Activities in Helium Transport, Carbon Diffusion, SiC/SiC Isochoric Heating, & SiC Properties Database

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OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

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Outline

Helium Modeling (**McHEROS**)

Carbon Diffusion Modeling

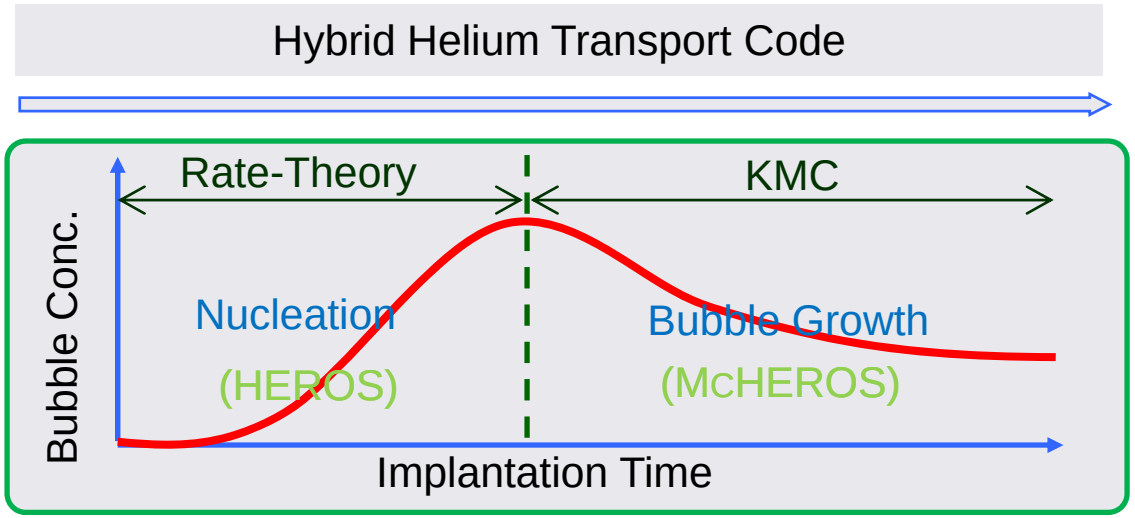
SiC Spallation Testing for Isochoric Heating

SiC Material Properties Database (**FusionNET©**)

Helium Transport Code Development

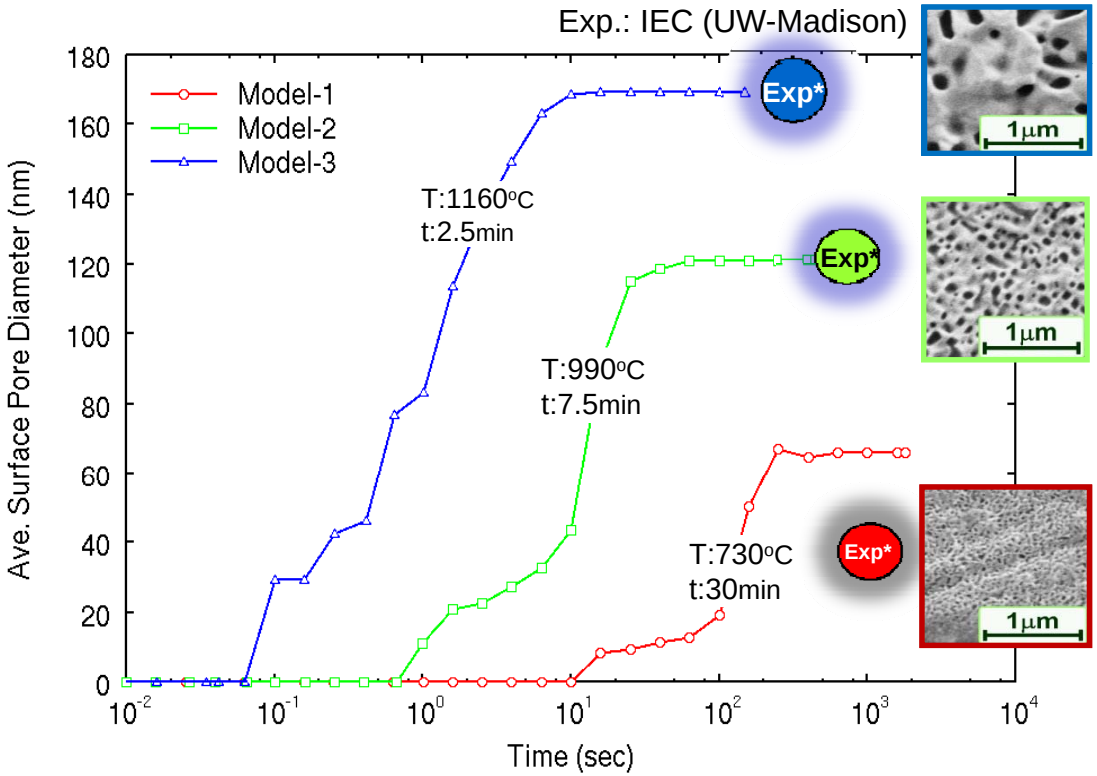
- Helium Transport requires Multiscale Modeling (atomic clusters → bubbles)
- Rate Theory uses unified field parameters
- KMC Simulation can model geometric features

Code	Method	Phenomena	Comments
HEROS	Rate Theory	Nucleation, Growth, Transport	2-D; Unified Field Parameters in Bulk Material
McHEROS	Kinetic **MC**	Growth, Transport	3-D; Discrete bubbles; Material Geometric Features; Surfaces



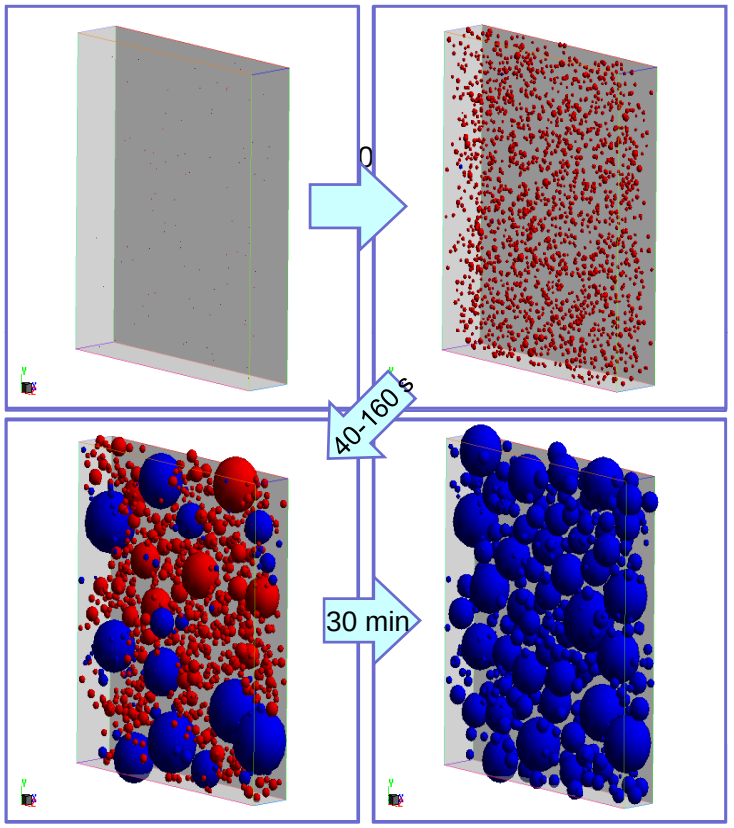
McHEROS Code Simulates IEC Surface Pores*

	Temperature (°C)	Implantation Rate (He/cm^2-s)	L_x (μm)	L_y (μm)	L_z (μm)
Model-1	730	2.2x10^{15}	0.2	1.0	1.0
Model-2	990	8.8x10^{15}	0.2	2.5	2.5
Model-3	1160	2.6x10^{16}	0.2	5.0	5.0



*A. Takahashi et al., TOFE Albuquerque, NM, 2006

2.2x10^{15} He/cm^2-s; 730 °C; t:30min (IEC)

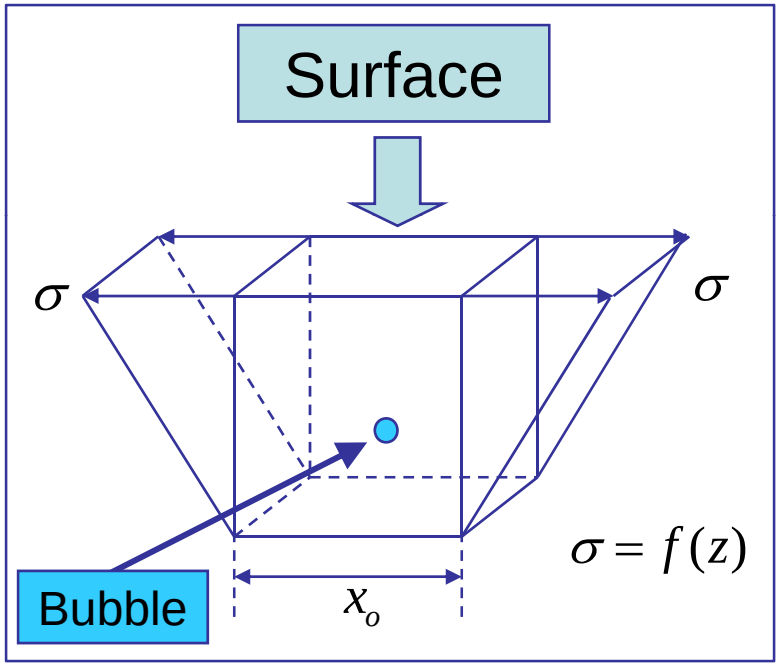


McHEROS Results:

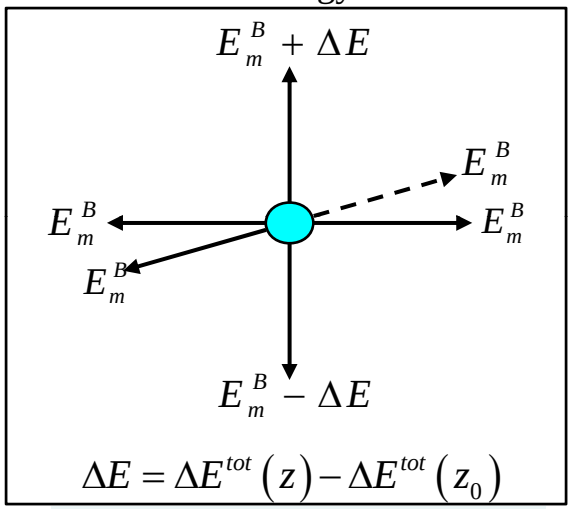
- **Good Agreement between McHEROS Simulation and Experiment**
- **McHEROS provides an *EXPLANATION* for the oversized Surface Pores**

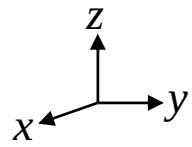
McHEROS Code Upgrade

- McHEROS Code now includes the effect of **stress gradients**.
- Stress gradients act as a driving force (F_p) on bubbles (strain energy): Bubbles move up the stress gradient



"Delta-Energy Rule"





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

v_p: Bubble volume
δ: Jump distance
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

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

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

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

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

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

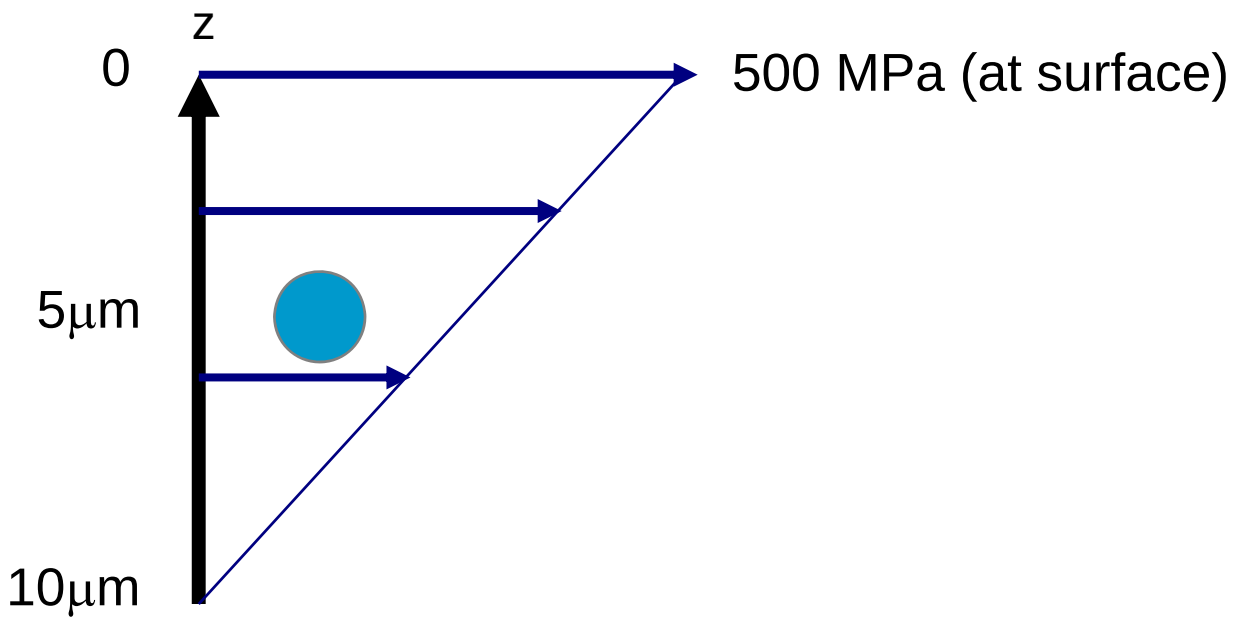
I. The net migration energy (E^{eff}_m) of the bubble due to a stress-field can be calculated using the bubble diffusion coefficient (D^{eff}_p).

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

McHEROS with Stress Gradient

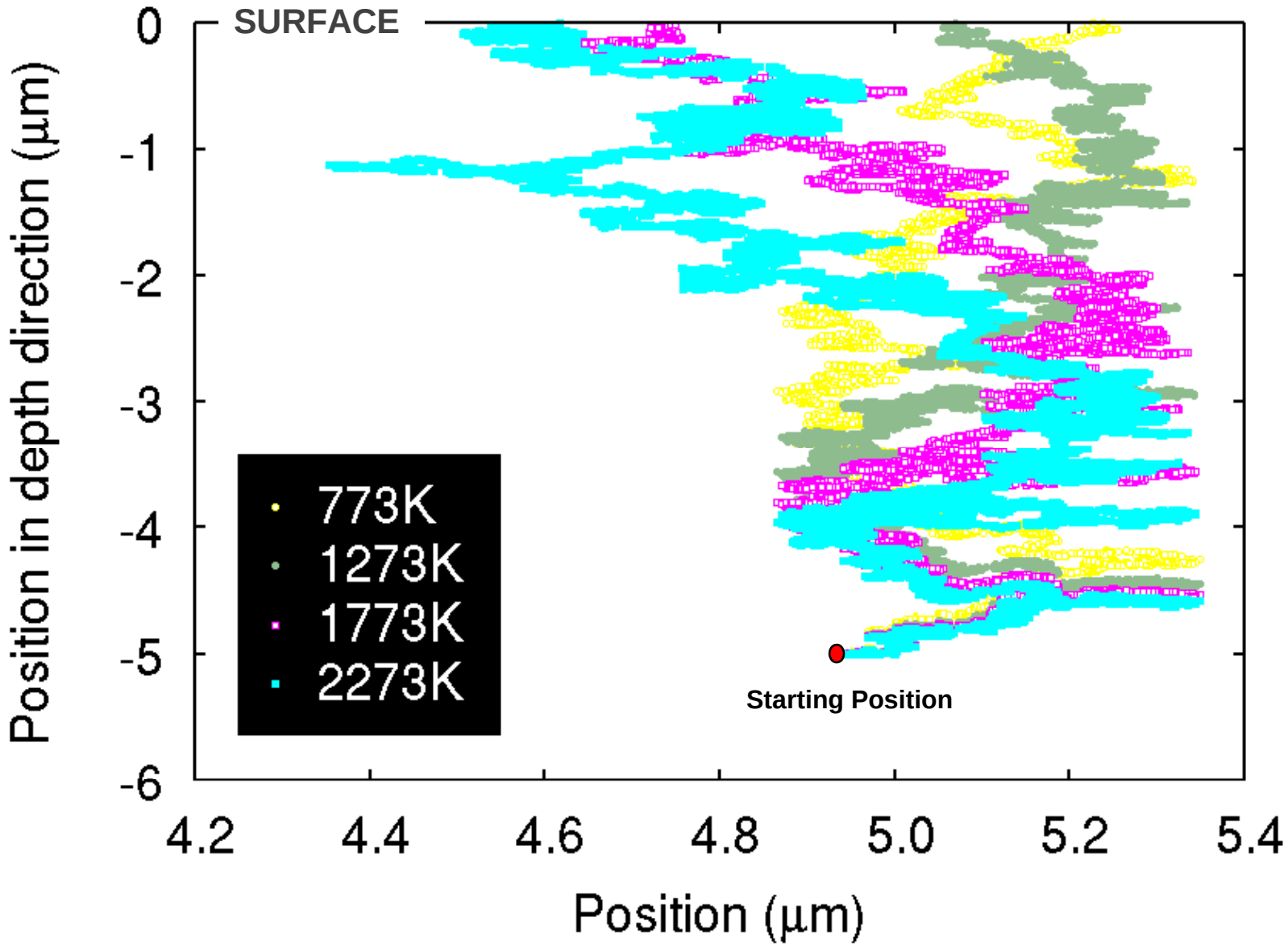
Numerical Example:

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



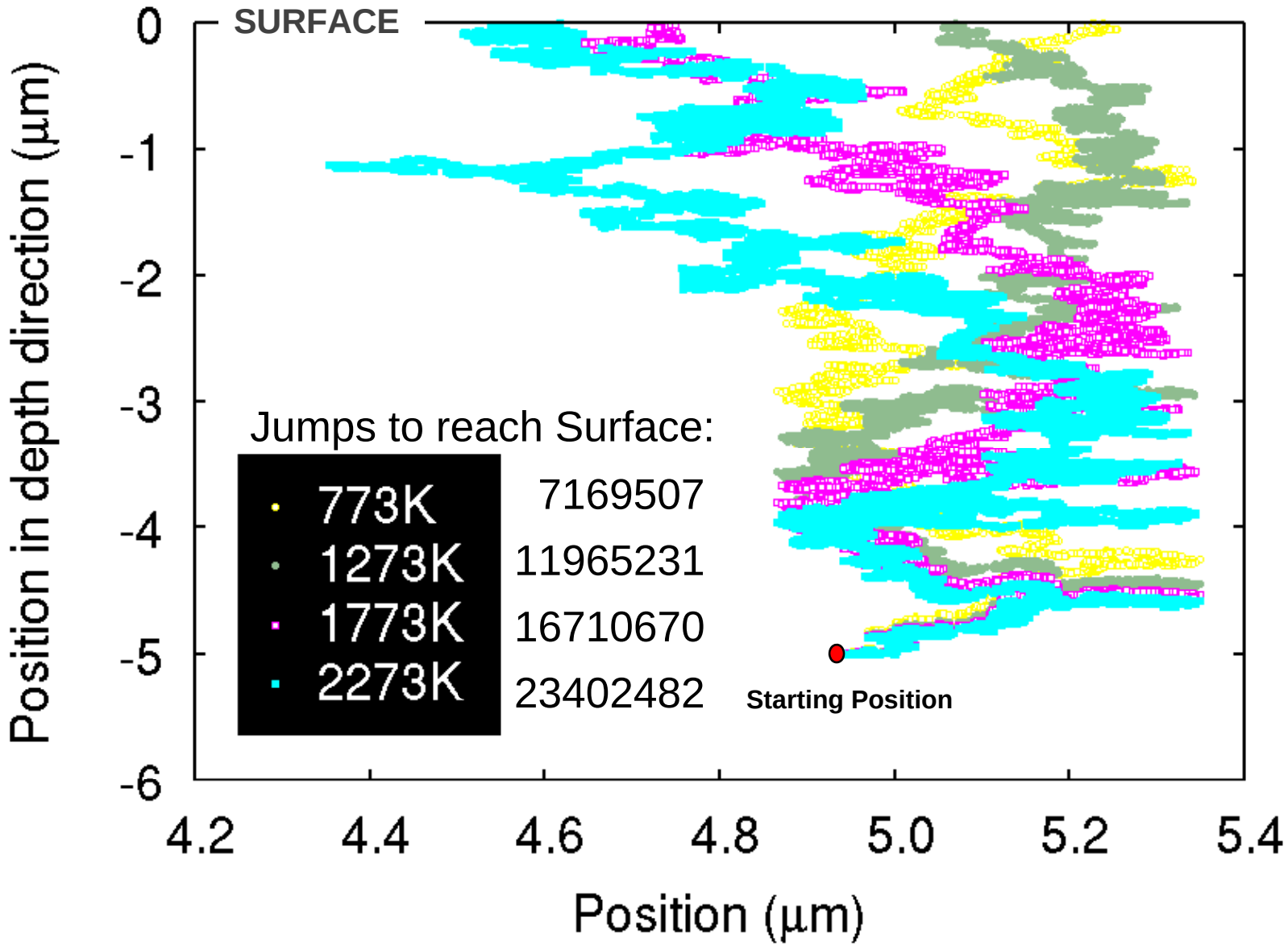
McHEROS with Stress Gradient

Tracking a single bubble in a stress gradient at various temperatures



McHEROS with Stress Gradient

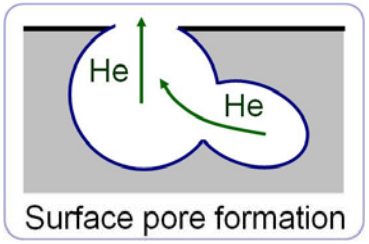
Tracking a single bubble in a stress gradient at various temperatures



Planned Activities

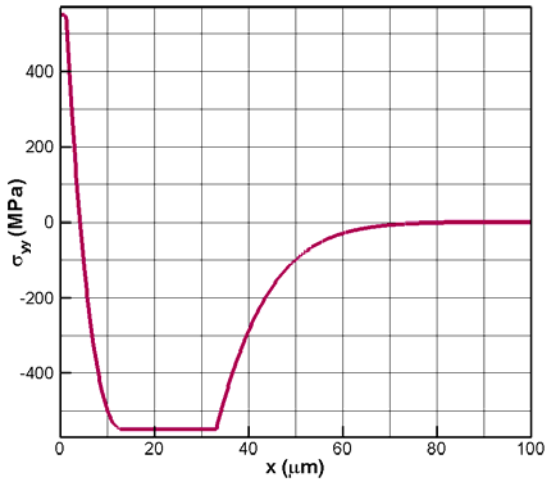
- Near Term:
  - Superimpose **near-surface** strain field gradient
  - Simulate Bubble Migration/Coalescence (MC) for HAPL **transient stress gradient**.
  - Add temperature field to MCHEROS Code
  - Simulate **transient temperature gradient** effect on bubble MC

- Long Term:

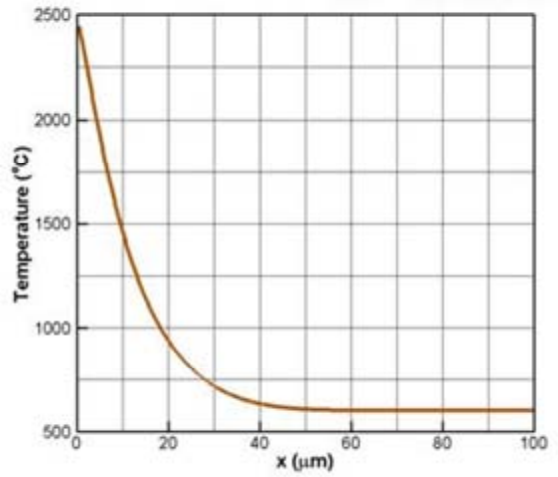


  - Add Near-surface **Bubble- Threading**
  - Include 3-D **Grain Structure** Features
  - Add HEROS-based **Bubble Nucleation** (Rate Theory Eqs.) to MCHEROS

Stress σ(x,t): Time = 0.4281E-05 sec



Temp. T(x,t): Time = 0.2760E-05 sec



Outline

Helium Modeling (**HEROS – McHEROS**)

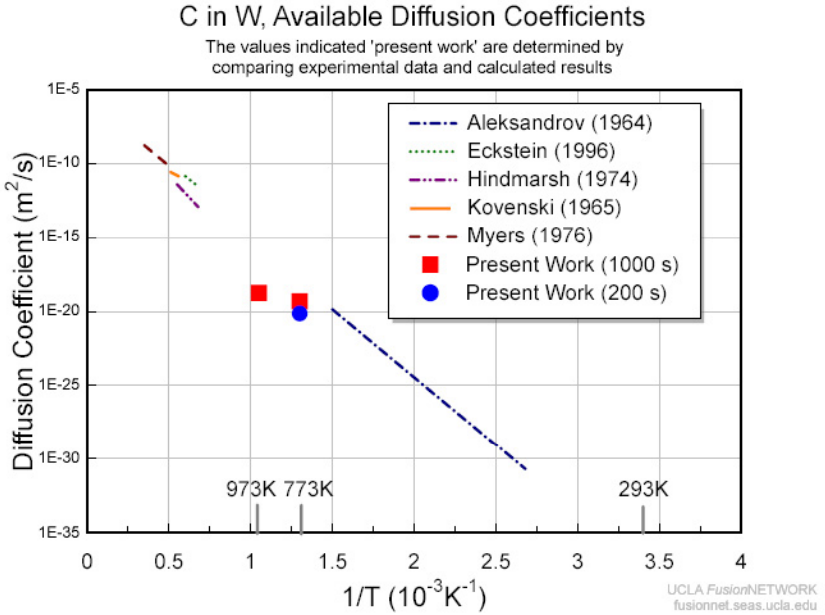
Carbon Diffusion Modeling

SiC Spallation Testing for Isochoric Heating

SiC Material Properties Database (**FusionNET©**)

Carbon Diffusion in Tungsten

- Previous modeling of Carbon diffusion assumed homogeneous W- material; no Grain Boundary (GB).
- Experiments show C concentrating along GB (16th HAPL, UNC)
- Need to account for fast diffusion along GBs
- Geometric features requires 3-D diffusion modeling



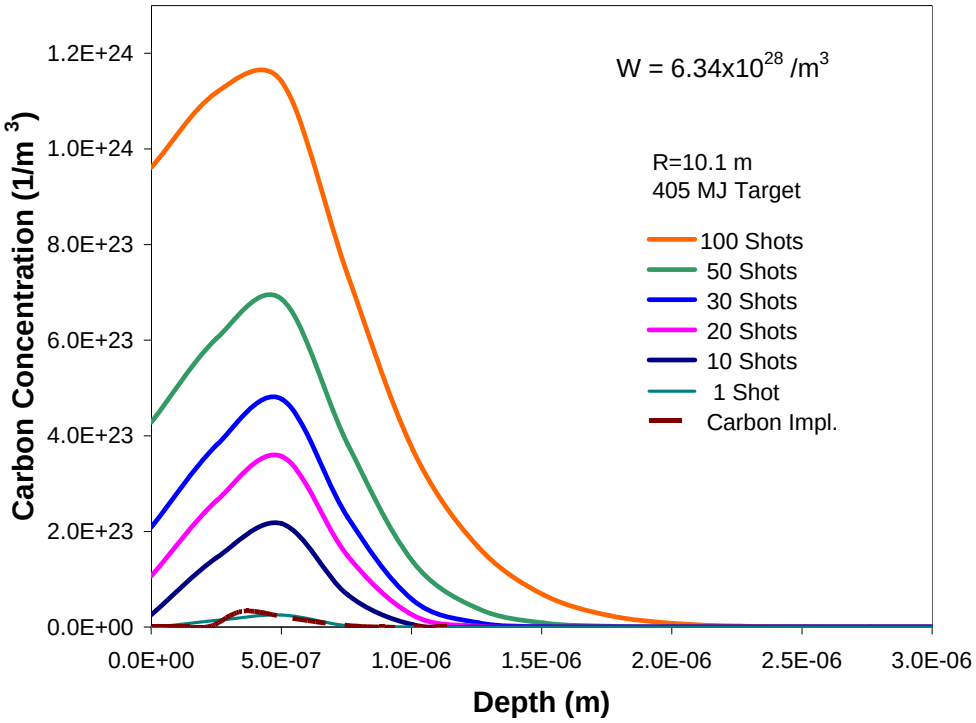
$$\frac{\partial C}{\partial t} = D(T)\nabla^2 C + R$$

where D_0: pre-exponential
R : reaction
Q: activation energy

$$D(T) = D_0 \exp\left(-\frac{Q}{kT}\right)$$

Typical Diffusion Length:

$$L = \sqrt{D\,t}$$

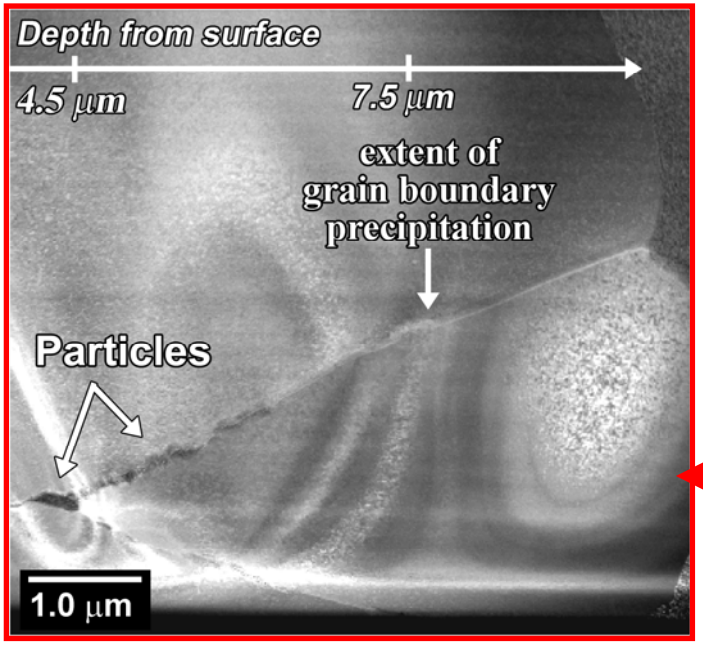


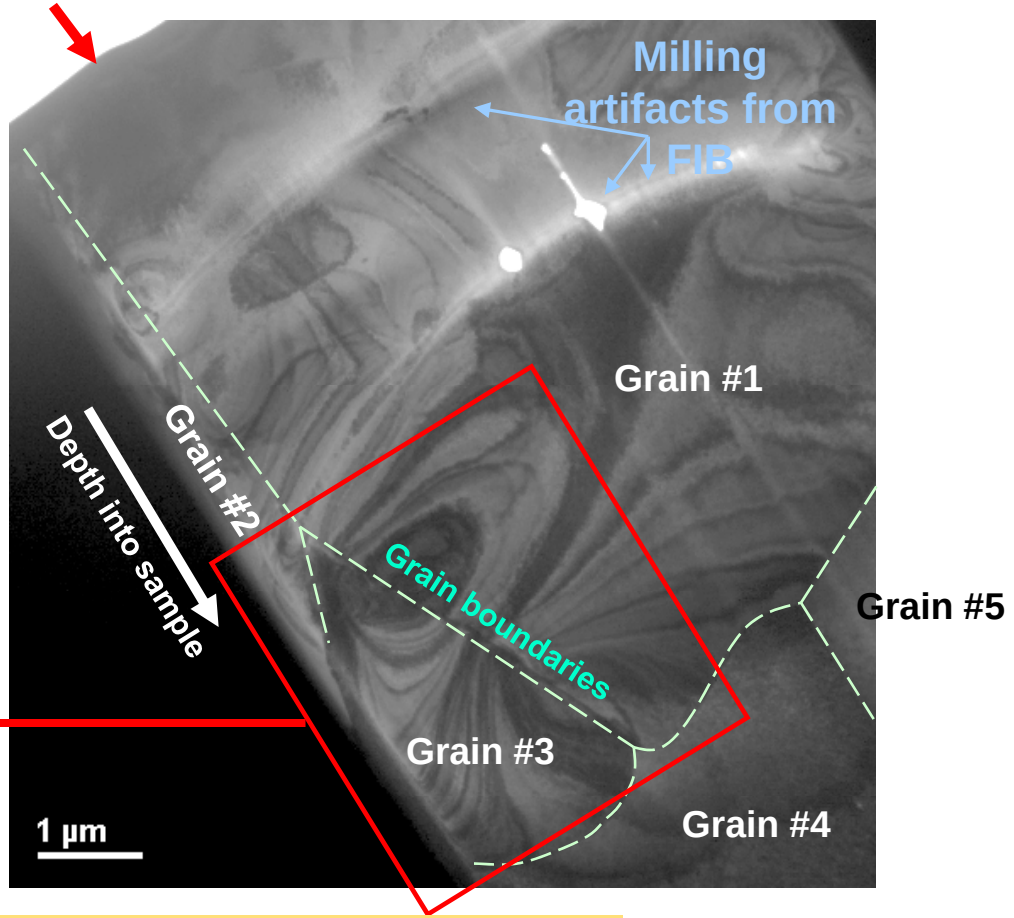
Carbon Implantation in Tungsten*

Step 1:
- Carbon implantation
- Polycrystalline W
- 1.4×10^{19} cm^{-2}
- Room temperature

Particles observed along grain boundaries.
- **Observed to a depth of 7.6 μm from surface.**

Step 2:
- Thermal anneal
- Electrical resistance heating
- 2000ºC; 5 minutes

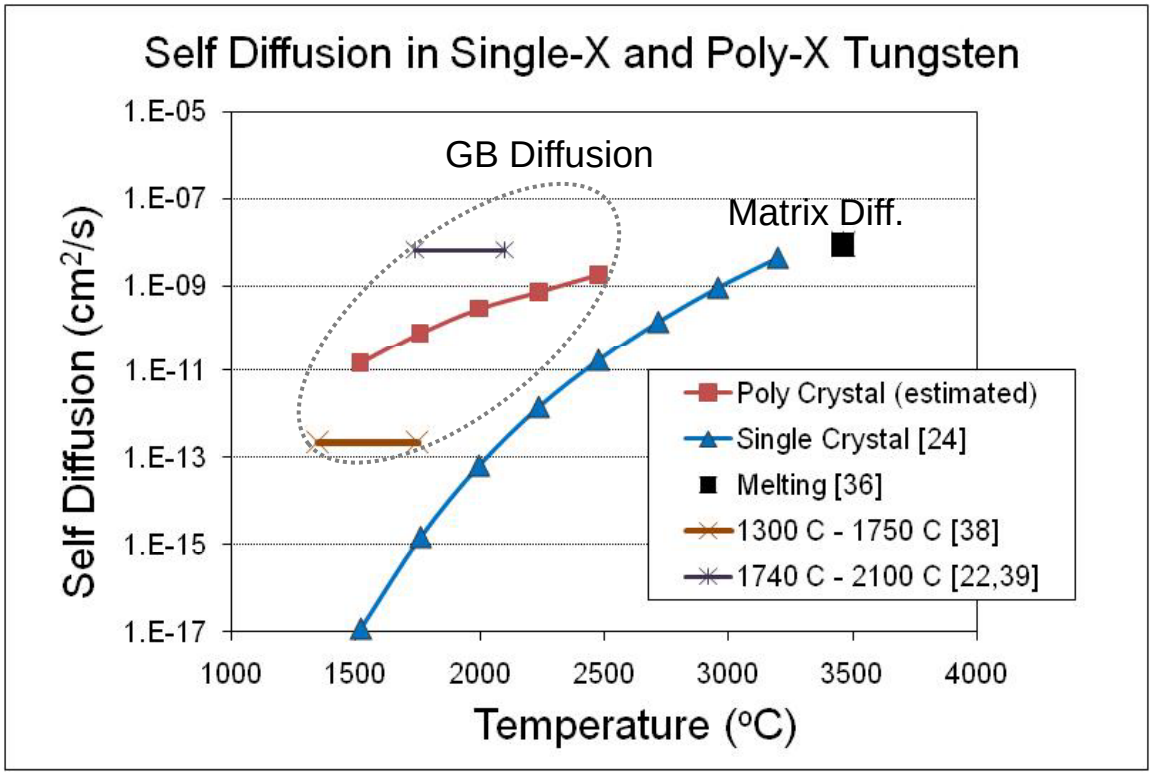




*UNC (presented at 16th HAPL, L.L.Snead)

Diffusion along GB in Tungsten

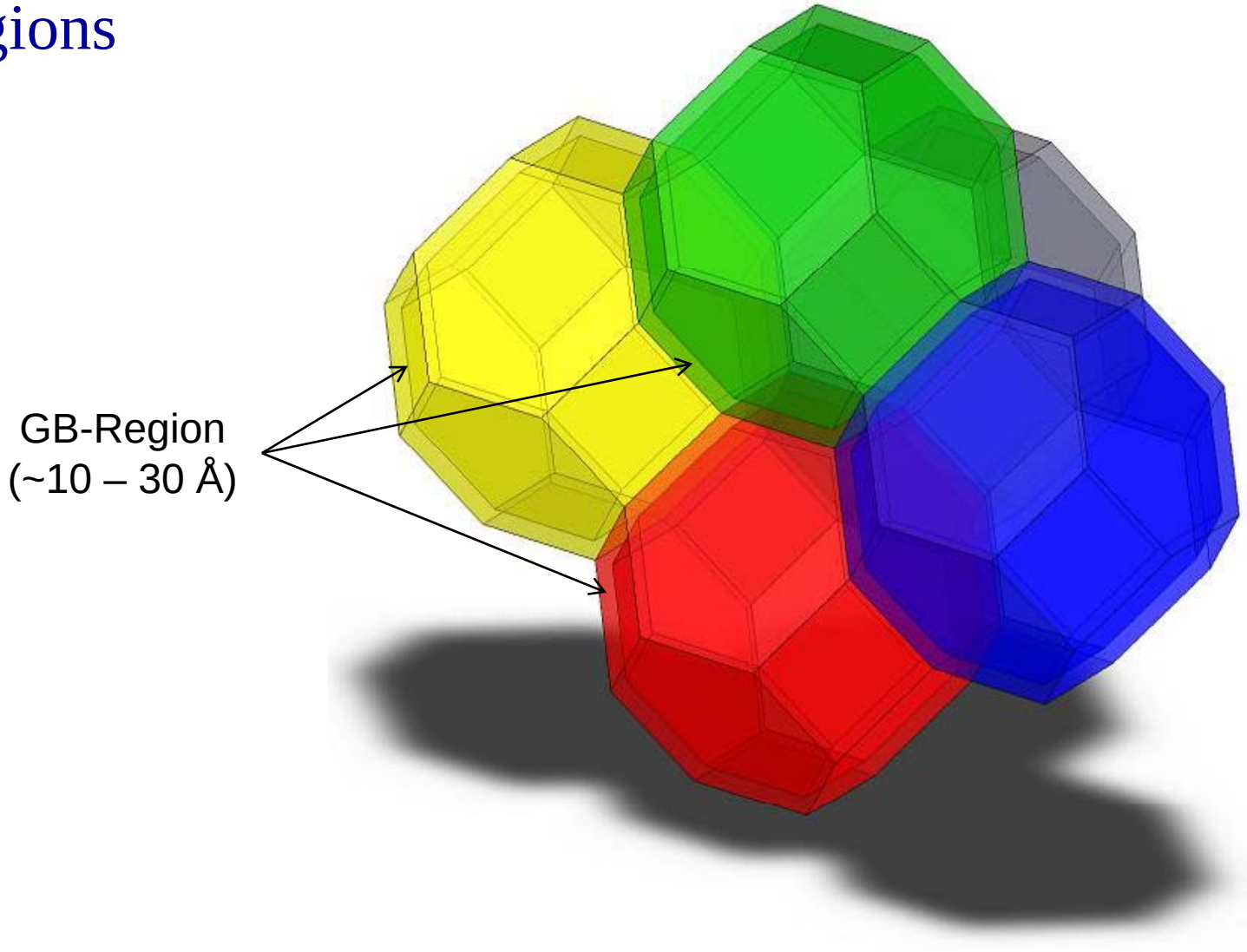
- GB Diffusion is the dominant diffusion mechanism in POLYCRYSTALLINE tungsten below 2100 C
- Self diffusion in GB is 3– 4 orders of magnitude faster than in matrix



- Similarly, C-diffusion is also faster in GB compared with matrix.

3-D Grain Model

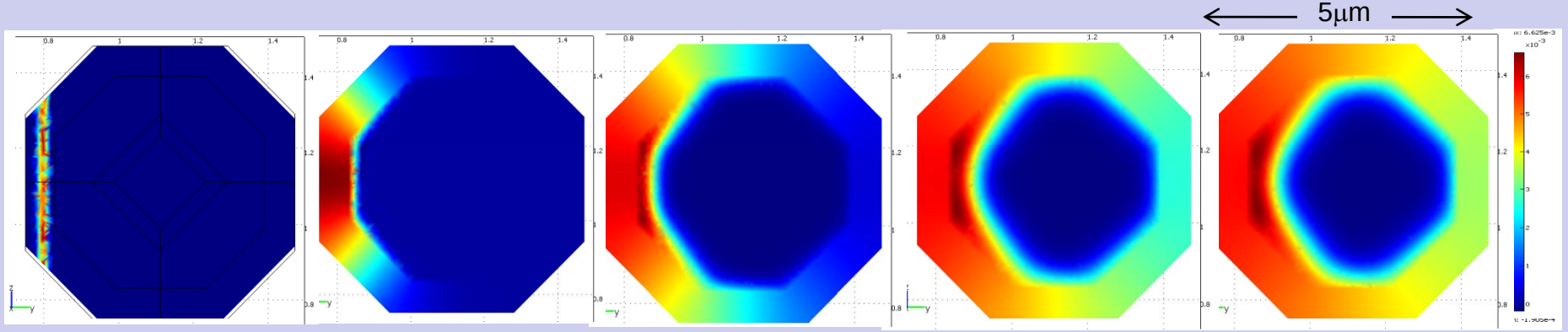
- A 3-D Grain Structure Model with **Grain Boundary** (**GB**) regions



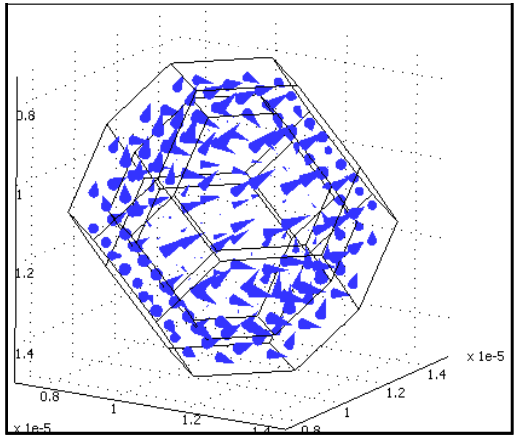
Initial Results of 3-D Carbon Diffusion Model

- Assigned higher diffusion coefficient (× 100) to GB-region
- Single crystal shows rapid diffusion along GB.

MIDPLANE: Time sequence of 3-D Carbon–Diffusion (T = 2000 ºC) through a W-Crystals



Diffusive Flux, C[mol/(m^2-s)]



- Planned Activities:
  - Calibrate Diff. coeff. with UNC experiments
  - Create realistic Tungsten Multi-Grain Model.
  - Add strain-gradient effect on C-diffusion
  - Model WC_2 formation and add to C-Diff.
  - Simulate HAPL conditions (T-gradients)

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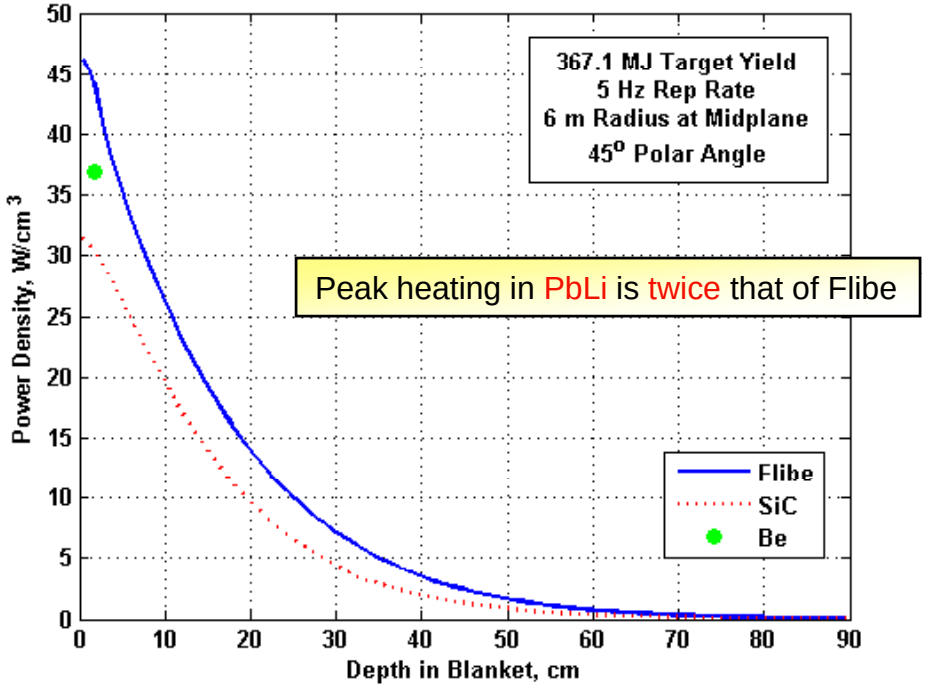
Isochoric Heating Conditions

Blanket Nuclear Heating*:



At 5 Hz:

- Peak power density in PbLi is ~92 W/cm^3
- Peak power density in SiC is 31 W/cm^3

M. Sawan, 16th HAPL, Dec. 2006

SiC/SiC Tube filled with PbLi

- Volumetric Energy per shot:
  PbLi: 18.4 MJ/m^3
  SiC : 6.2 MJ/m^3
- Isochoric heating results in rapid expansion of SiC and PbLi

- Integrity of SiC/SiC is a concern

Pressure Due to Isochoric Heating

- Pressure (p):

$$p = \gamma \frac{E}{V}$$

E: Energy; V: Volume;

γ is the Gruneisen constant: (thermal expansion coefficient multiplied by the volume divided by the heat capacity and compressibility):

$$\gamma = \frac{\alpha v}{C_p \kappa_s}$$

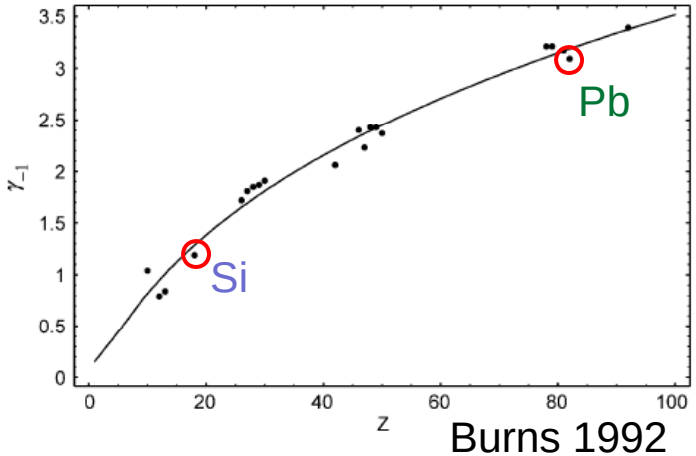
γ_{SiC} ~ 0.9 (<1000 K)

γ_{Pb} ~ 3.1 (RT)

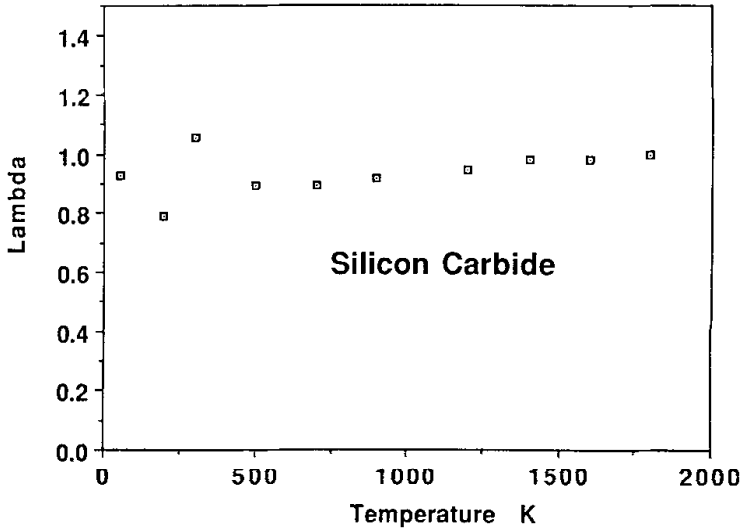
γ_{Li} ~ 0.3 (RT)

γ_{PbLi} ~ 2.6 (RT)

Gruneisen Parameter



Burns 1992



Burakovsky 2004

Pressure Due to Isochoric Heating

Material	γ	E/V (MJ/m^3)	P (MPa)
PbLi	2.6	18.4	48.3
SiC	1	6.2	6.2

- Ignoring isochoric heating in SiC: ~50 MPa pressure is applied to the inside wall of the coolant channel within a Δt~ 10 ns
- Concerned about impulse loading of SiC/SiC
- SiC/SiC – PbLi Interface: CVD SiC layer (~1 mm)
- Matrix cracking strength ~120 MPa for SiC/SiC

Planned Activities:

- Perform **Spallation Experiment** to test impact of nanosecond pressure pulses **(1) CVD SiC** [for calibration] and **(2) SiC/SiC samples**
- Expose 1-mm thick CVD SiC to: 50, 100, 150, and 200 MPa (~ 10 ns)
- CVD-SiC Samples are being prepared for experiment

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Carbon Diffusion Modeling

SiC Spallation Testing for Isochoric Heating

SiC Material Properties Database (FusionNET©)

SiC Material Properties Database

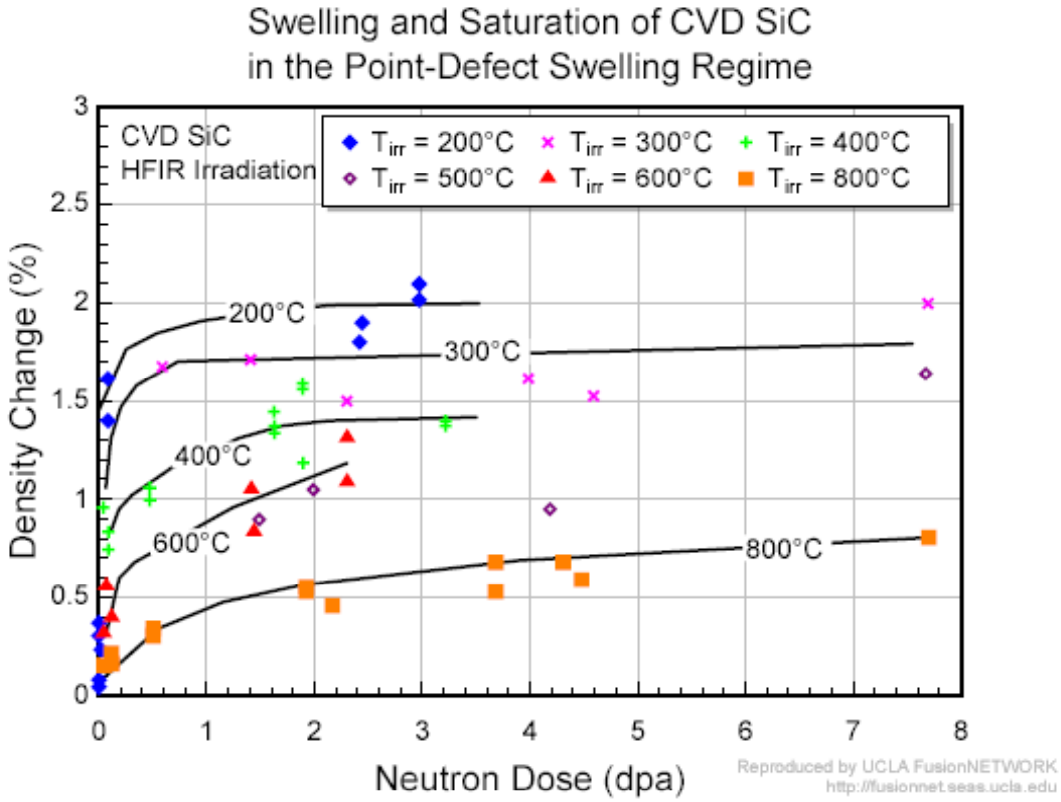
FusionNET© is an Interactive Web-based Fusion Material Properties Database

- Currently being maintained with help from two students:
  Evelyn Zarraga and Sandy Chow
- http://fusionNET.seas.ucla.edu or http://fusionet.seas.ucla.edu
- Best viewed using **IE-browser** due to lack of "Scalable Vector Graphics" (SVG) support by Mozilla,
- In support of HAPL, FusionNET© is reproducing data from the SiC-Handbook (ORNL)

- Keeping with the tradition of FusionNET© the SiC data contains all of FusionNET's features, e.g.:
  - Scalable Vector Graphics
  - Down-loadable Tabulated Data
  - Computable Correlations
  - References

Sample of FusionNET© SiC Data

http://fusionnet.seas.ucla.edu - Data Summary - Microsoft Internet Explorer



CAPTION: Swelling and Saturation of CVD SiC in the Point-Defect Swelling Regime (linear plot)
Author: Snead, L.L., T. Nozawa, Y. Katoh, T-S. Byun, S. Kondo, D.A. Petti,
Title: Handbook of SiC Properties for Fuel Performance Modeling
Journal: Journal of Nuclear Materials, 2007, Volume 371, Page 329-377

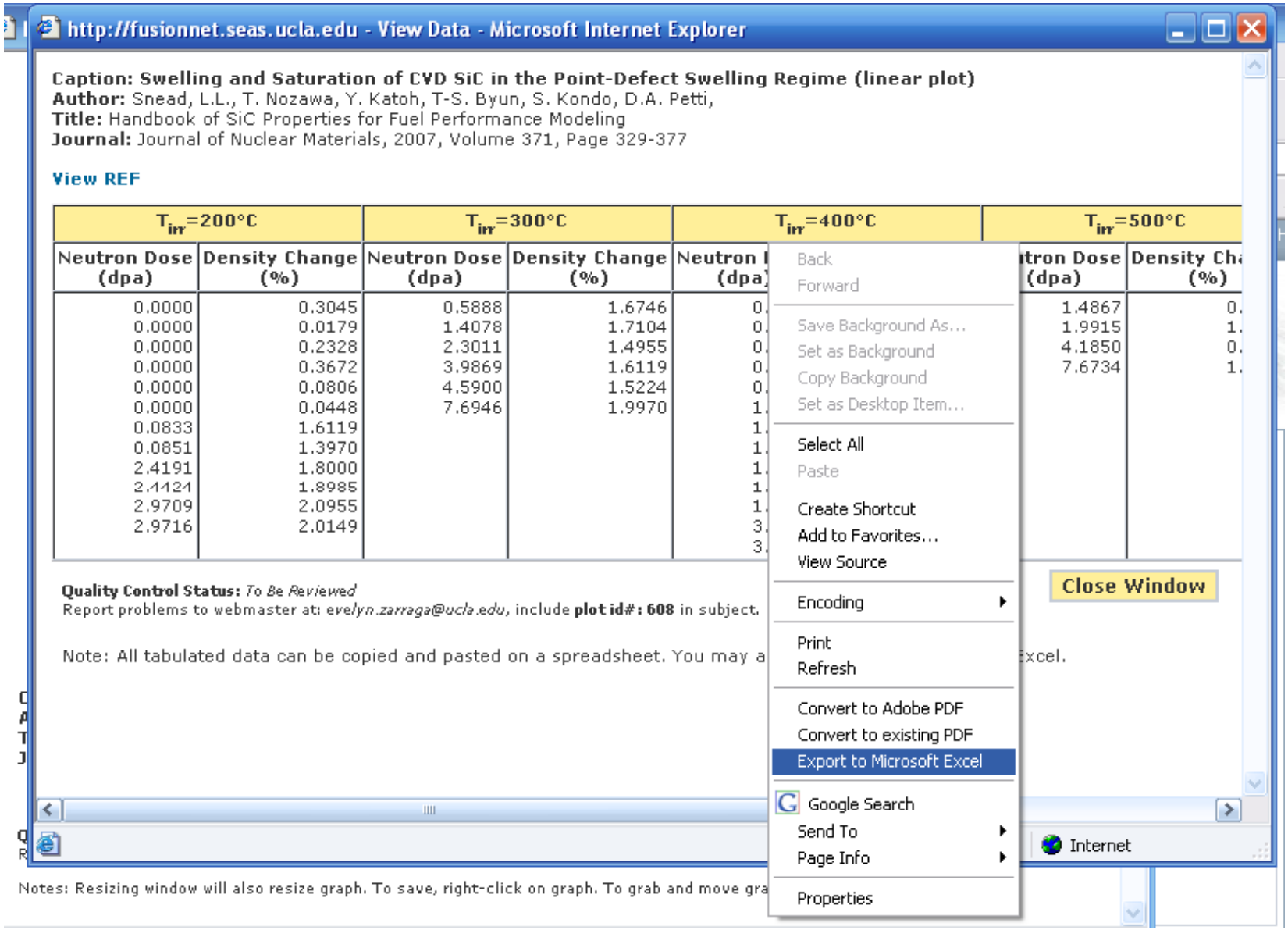
View REF | **View Data** | Print page | Close Window

Quality Control Status: *To Be Reviewed*
Report problems to webmaster at: *evelyn.zarraga@ucla.edu*, include **plot id#: 608** in subject.

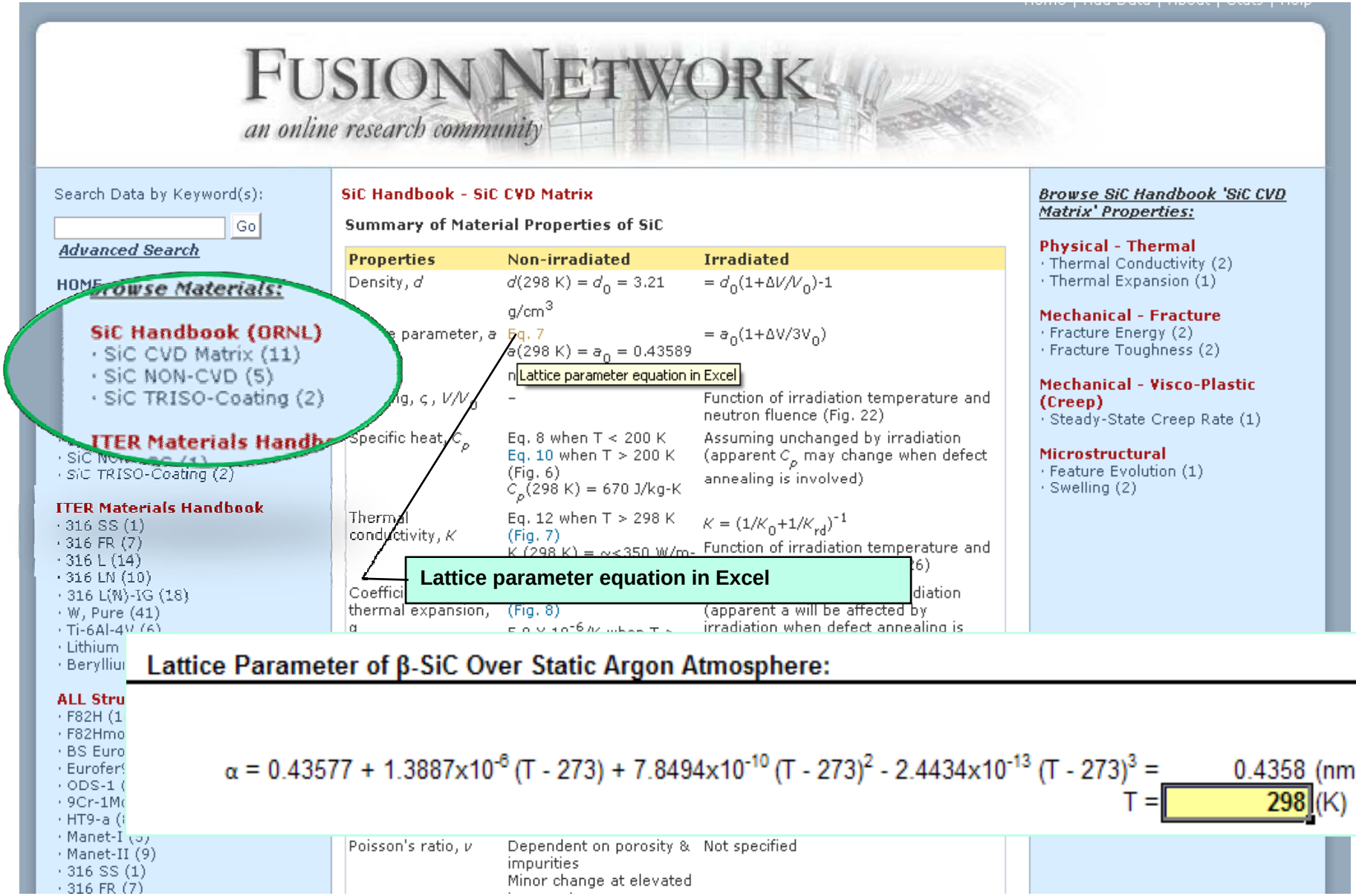
Notes: Resizing window will also resize graph. To save, right-click on graph. To grab and move graph while zoomed in, Hold Alt.

Done | Internet

Sample of FusionNET© SiC Data



Sample of FusionNET© SiC Data



FusionNET© SiC Database

Planned Activities:

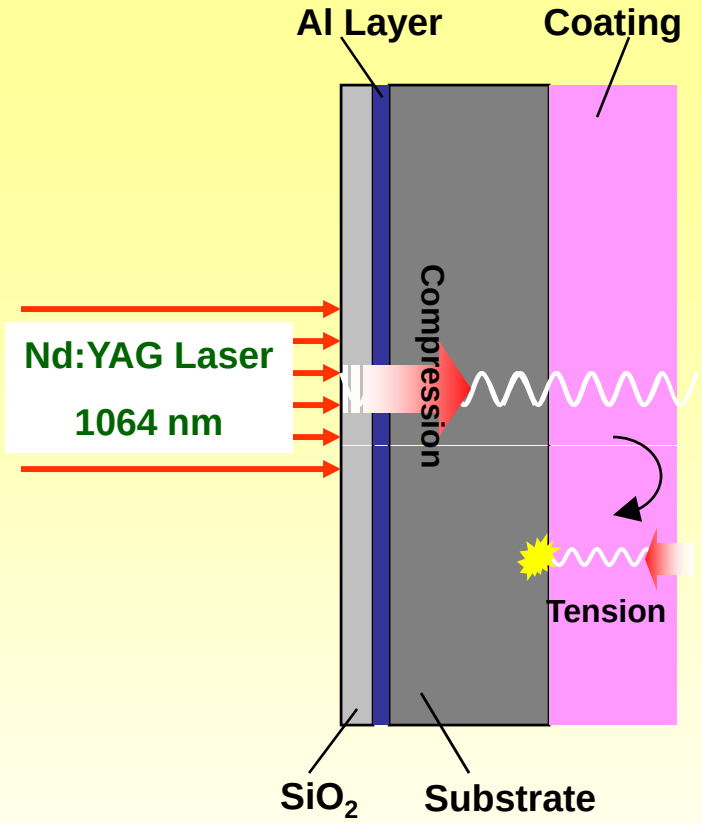
- Complete reproducing all 35 graphs (have completed ~1/2)
- Add 4 more Tables of property summaries (completed 1)
- Hyperlink all entities in Tables (Figures and Equations) to FusionNET entities.

Summary

- Helium Modeling (MCHEROS):
  Stress- & Temp. Gradient effects and capability of modeling material features (GB, surface) under development
- Carbon Diffusion Modeling:
  3-D Grain models including Grain-Boundaries for more accurate C-diffusion simulation is under development
- SiC Spallation Testing for Isochoric Heating:
  CVD-SiC plate is being prepared for spallation energy calibration and testing
- SiC Material Properties Database (FusionNET©):
  CVD-SiC material properties is being completed

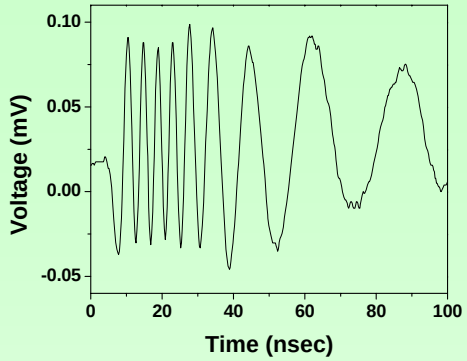
Backup Slides

The Laser Spallation: Determine Interface Bond Strength

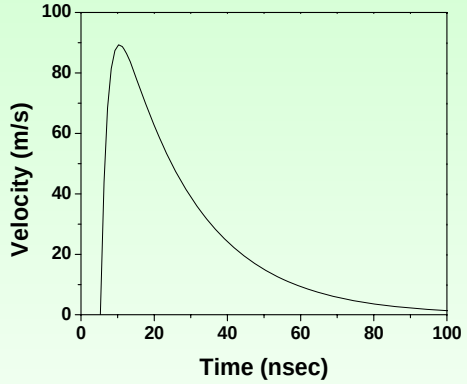


1. Al layer melts and rapidly expands
2. Launching a compressive stress waves through substrate into film layer
3. Compressive waves are reflected as tensile waves from free surface
4. If tensile stress is sufficient interface failure will occur.

Photodiode voltage is used to determine the Displacement profile of the coating surface



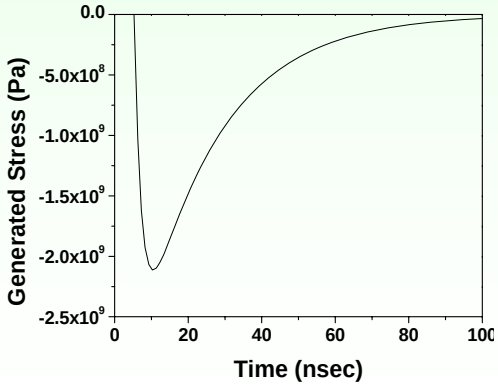
Coating surface velocity is calculated by differentiating the displacement profile



The stress can then be calculated using:

$\sigma = \frac{1}{2}(\rho\, c\, v)$

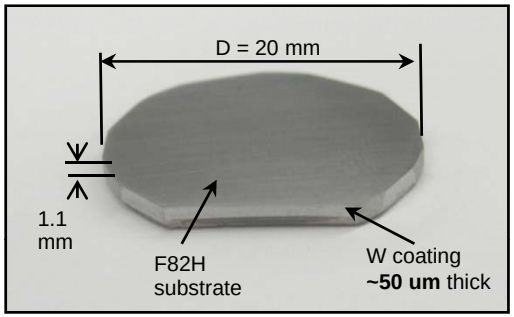
Finally, tensile failure stress failure is then evaluated using FEM



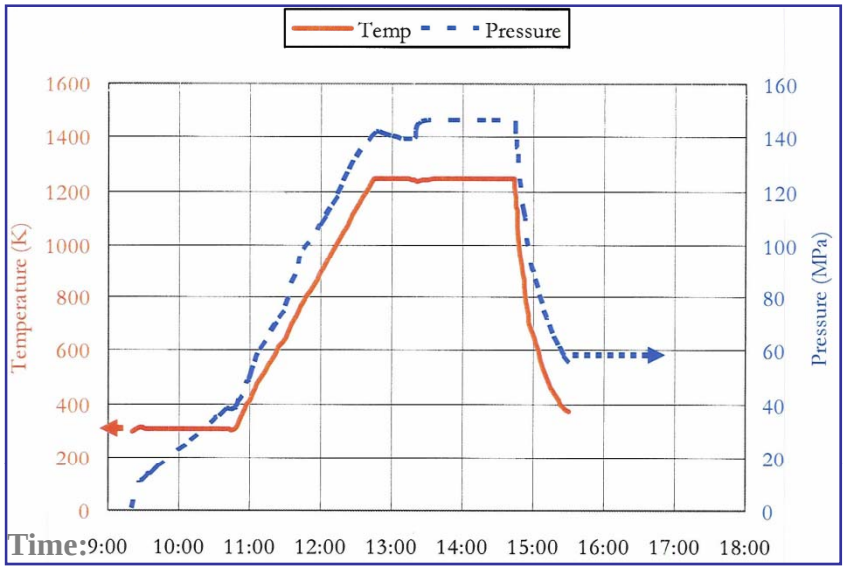
Density and Elastic Properties of both coating and substrate are required to determine accurate failure stresses

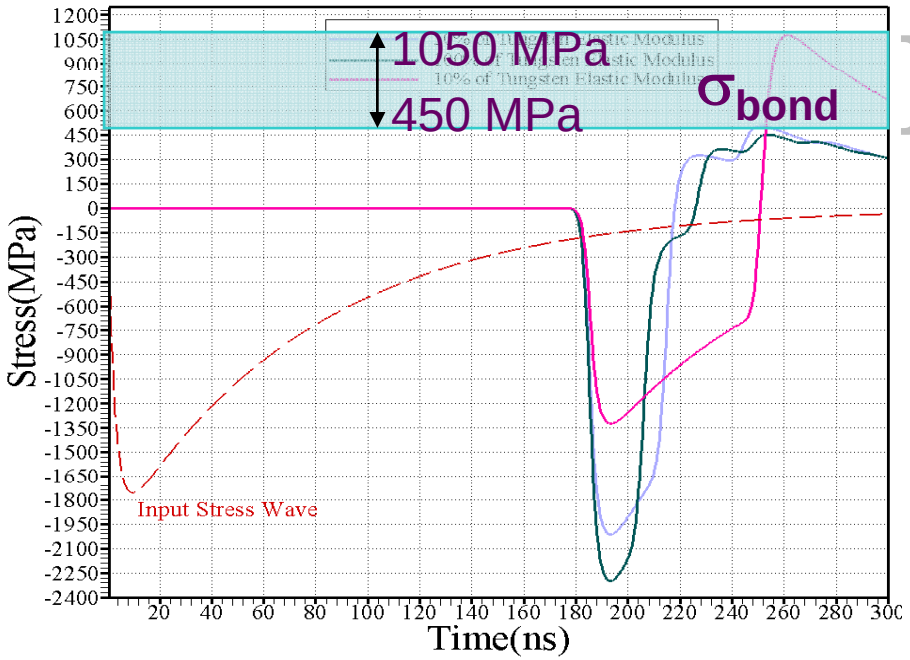
HIP'd W-F82H Sample (ITER, JAEA)

- Hot Isostatic Pressure (HIP) bonded Tungsten to F82H

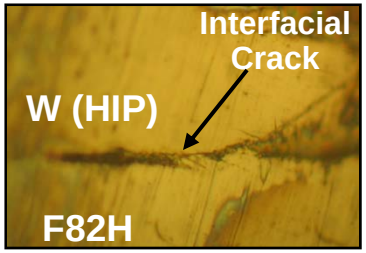


Sample from ITER Development JAEA (Japan)





Bond Strength:
Depends on Coating Elastic Properties & Density



Since **Elastic properties** of the coating depend on processing in a statistical manner → Predicted interfacial strengths will have statistical variations

$$\sigma_{BOND} = 1050\ MPa\ (10\%\ W - Young's)$$
$$\sigma_{BOND} = 450\ MPa\ (100\%\ W - Young's)$$

Reported 14th HAPL

VPS-W Test Matrix (PPSI/ORNL)

- Vacuum Plasma Sprayed (VPS) samples supplied by **PPI** (S. O'Dell).
- W-Coatings were polished to ~50 μm thickness at **ORNL** (G. Romanoski)

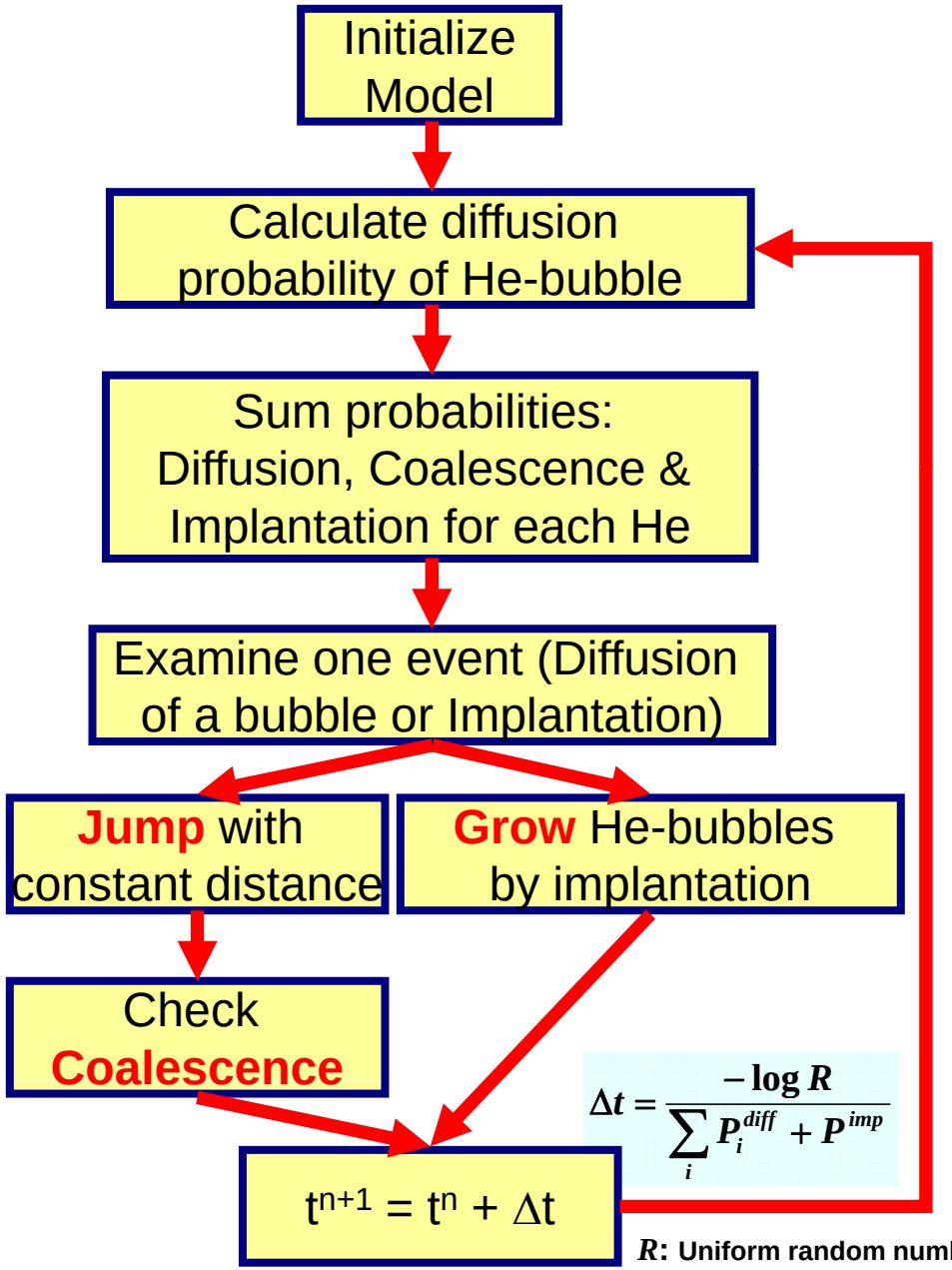
TEST MATRIX: VPS W-Coated Steel Samples

Sample Name	Sample Number	Total Thick. (mm)	Steel Substrate (mm)	W-Coating (mm)
V2-03-370	Sample01	1.14 (±0.01)	1.0939	0.04610
V2-03-392*	Sample02	1.20 (±0.08)	1.1510	0.04900
V2-04-388	Sample03a			0.04945
V2-04-388	Sample03b			0.04960
V2-03-393	Sample04	0.99 (±0.01)	0.9494	0.04060
V2-05-153	Sample05	1.22 (±0.01)	1.1706	0.04940
V2-05-155	Sample06	1.20 (±0.02)	1.1511	0.04890
V2-05-176	Sample07	1.21 (±0.01)	1.1609	0.04910
V2-05-184	Sample08	1.18 (±0.04)	1.1326	0.04745
F82H Substrate	Sample09a	1.16 (±0.01)	1.1600	
F82H Substrate	Sample09b	1.17 (±0.01)	1.1700	
HIP	HIP	1.15 (±0.01)	1.1000	0.05000

* 600°C Preheat

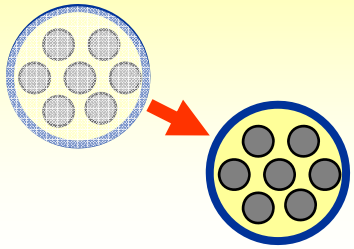
Yellow = Tested

MC – Calculation Procedure



R: Uniform random number (0:1)

Diffusion Migration:



Surface diffusion rate

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

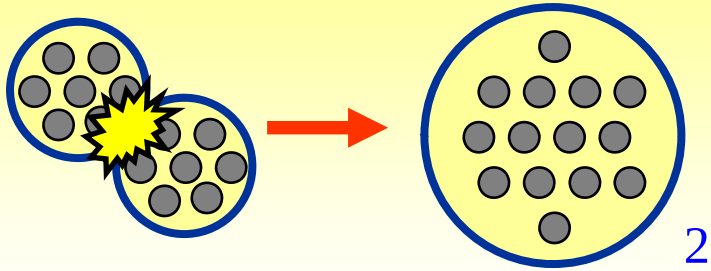
Bubble diffusion rate

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

Es: Activation energy, 2.5eV*

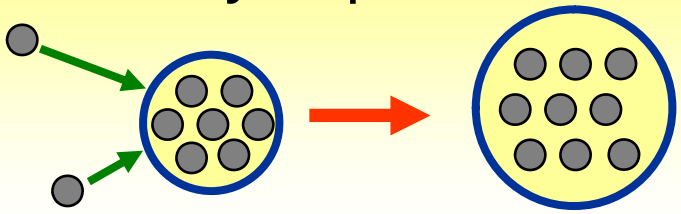
D_0: Pre-expon 1.25x10^{-2}cm^2/s

Coalescence:



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

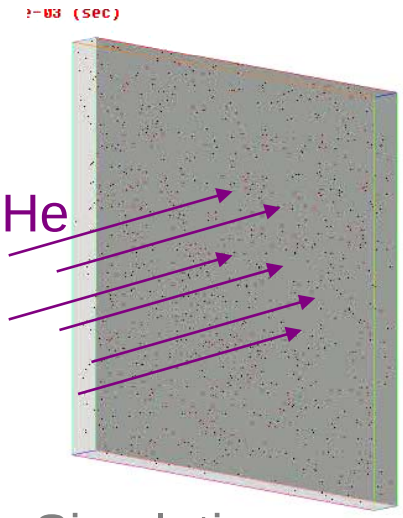
Growth by Implantation:



*A. Takahashi, TOFE 2006

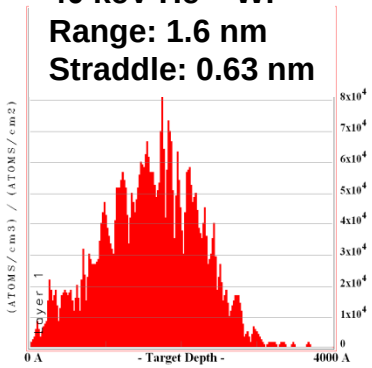
KMC Model for the 730 °C IEC Case:

Gaussian Density Distribution

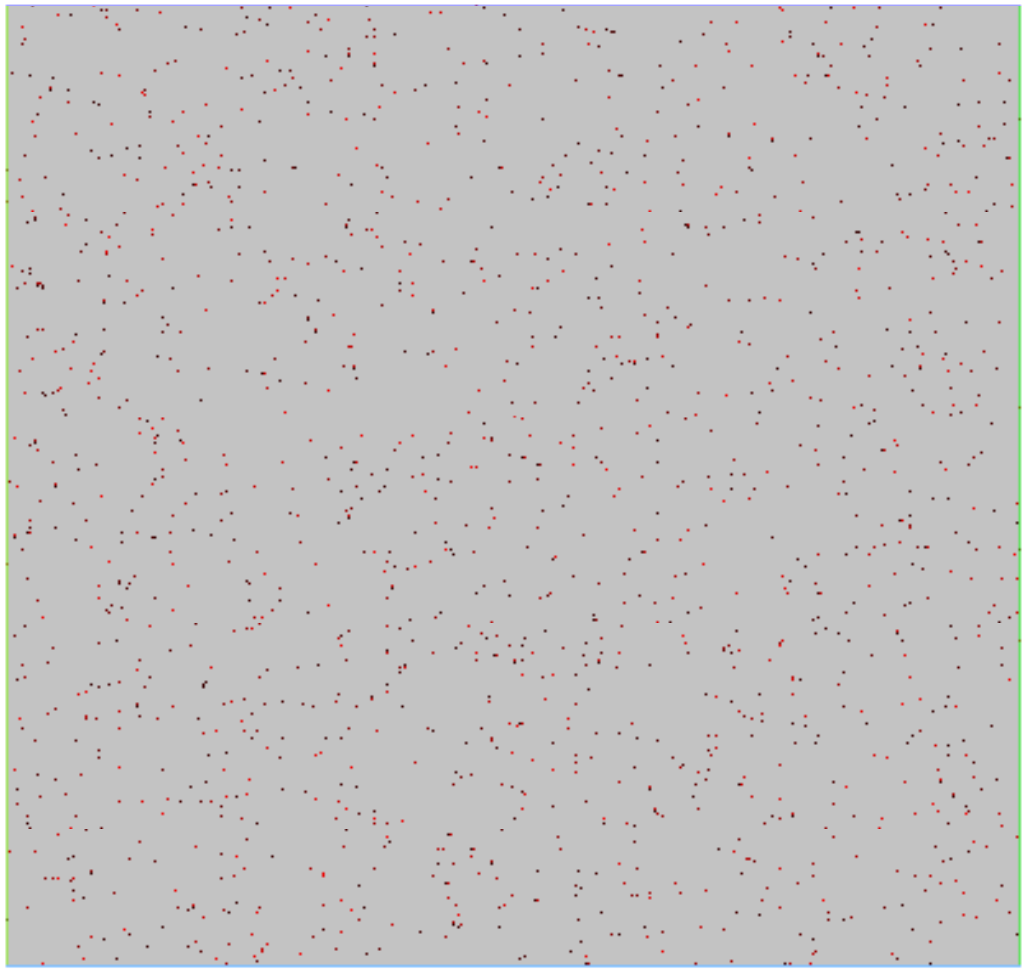


Simulation Volume

40 keV He – W:
Range: 1.6 nm
Straddle: 0.63 nm

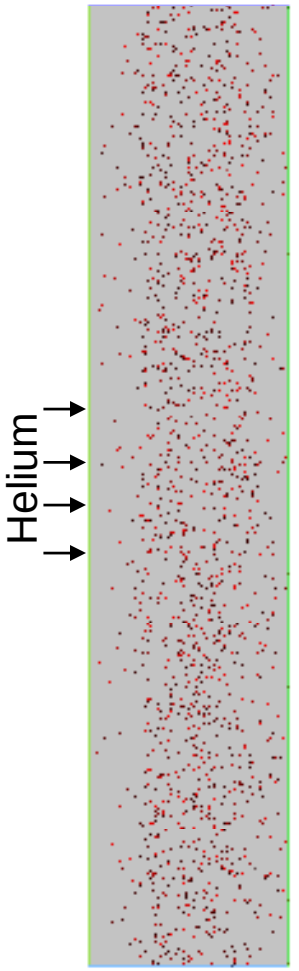


Front View



1 μm

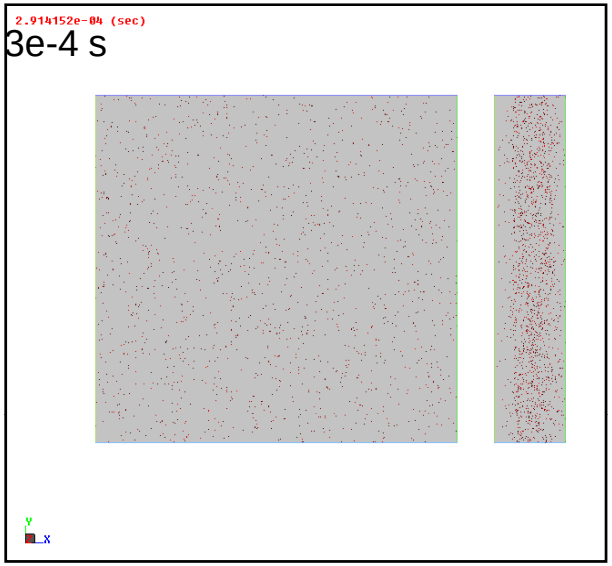
Side View

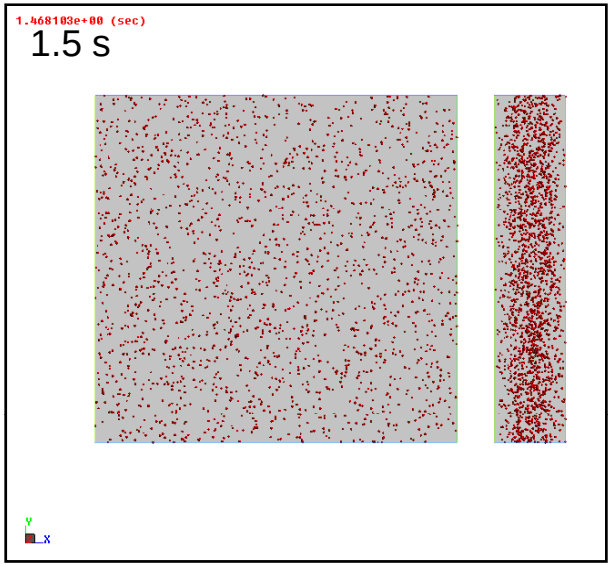


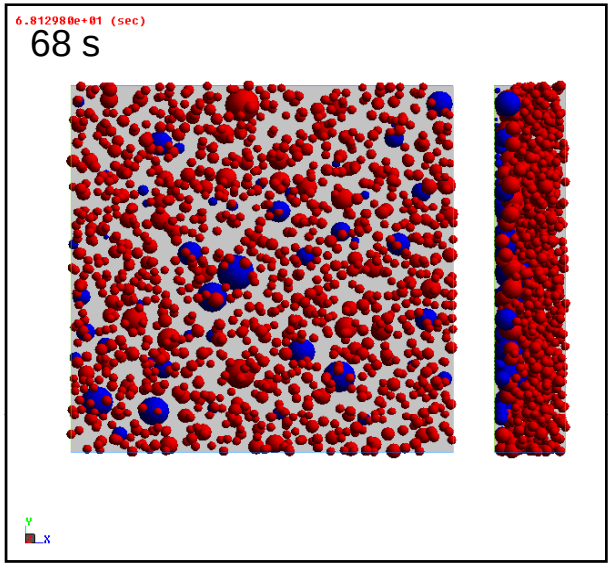
0.2 μm

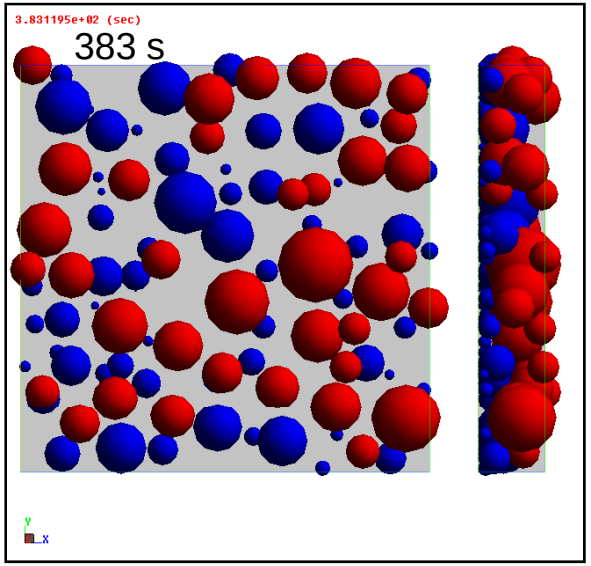
Temperature	Bubble Density	He-Implantation	Init. Radius	Simulation Volume
730 C	10^{17} 1/cm^3	2.2 x 10^{15} 1/cm^2-s	0.5 nm	0.2 x 1.0 x 1 mm^3
990 C	10^{15} 1/cm^3	8.8 x 10^{15} 1/cm^2-s	1.0 nm	0.2 x 2.5 x 1 mm^3
1160 C	10^{14} 1/cm^3	2.6 x 10^{16} 1/cm^2-s	1.5 nm	0.2 x 5.0 x 1 mm^3

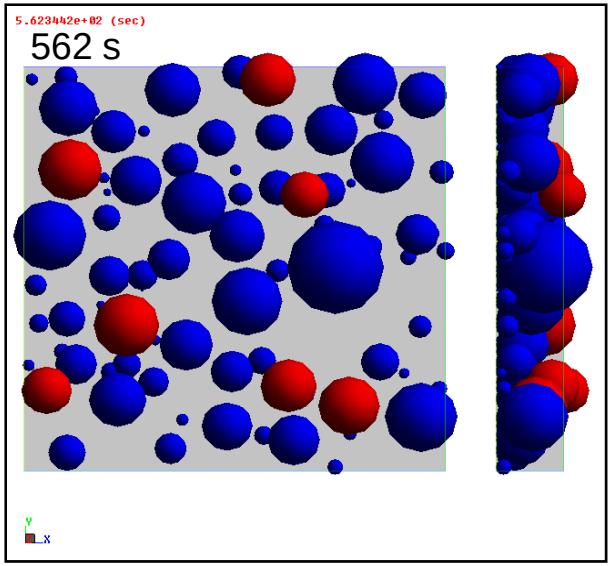
Time Sequence of Pore Evolution (IEC Conditions,730 ºC)

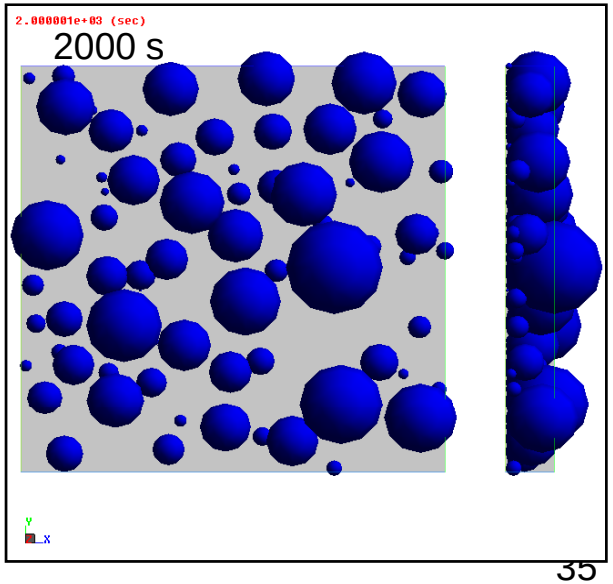




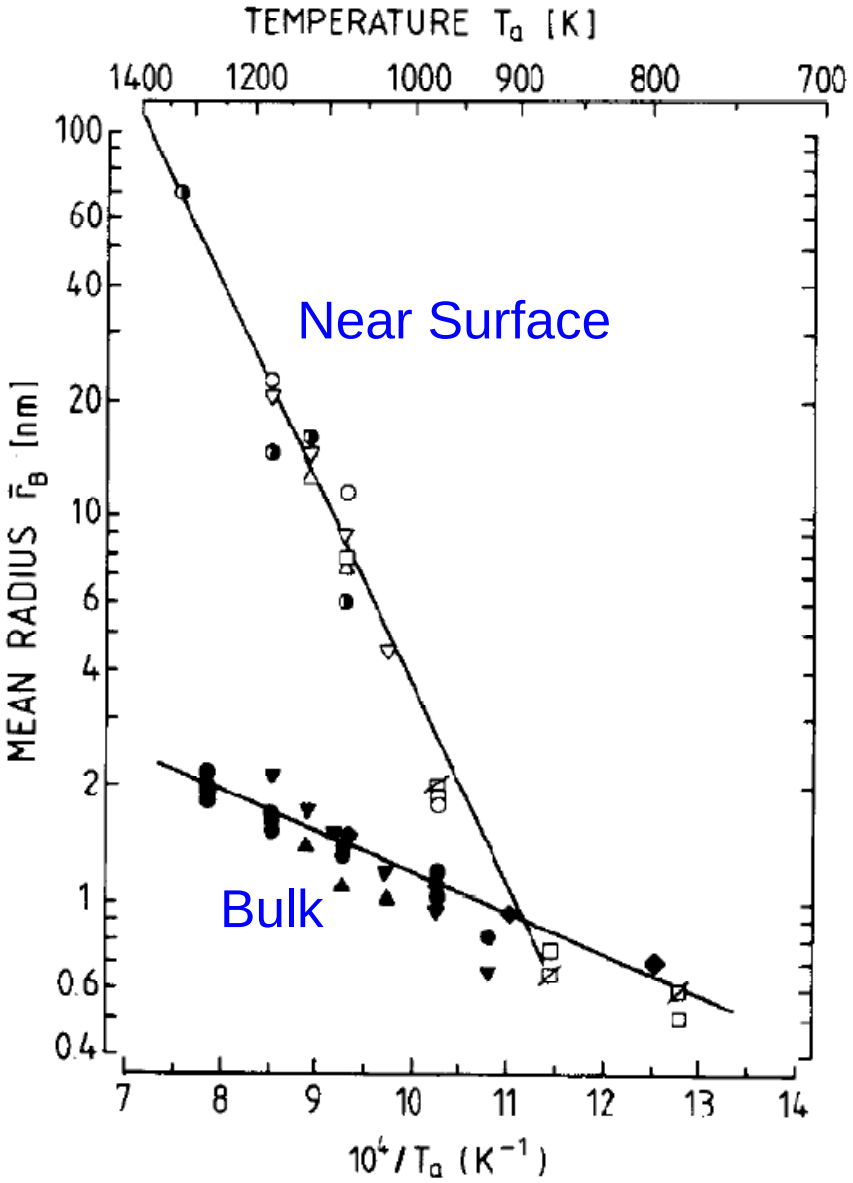








Bubble Size Near Surface vs Bulk *



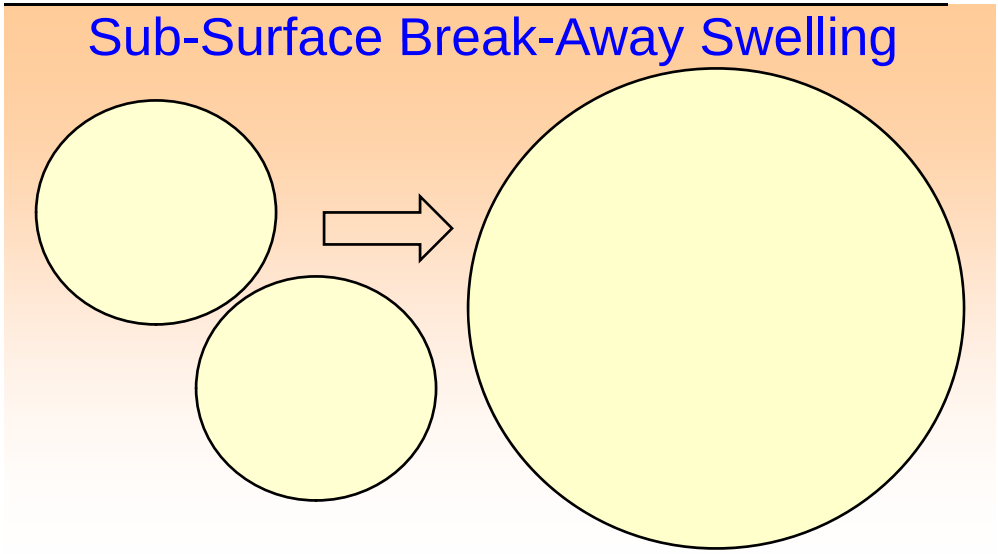
- 1000 appm He Implanted in Ni at RT.
- Uniform He implantation using degrader Al-foil (28 MeV He)
- Annealing time: 0.5 – 1.5 hr

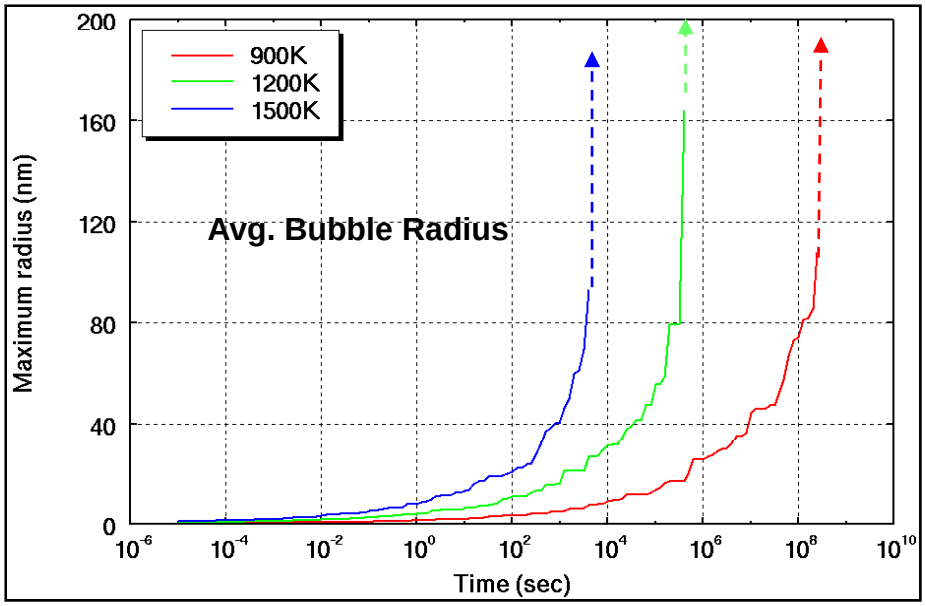
Abundance of Near Surface Vacancies promotes rapid and large bubble growth

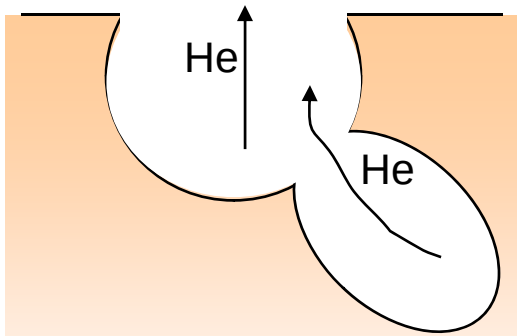
*CHERNIKOV, JNM 1989

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.**







Surface Pore Formation

Probable Explanation of IEC 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

Effects of Carbon Implantation (ORNL/UNC/UCLA)

- **Issue:** About 6.8×10^{19} per shot Carbon atoms are released from the 365 MJ Target (10 m Chamber):
  - ~1.7 appm per shot Carbon in Tungsten ➔ in about 1×10^6 shots C/ W ~ 1.7 (1.2 days @ 10 Hz)
  - ~0.7 appm per shot Carbon in SiC ➔ in about 1×10^6 shots C/ W ~ 0.7 (1.2 days @ 10 Hz)
- **Goals:**
  (1) Investigate the Behavior of Carbon Implantation :
  - Free or bound Carbon (WC and W_2C) ?
  - Release of Carbon from surface or Diffusion of Carbon toward W/Steel Interface ?

  (2) Investigate Helium Release from Carbon Implanted Region :
  - Helium release
- **Experiments:**
  Follow Sample Handling Procedure
- (1) UNC Carbon Implantation (Single-X W) Steady State followed by 1 Annealing Cycle:
  - Implantation at T = 850˚ C, <0.5 MeV
  - Total C-Fluence = 1.6×10^{22} C/m^2 (eq. to ~3×10^5 shots or ~ ½ day at 10 Hz) → C/ W ~ 0.5
  - Anneal at 2000˚ C for ~430 sec (total time above 1000 C for ~3×10^5 shots)
  - Determine depth profile and density of Carbon & Perform Hardness measurements

  (2) UNC Helium Implantation (use Carbon exposed SX-W). Step wise He followed by 2000 C annealing:
  - Implant 1×10^{19} ^{3}He/m^2 at 850˚ C, flash anneal at 2000˚ C in 1000 or 100 steps
  - Determine Helium release and depth profile.
- **Modeling:**
  - Modify Carbon Diffusion model (UCLA) to include WC and W2C formation
  - Add Carbon Implantation/Carbide Formation to the HEROS code He model (UCLA):
    - Account for large damage rates caused during C-implantation and short time at T.