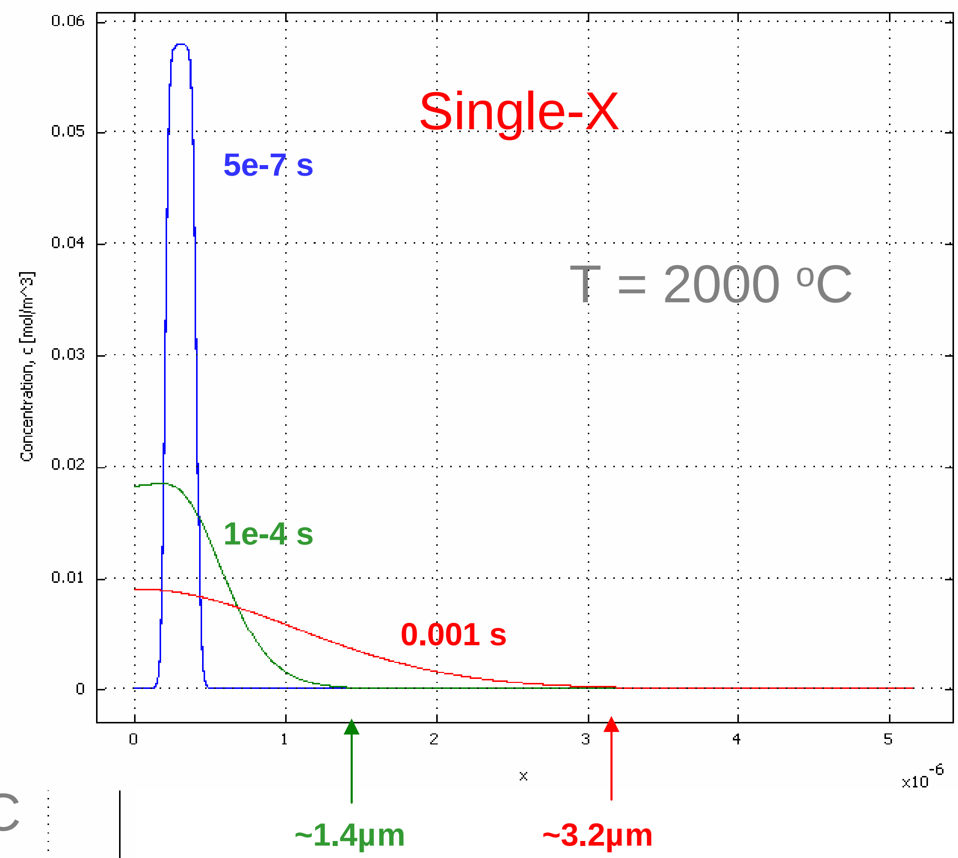


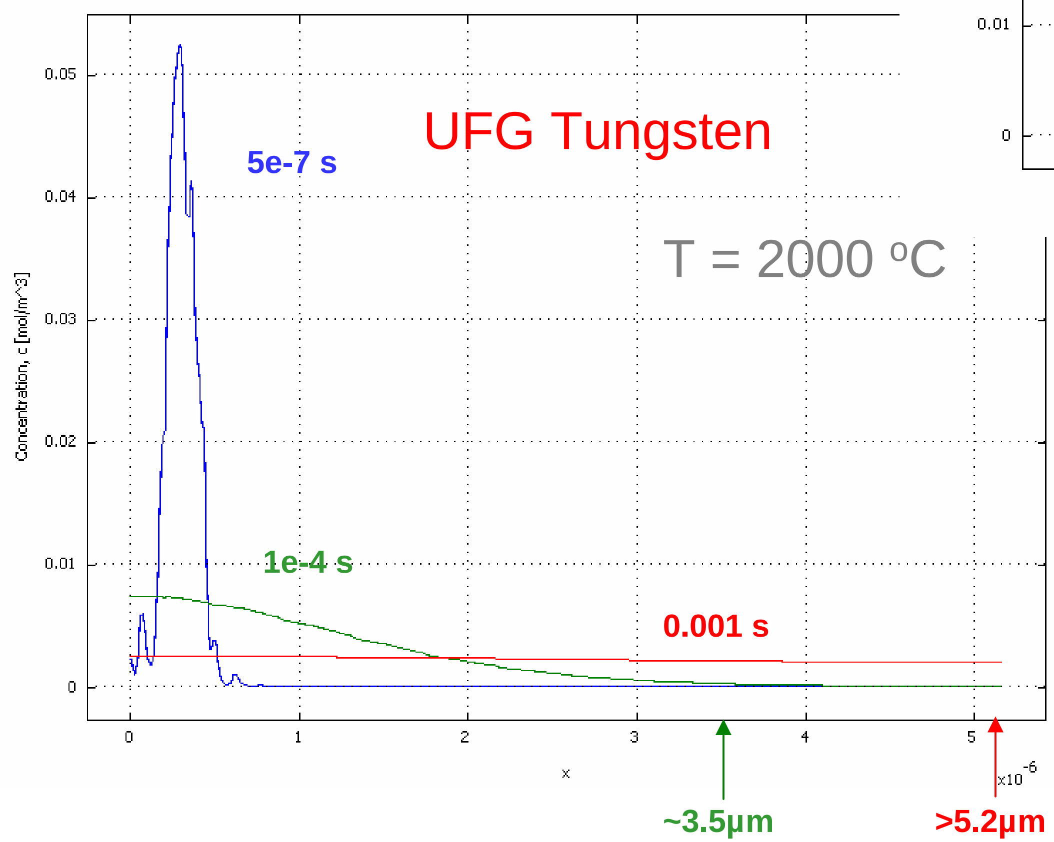
- 5.16 µm long **single crystal** (D = $5.24X10^{10}$ m^2/s)
- The plot shows initial C implantation with the red region ($3.5x10^{16}$ C/cm^3)



Time=0 Surface: Concentration, c [mol/m 3]
Initial state of fine grains model
Multiple fine grains spanning 5 microns
Max: 0.05
Time=0.001 Surface: Diffusive flux, c [mol/(m 2·s)]
Single Crystal spanning 5 microns
Final result: t =0.001 s
Min: 5.512

C-concentration along the Centerline
(x direction)





C diffuses through the entire UFG-W sample (5 µm) as there is rapid diffusion along grain boundaries

Summary

- Grain Boundary diffusion is significantly faster than in the matrix
- Realistic Grain structure was modeled based on UFG-W
- Modeled C-diffusion for annealing (T=2000^{o}C) in UFG-W
- Modeled C-diffusion with HAPL temperature transient
- Compared UFG-W with Single-X W

Findings:

- C-diffuses rapidly (<10^{-4} s) at 2000 ^{o}C through the UFG sample (1.3 μm)
- **Near surface high temperature transients move Carbon towards surface and reduces diffusion into the W**
- C concentration remains peaked for Single-X, while in UFG-W C diffuses throughout the thickness (5 μm) for a 2000 ^{o}C anneal in < 0.001 s.

TOFE 2008: Submitted Abstracts

- **A Unified Model for Ion Deposition and Thermomechanical Response in Dry Wall Laser IFE Chambers,** J. Blanchard, Q. Hu, and N. Ghoniem
- **Roughening of Surfaces under Intense and Rapid Heating**," M. Andersen, A. Takahashi, N. Ghoniem
- **Thermo-mechanical Analysis of the Hibachi Foil for the Electra Laser System,"** A. Aoyama, J. Blanchard, J. Sethian, N. Ghoniem, and S. Sharafat
- **A Simulation of Carbon Transport in Implanted Tungsten**," M. Narula, S. Sharafat, and N. Ghoniem
- **A KMC Simulation of Grain Size Effects on Bubble Growth and Gas Release of Implanted Tungsten**, A. Takahashi, K. Nagasawa, S. Sharafat, and N. Ghoniem
- **Simulation of Pressure Pulses in SiC due to Isochoric Heating of PbLi Using a Laser Spallation Technique,** J. El-Awady, H. Kim, K. Mistry, V. Gupta, N.Ghoniem, S. Sharafat

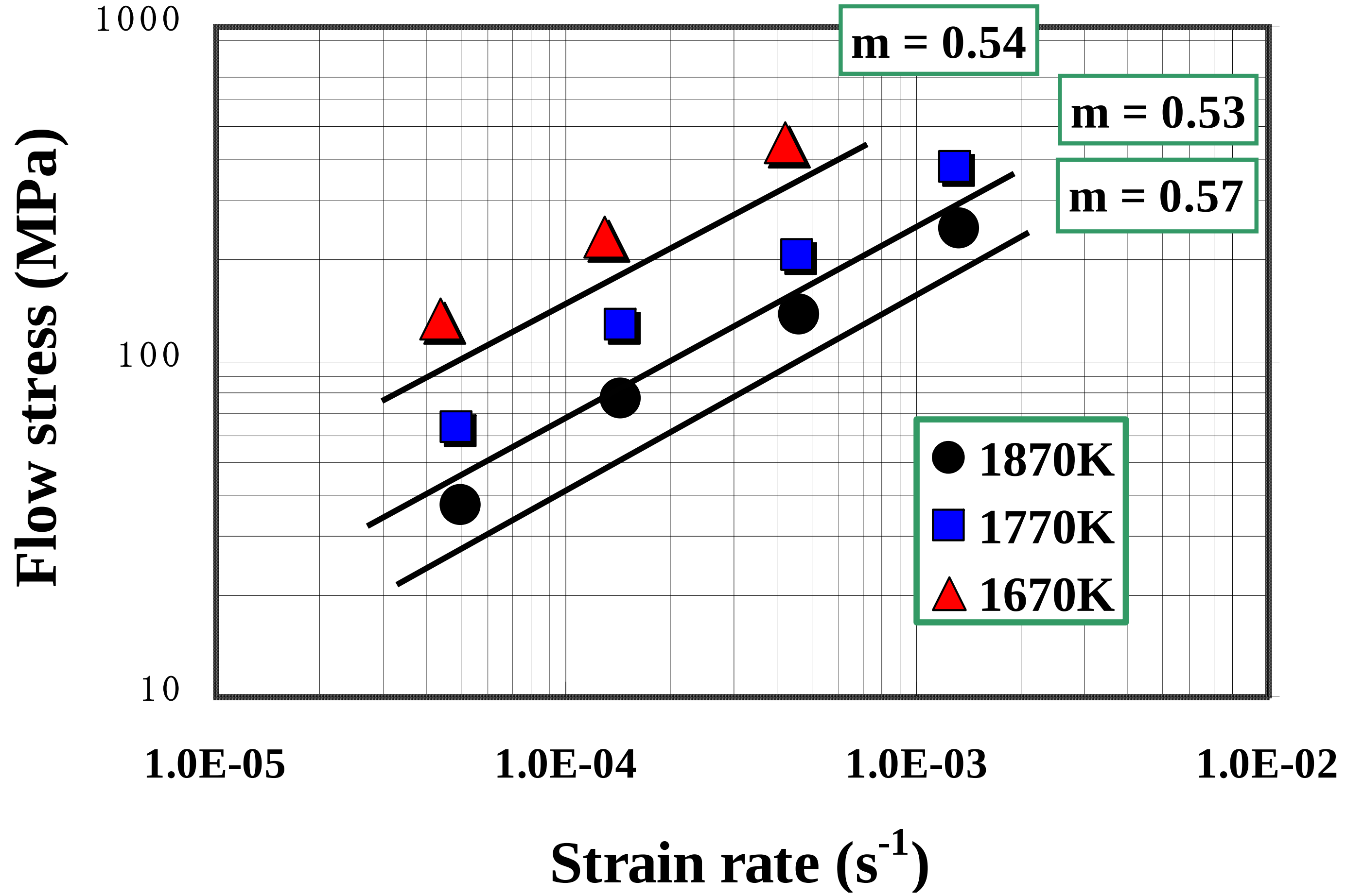
Backup Slides for C-diffusion modeling

Development of UFG Tungsten

- What is ultra fine grained tungsten?
  - Tungsten materials with very small grains (<100 nm) with some TiC dispersoids.
  - Development by Dr. Kurishita (Tohoku University)
- Fabrication
  - Mixing of powder of tungsten and TiC in Ar or H_2 atmosphere without oxygen.
  - Mechanical alloying
  - Degassing in vacuum
  - HIP process
- Advantages for plasma facing material
  - Little or no radiation (neutron, He) hardening
  - No significant blistering (H_2, He)
  - Superplasticity ~160 % (T>1670 K)
  - Higher re-crystalliation temperature (claim)

Strain rate dependence of flow stress

W-0.5TiC-H_2

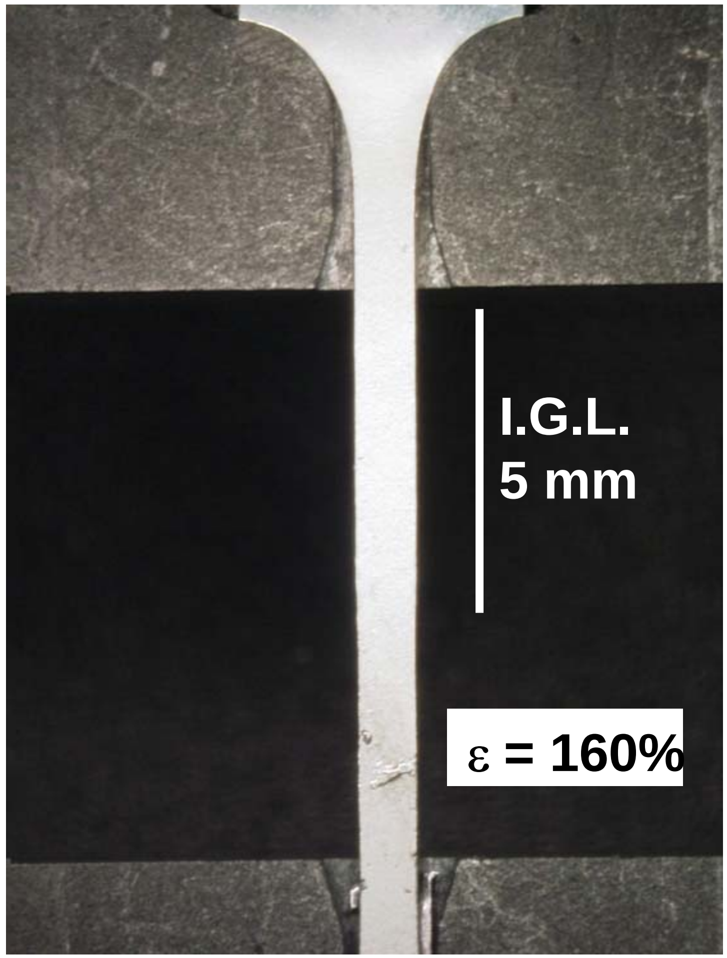


W-0.5TiC-H_2 exhibits superplasticity at and above 1670K, with a large strain rate sensitivity, *m*, of 0.5~0.6, that is characteristic of superplastic materials.

* Y. Ueda et al., 2006 US-J Workshop on Fusin High Power Density components and system and Heat Removal and Plasma-

Superplastic deformation of UFG W-0.5TiC-H_2

G.S.: 0.5 mm x 1.2 mm x 5 mm



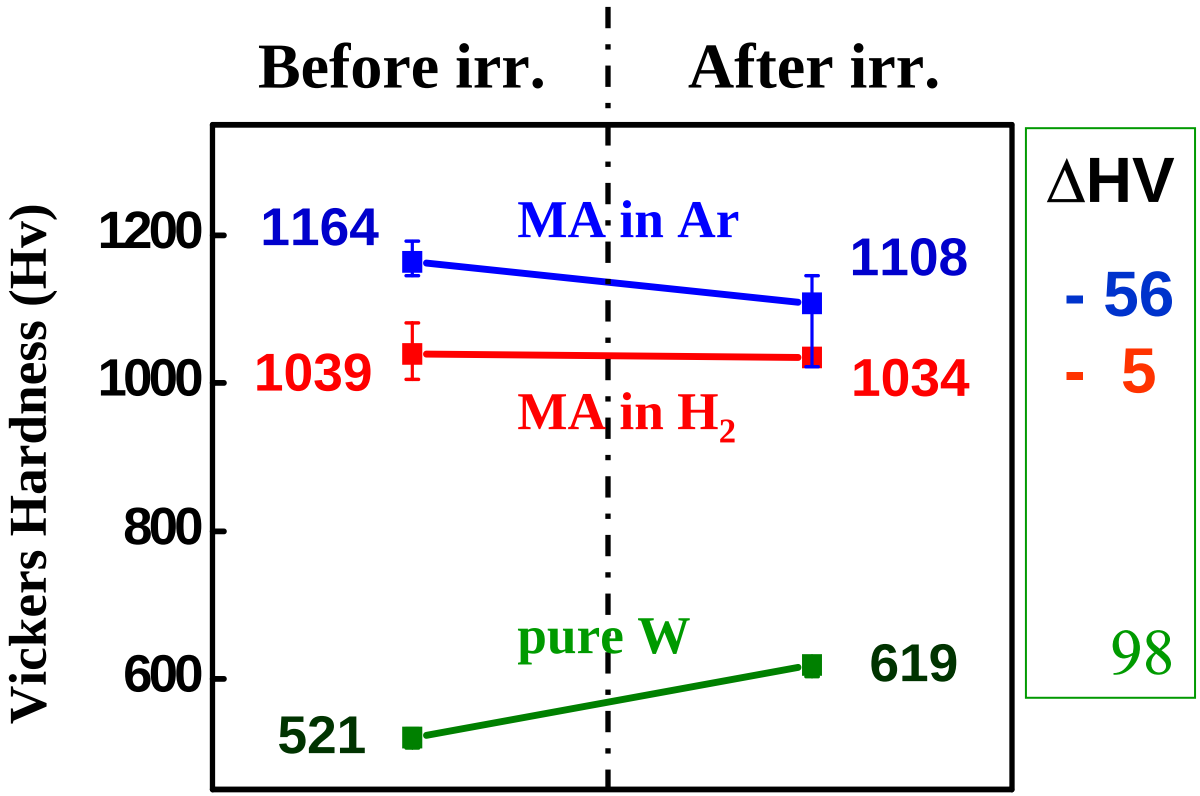
1970K

an initial strain rate of 5×10^{-4} s^{-1}

Crosshead is arrested at ε = 160% to examine the specimen surface.
I.G.L. stands for the initial gauge length of the tensile specimen.

* Y. Ueda et al., 2006 US-J Workshop on Fusin High Power Density components and system and Heat Removal and Plasma-

Radiation hardening in pure W and UFG W-0.5TiC



Vickers microhardness before and after irradiation

Radiation hardening occurred in pure W, but not in W-0.5TiC-H_2 and W-0.5TiC-Ar.

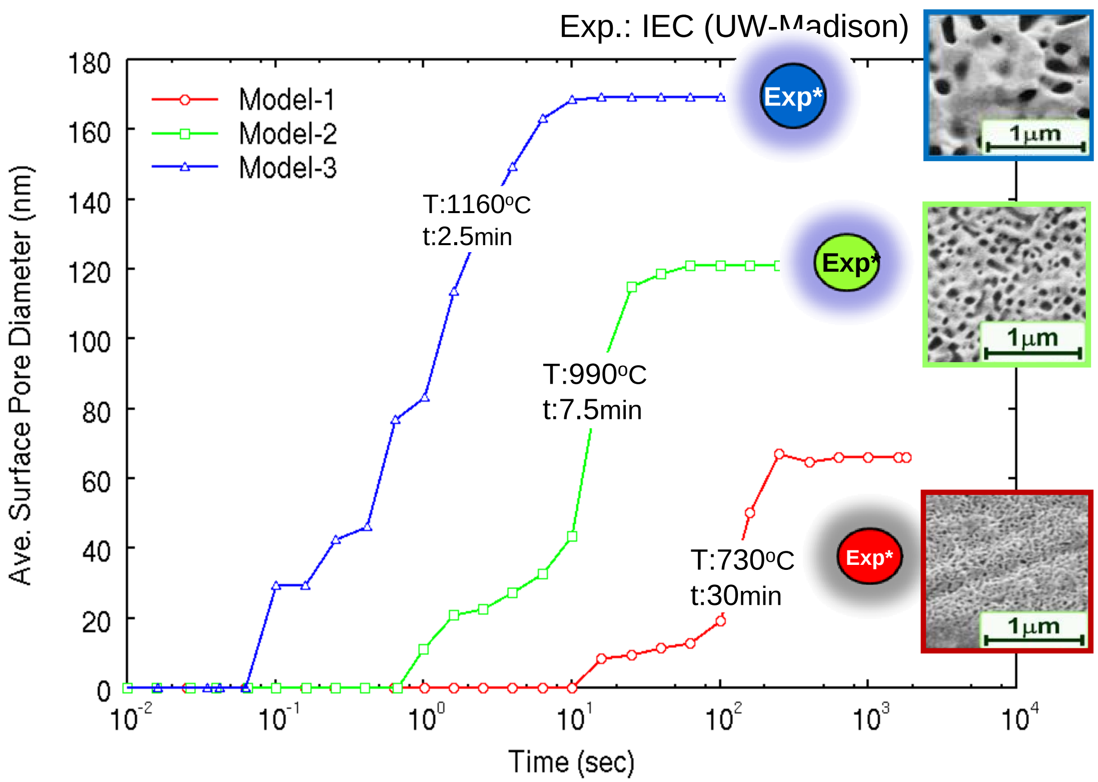
T_{irr} = 873K and fluence of 2×10^{24} n/m^2 (E_n > 1 MeV). (JMTR)

* Y. Ueda et al., 2006 US-J Workshop on Fusin High Power Density components and system and Heat Removal and Plasma-

Backup Slides for He-bubble Migration and Coalescence in a Stress Gradient

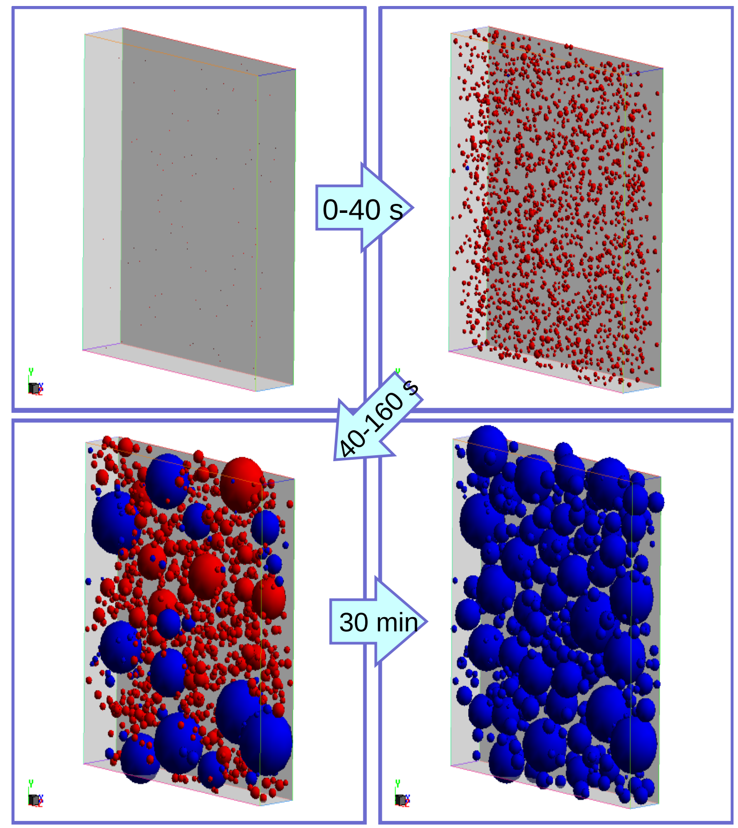
McHEROS Code Simulation of IEC Surface Pores

	Temperature	Implantation Rate (He/cm^2-s)	L_x (μm)	L_y (μm)	L_z (μm)
Model-1	730	2.2×10^{15}	0.2	1.0	1.0
Model-2	990	8.8×10^{15}	0.2	2.5	2.5
Model-3	1160	2.6×10^{16}	0.2	5.0	5.0



Kulcinski et al., 2005 IEC Facitlies, UW-Madison

1.6×10^{18} He/m^2-s; 730 °C; t:30min (IEC)



McHEROS Results:

- **Good Agreement between McHEROS Simulation and Experiment**
- **McHEROS provides an *EXPLANATION* for the oversized Surface Pores**

McHEROS Stress Gradient: Methodology

Diffusion coefficient of a bubble (D_p) based on the surface diffusion (D_s) mechanism:

$$D_s = D_0 \exp\left(-\frac{E_m}{kT}\right) \qquad D_p = \frac{3\Omega^{4/3}}{2\pi r^4} D_s$$

Velocity and mobility of a bubble in a stress gradient field

$$V_p = B_p F_p \qquad B_p = \frac{D_p}{kT}$$

Effective diffusion coefficient of a bubble in a stress gradient field

$$\boxed{D_p^{eff} = V_p \delta = B_p F_p \delta = \frac{D_p}{kT} F_p \delta = D_p \frac{F\delta}{kT} = D_o^p exp\left(-\frac{E_m^{eff}}{kT}\right)}$$

The pre-exponential diffusion coefficient of bubble is estimated using:

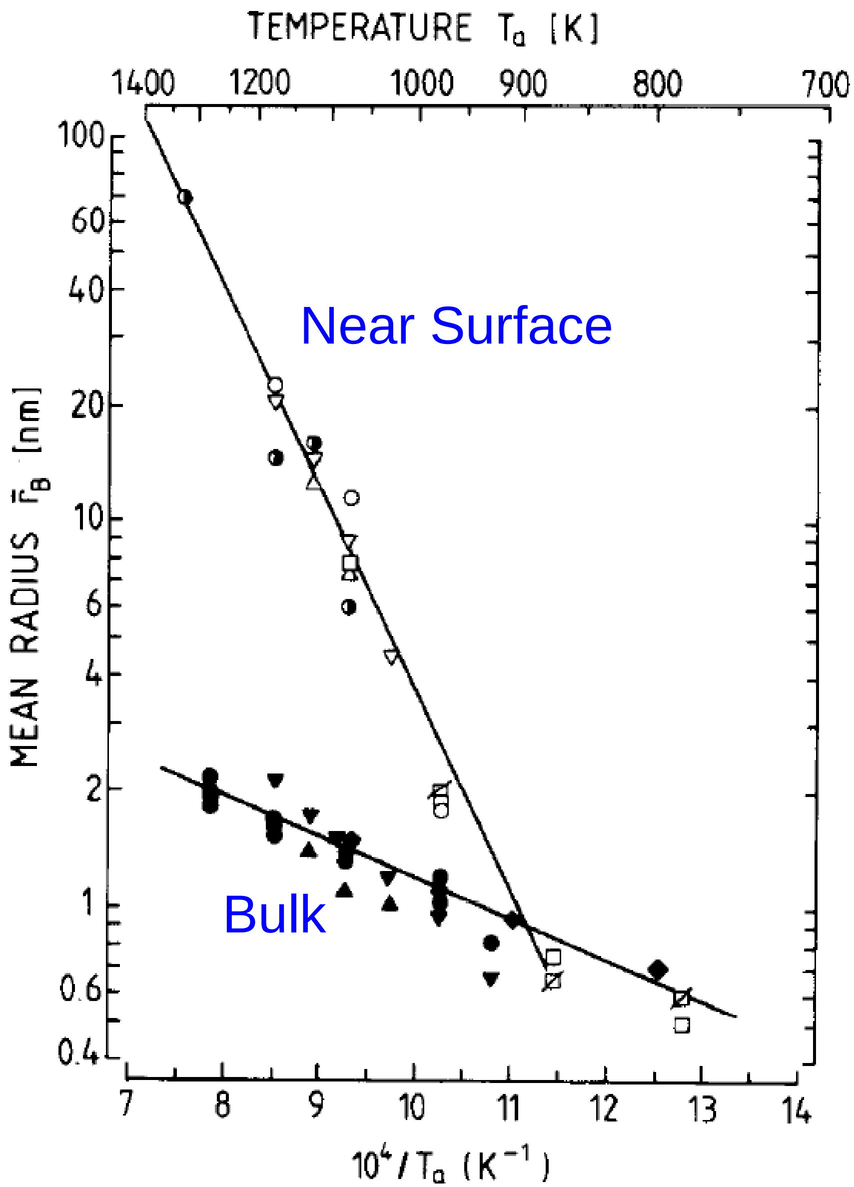
$$D_0^p = \frac{\nu_0 \delta^2 V^p}{6\Omega}$$

V^p: Volume of bubble
ν_0: Debye frequency

I. The net migration energy (E^{eff}_m) of the bubble due to a stress-field can be calculated using the bubble diffusion coefficient (D^{eff}_p).

II. Then we apply the "Delta-Energy Rule" to calculate the migration energy of the bubble in 6 different directions.

Bubble Size Near Surface vs Bulk *



- 1000 appm He Implanted in Ni at RT.
- Uniform He implantation using degrader Al-foil (28 MeV He)
- Annealing time: 0.5 – 1.5 hr

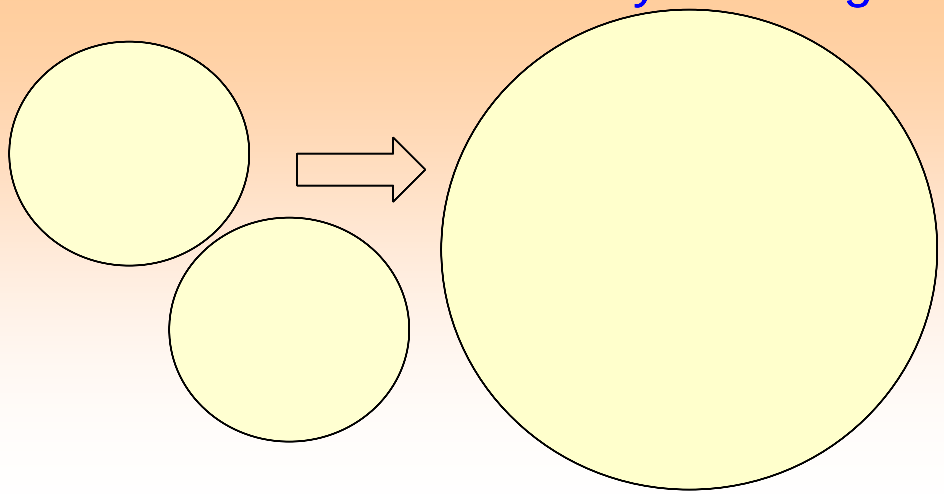
Abundance of Near Surface Vacancies promotes rapid and large bubble growth

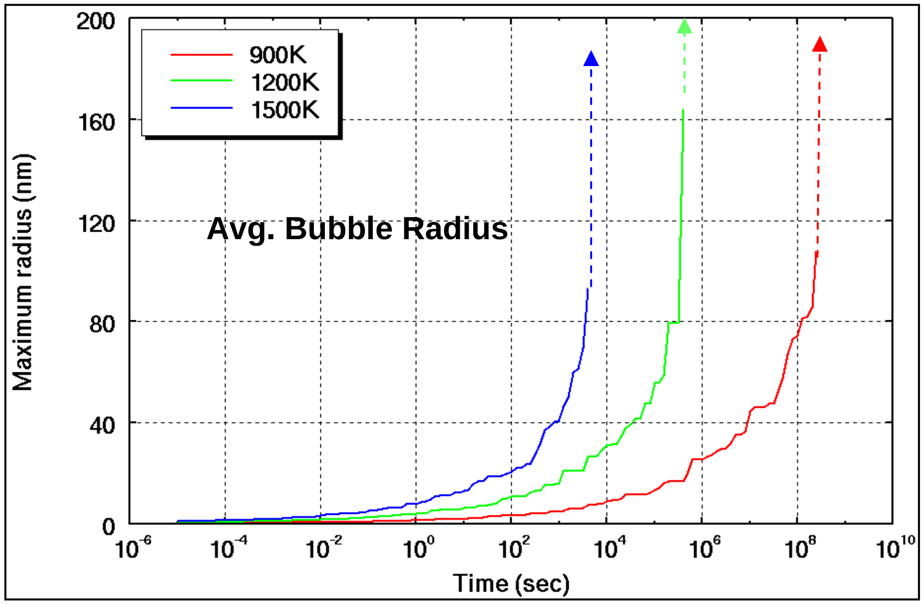
*CHERNIKOV, JNM 1989

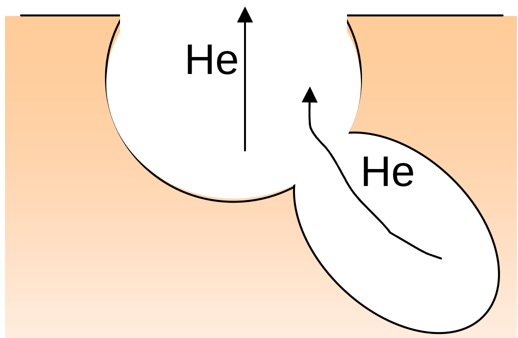
Sub-Surface Break Away Swelling Contribution

- **BREAK-AWAY Swelling (very rapid growth of bubbles) occurs at the subsurface**
- **However, because the bubbles bisect the surface the swelling is stopped by venting He.**
- **Time to BREAK-AWAY swelling DECREASES with higher Temps.**

Sub-Surface Break-Away Swelling







Surface Pore Formation

Explaining Low-E He-Implantation Results

- Abundance of **near surface** vacancies allow bubbles to grow rapidly to equilibrium size:
  → Large bubbles & low He-pressure

- **Near the surface, Migration & Coalescence (M&C) plus rapid growth results in super-size bubbles.**

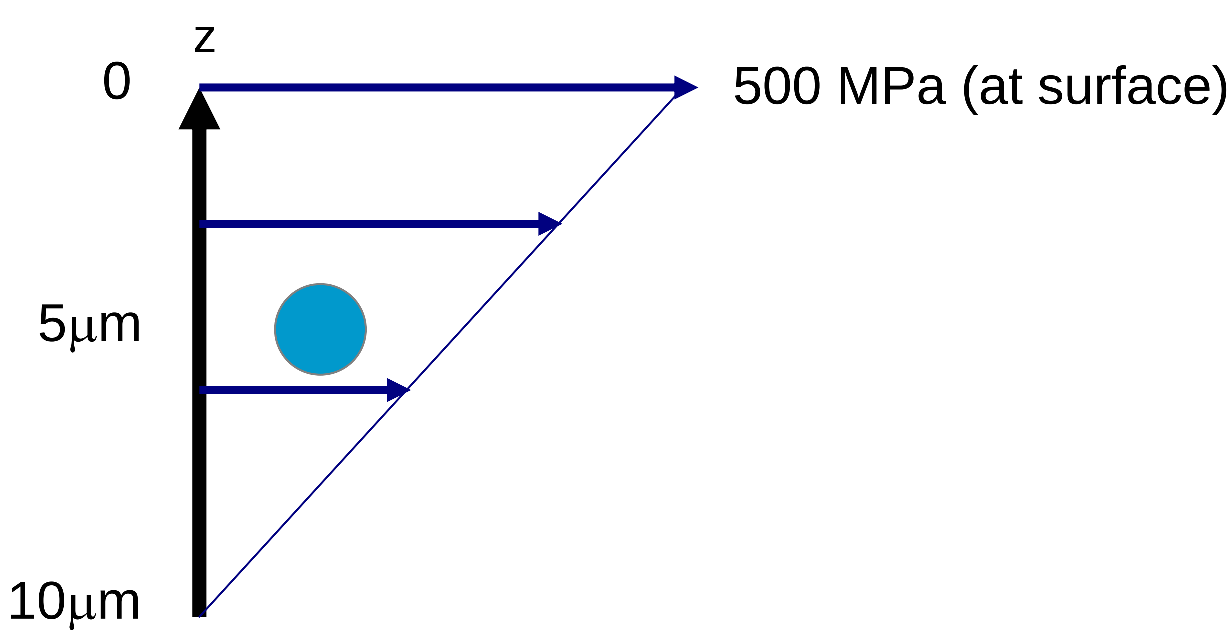
- **Super-large** bubbles bisect the surface, thus providing a probable explanation for surface deformation and large subsurface bubbles.

- A network of deep interconnecting surface pores is rapidly set up which results in drastic topographical changes of the surface

McHEROS with Stress Gradient

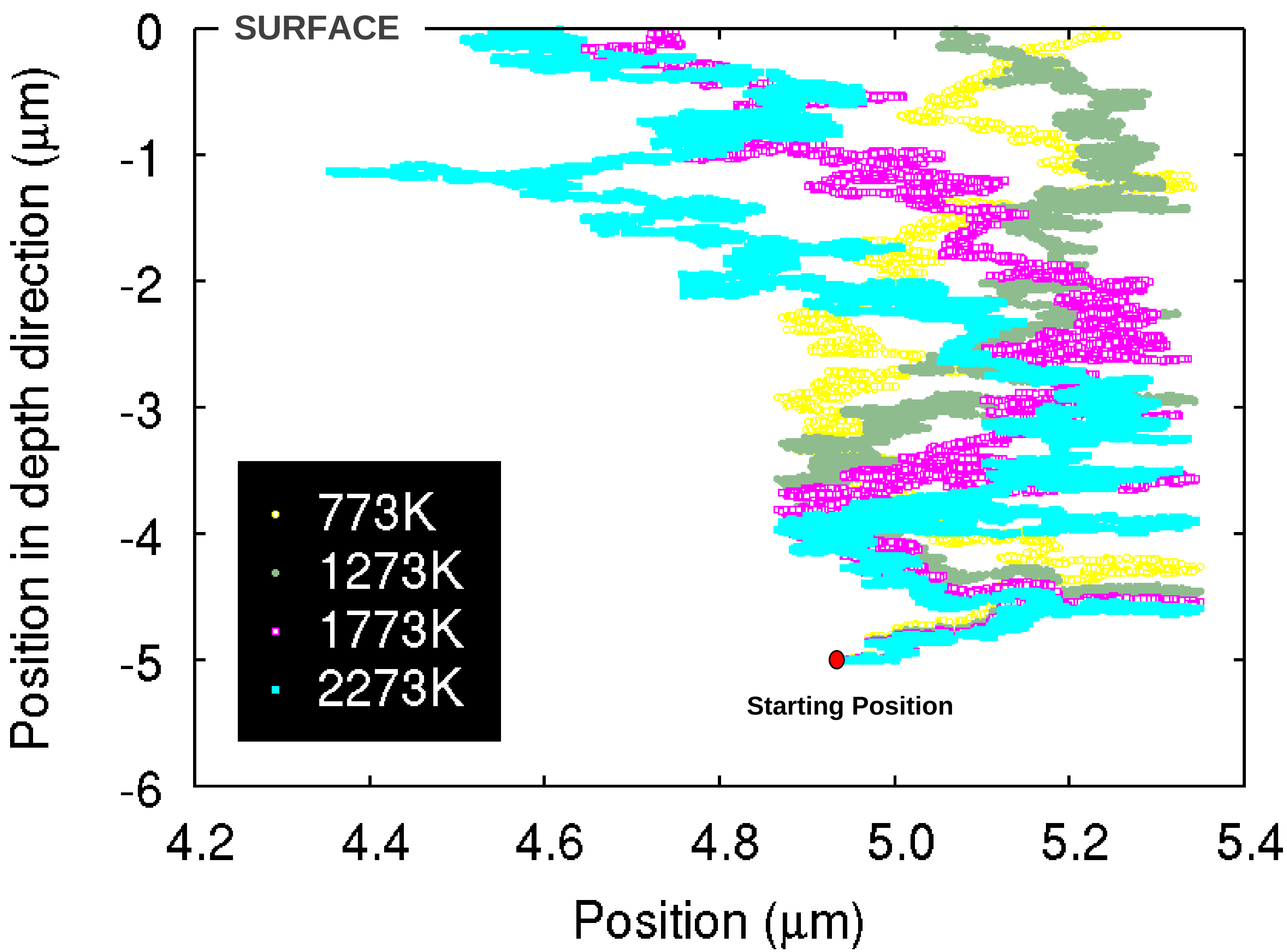
Numerical Example:

- Diffusion of single bubble
  - Radius: 10nm
- Stress gradient in depth direction



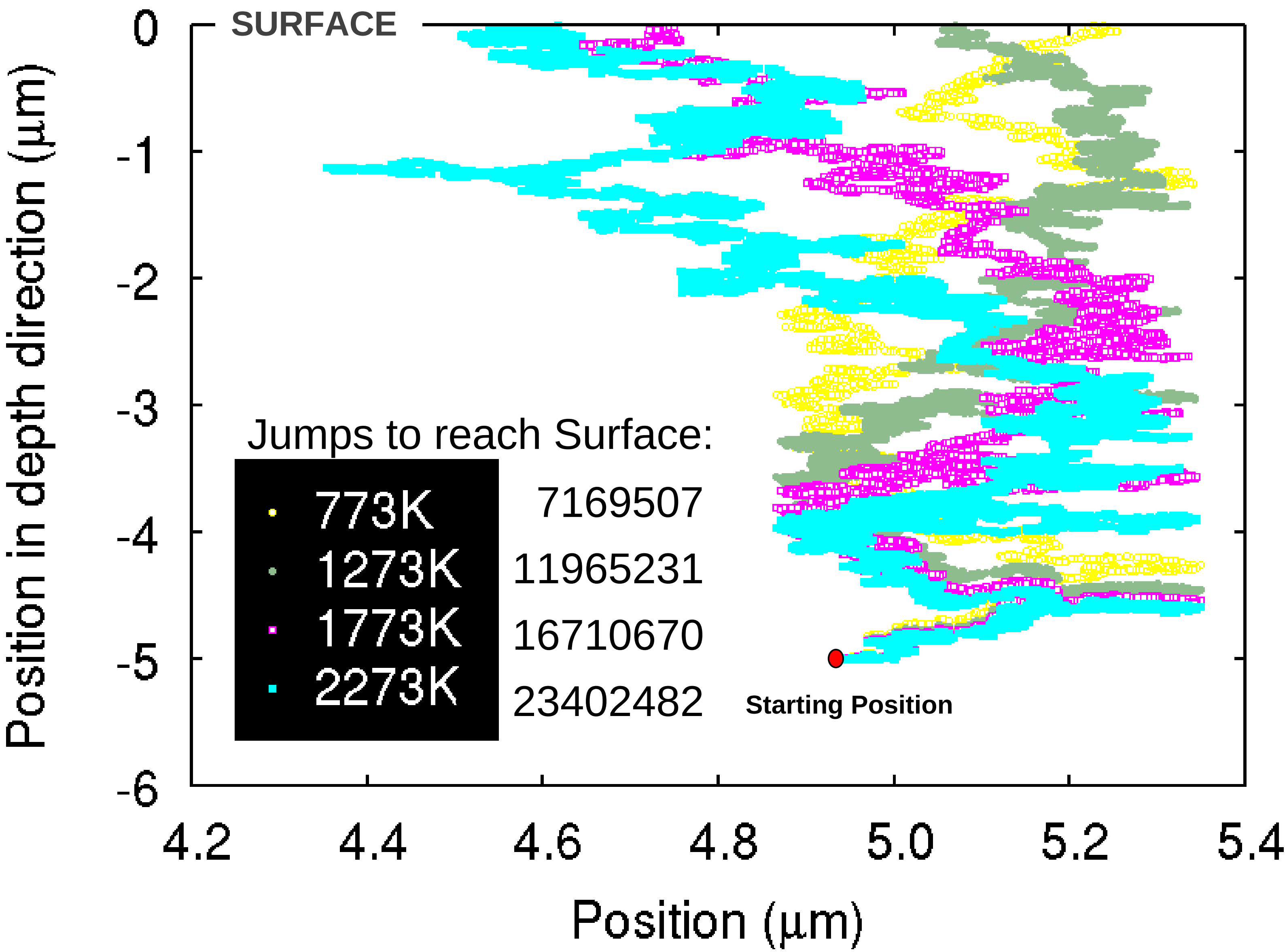
McHEROS with Stress Gradient

Tracking a single bubble in a stress gradient at various temperatures

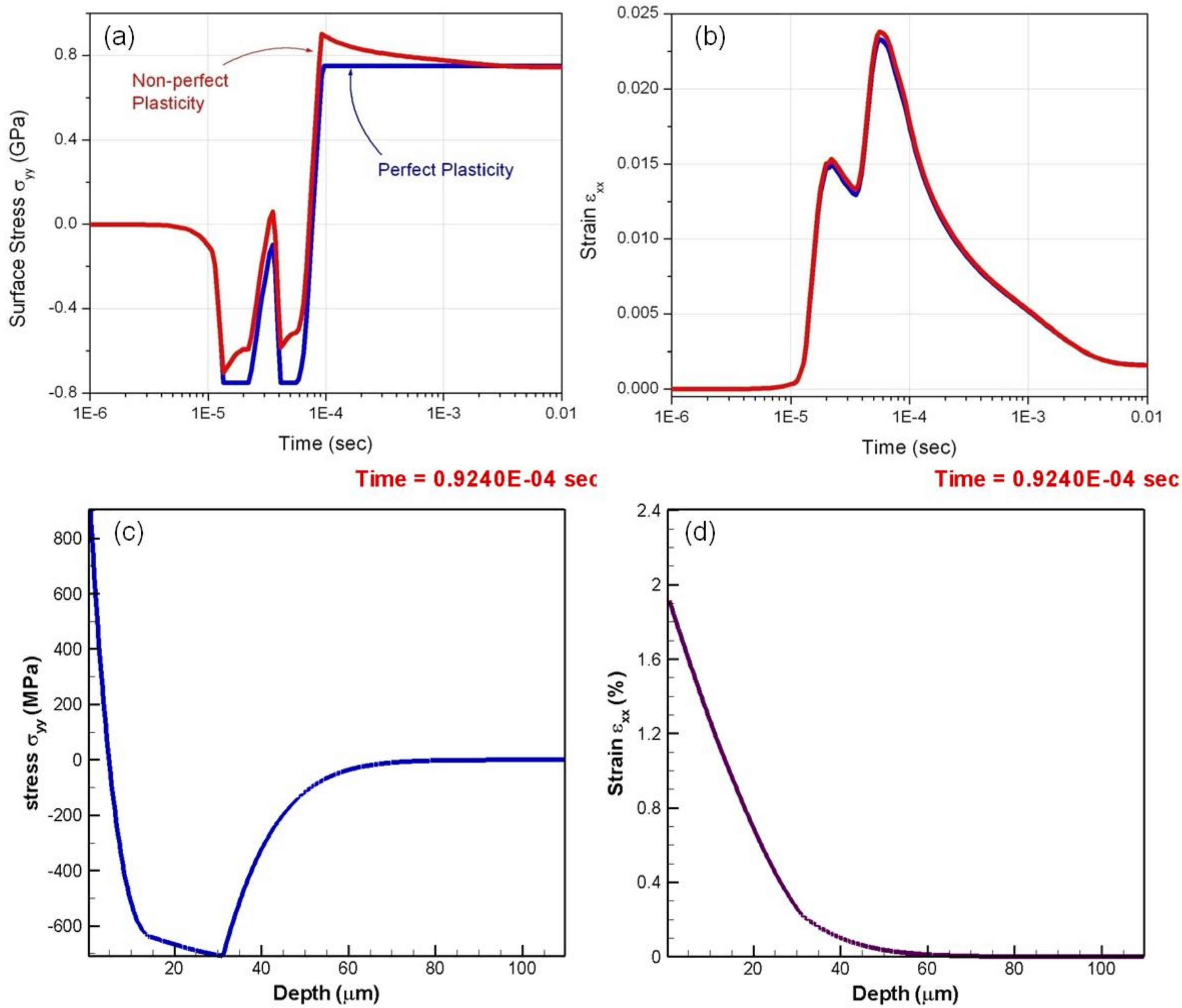


McHEROS with Stress Gradient

Tracking a single bubble in a stress gradient at various temperatures



Calculated Stress/Strain Transients in IFE FW



KMC – Calculation Procedure

Initialize Model

↓

Calculate diffusion probability of He-bubble

↓

Sum probabilities: Diffusion, Coalescence & Implantation for each He

↓

Examine one event (Diffusion of a bubble or Implantation)

↓

Jump with constant distance → Check **Coalescence**

Grow He-bubbles by implantation

↓

$t^{n+1} = t^{n} + \Delta t$

$$\Delta t = \frac{-\log R}{\sum_i P_i^{diff} + P^{imp}}$$

R: Uniform random number (0:1)

Diffusion Migration:

Surface diffusion rate

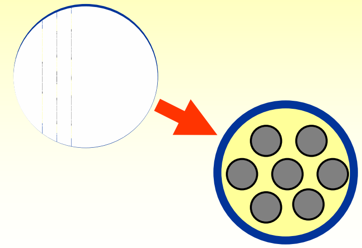
$$D_s = D_0 \exp\left(-\frac{E_s}{kT}\right)$$

Bubble diffusion rate

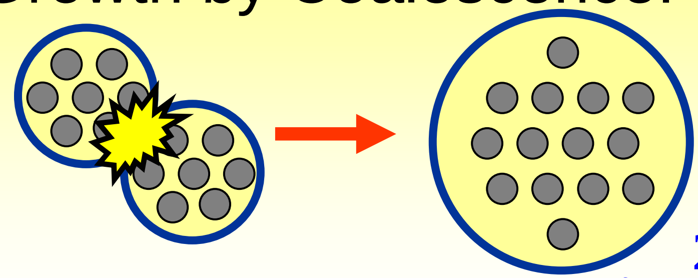
$$D_b = \left(\frac{3\,\Omega^{4/3}}{2\pi r^4}\right) D_s$$

E_s: Activation energy, 2.5eV*

D_0: Pre-expon 1.25×10^{-2} cm²/s

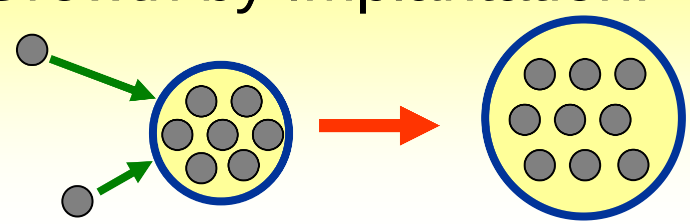


Growth by Coalescence:



Instantaneous Equilibrium Size: $p = \dfrac{2\gamma}{r}$

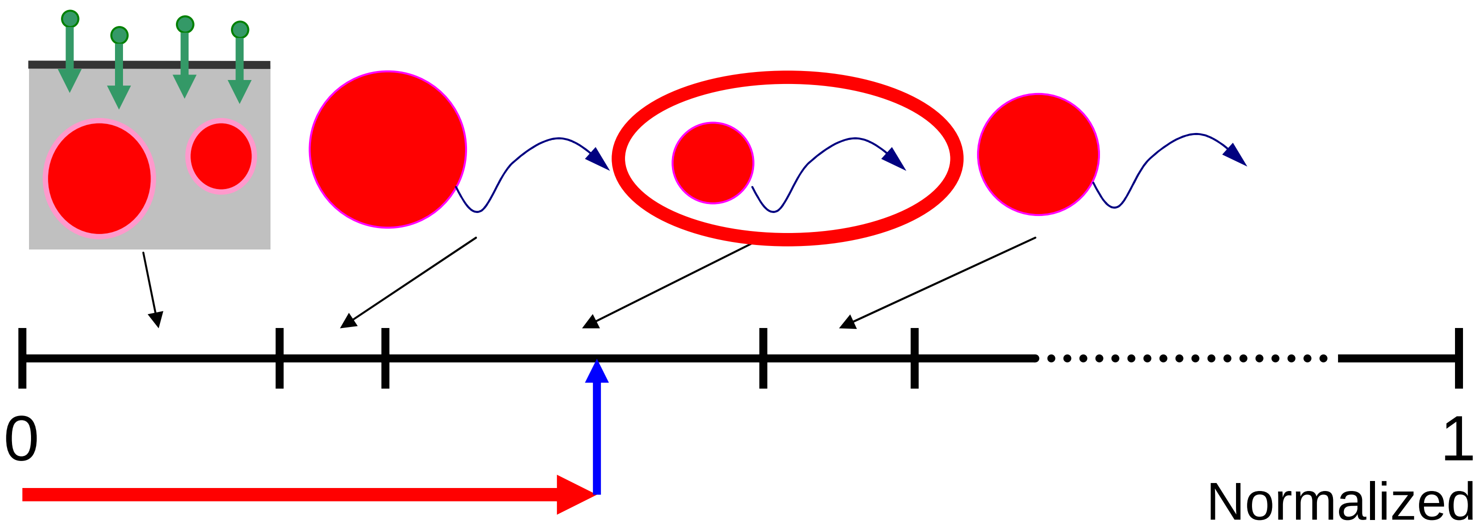
Growth by Implantation:



*A. Takahashi, TOFE 2006

Event Kinetic Monte Carlo

- **How to pick an event**
  - Using the event rate ν_i and uniform random number

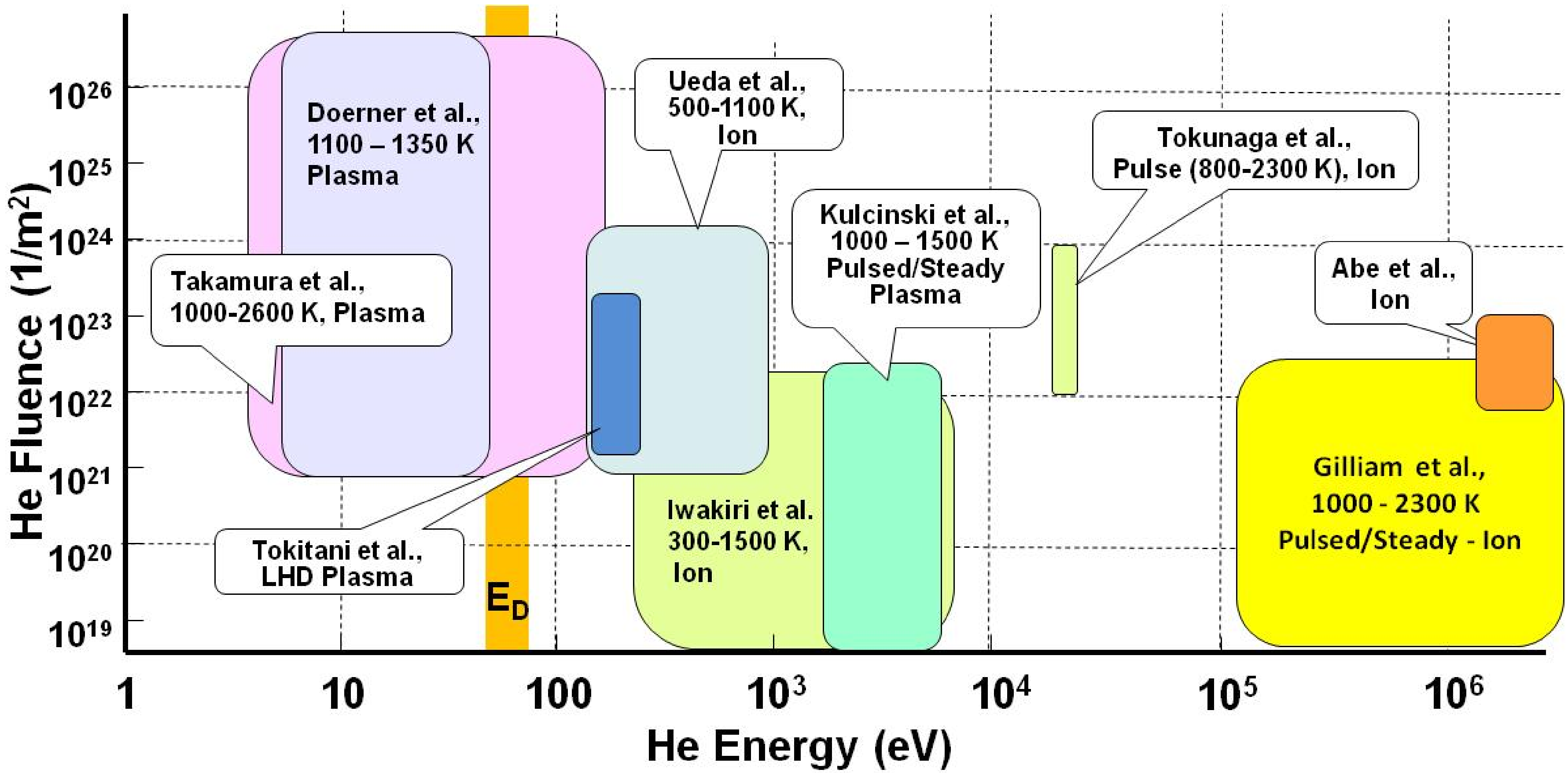


$$\frac{\nu_i}{\sum_j \nu_j}$$

- **Physical time calculation**

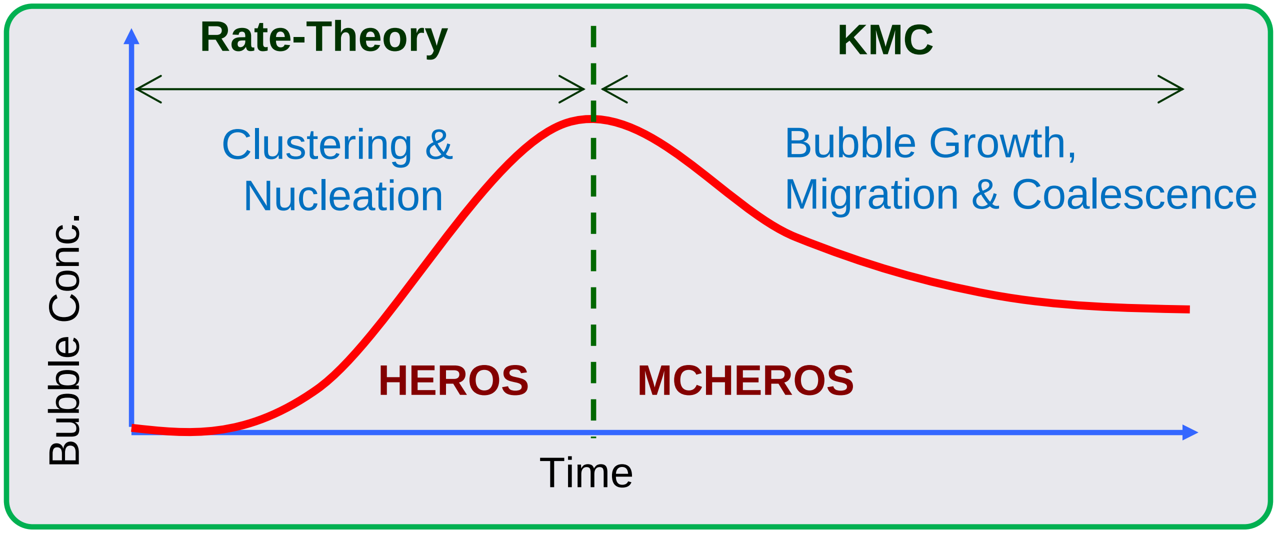
$$\Delta t = \frac{-\log R}{\sum_i \nu_i}$$

Summary of US and Japanese Experiments of He-Implantation in W



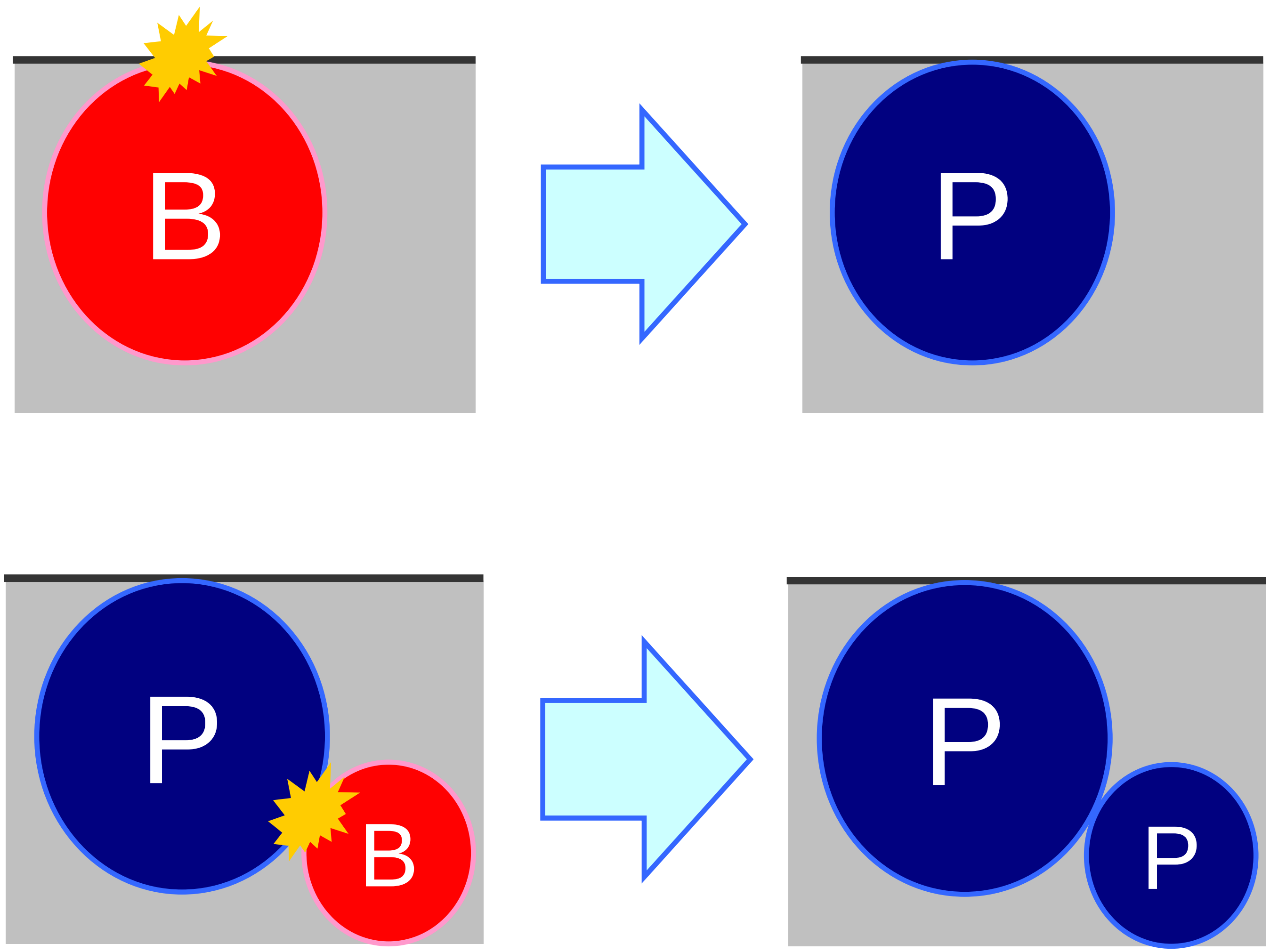
UCLA He-Transport Code Development

Hybrid Helium Transport Code



Code	Method	Phenomena	Comments
HEROS	Rate Theory	Nucleation, Growth, Transport	1-D; Unified Field Parameters in Bulk Material
McHEROS	Kinetic MC	Growth,Transport,Coalescence	3-D; Discrete bubbles; Material Geometric Features; Surfaces

Events (Surface pore formation)



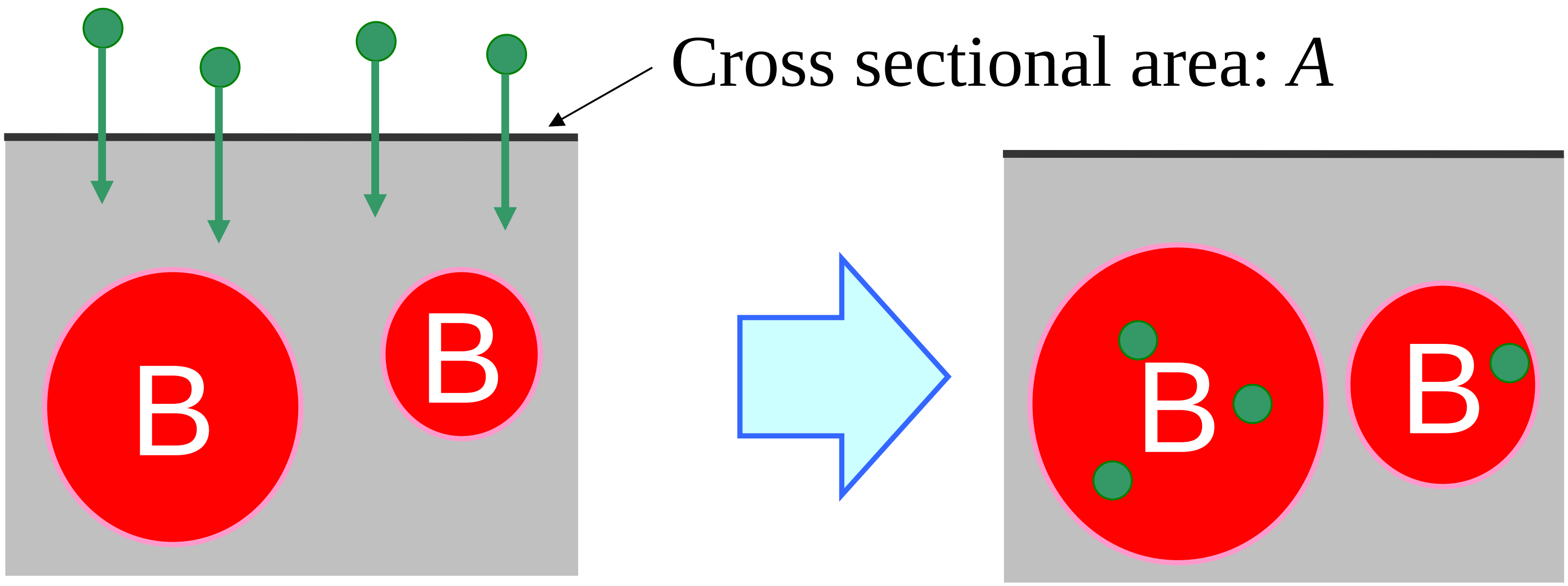
Surface pore is formed without coalescence

Events (Helium implantation)

- Helium implantation rate (= event rate)

$$\nu_{HeI} = \rho \times A$$

ρ: Implantation rate



- Helium bubbles capture implanted helium atoms
  - Linear relationship with the cross sectional area