A new spatially resolved model for defects and fission gas bubbles interactions

L. Verma, L. Noirot, P. Maugis

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Institut Matériaux Microélectronique Nanosciences de Provence
UMR CNRS 7334, Aix-Marseille Université, Univ. De Toulon

Aix Marseille université

A new spatially resolved model for defects and fission gas bubbles interactions

Lokesh VERMA[1,2] , L. NOIROT[1] , P. MAUGIS[2]

1: CEA, DEN, DEC, Cadarache, 13108 Saint-Paul-lez-Durance, France

2: Aix Marseille Univ, Univ Toulon, CNRS, IM2NP, Marseille, France

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Overview

- Motivation
- Introduction
- BEEP Model
- 2-D Analysis
- Conclusions & Prospects

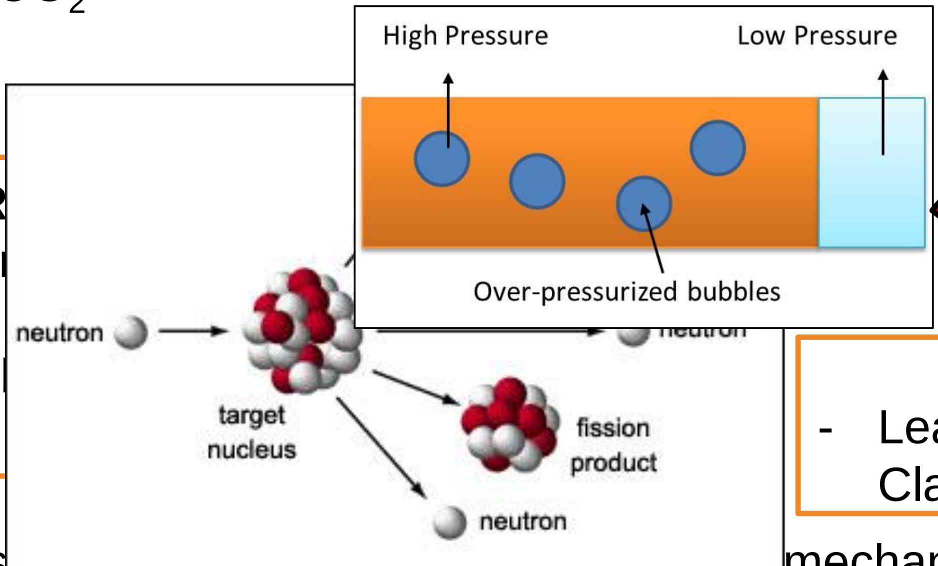
Motivation

- Fission gases are produced in the fuel during nuclear reactor operation
- Almost insoluble in UO_2

Precipitate as bubbles

Released

Fission Gas R
- Pressure withi rod increases
- Cladding is su stresses



Swelling
- Leads to Fuel-Cladding Interaction

- Swelling and Fission Gas Release affect the thermo-mechanical properties of the fuel rod

- Behaviour of fission gases and their interactions with defects need to be understood

- During post-irradiation annealing, the fission gas release (FGR) from nuclear fuels can be attributed to a two-step process:

1

The migration of gas within the grain towards the grain boundary

transport of intragranular gas to the grain surface >> predicted from effective diffusion theory

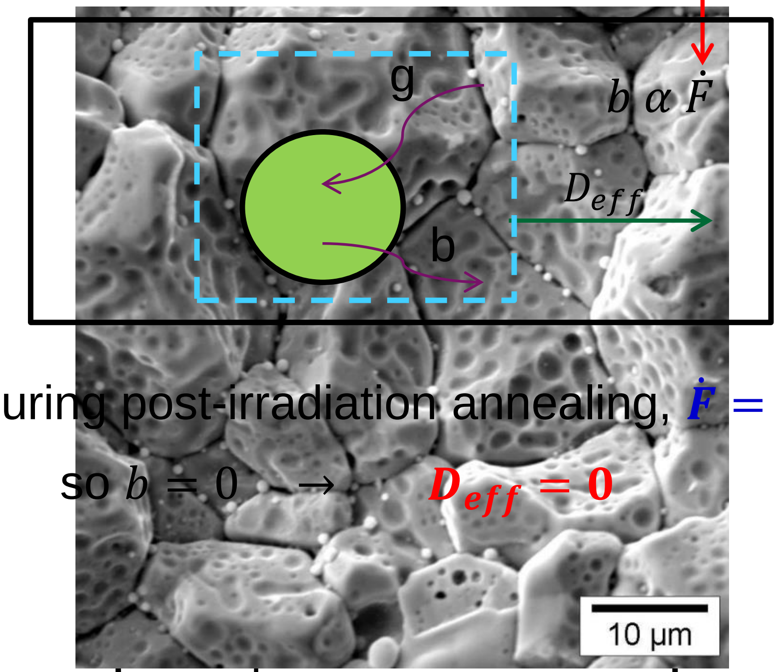
$$D_{eff} = \frac{b}{b+g} D_{Xe}$$

Well known at high temperatures (T>1400°C)

g: frequency of traping of gas atoms in the bubble

b: frequency of re-solution of gas atoms back into the bulk

Fission rate



During post-irradiation annealing, $\dot{F} = 0$,

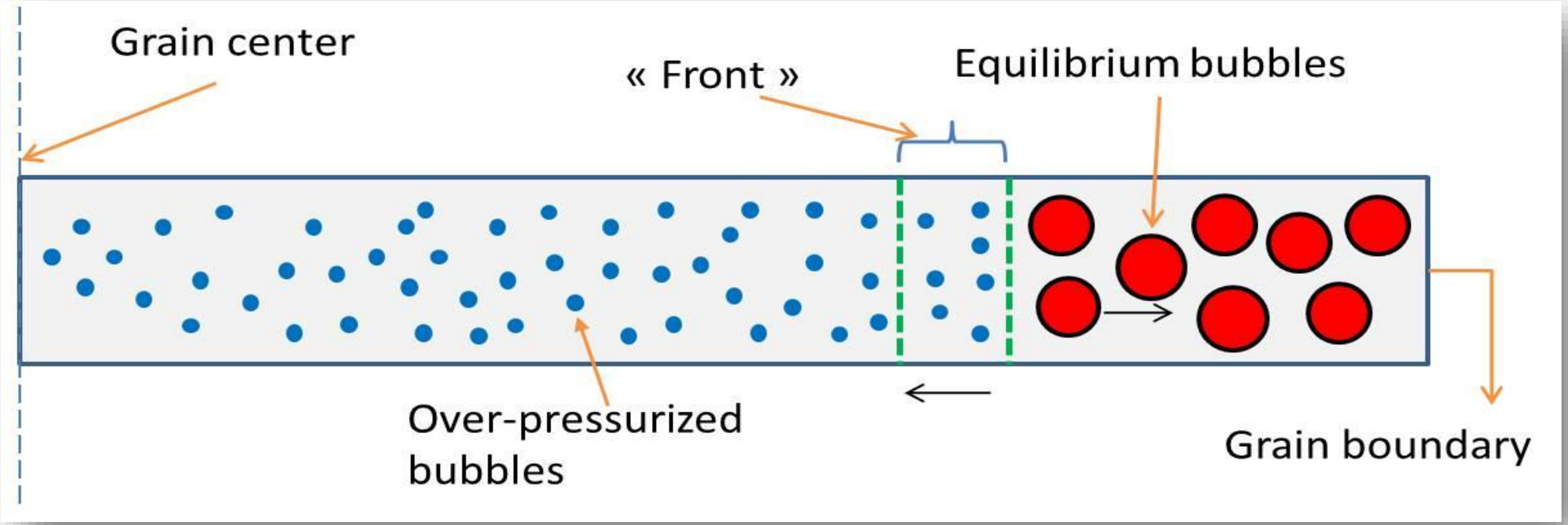
so $b = 0 \rightarrow D_{eff} = 0$

Time = 3 hours

FGR > 60%

S. Valin, Etude des mécanismes microstructuraux lies au relâchement des gaz de fission du dioxyde d'uranium irradie, Ph.D. thesis, Institut National Polytechnique de Grenoble, 1999.

- Various mechanisms have been suggested to explain the movement of gas within the grain to the grain boundary.



- Evans further proposed a model for the quantitative assessment of this mechanism, however, his model is not mechanistic.

- We are developing a new model, BEEP, which focuses on simulating the bubble interactions with the point defects and to analyze the fractional gas release.

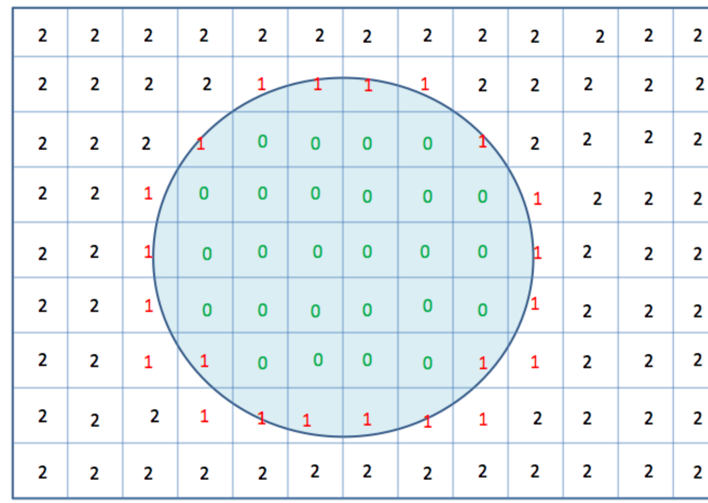
*J. H. Evans, The role of directed bubble diffusion to grain boundaries in post-irradiation fission gas release from UO_2: A quantitative assessment, J. Nucl. Mater. 238 (1996) 175-182.

BEEP Model

- BEEP code is designed to model the interaction between point defects and cavities (Xenon bubbles and free surfaces).

- It allows spatial representation of the microst

- Assumptions:
  - The solid is modeled as a mono crystal
  - No irradiation is considered, it is only a
  - Only vacancies are considered as poi
    present inside the cavities and not in th
  - Bubbles are assumed to be spherical a



- The domain is discretized on a regular mesh, represented by the two variables: _concentration field_ and _spin_

Spin = 0 for cavities ; **Spin = 1** for interface ; **Spin = 2** for solid

- The boundary condition imposed for the diffusion equation is that the ***concentration of vacancies in the interface cells are equal to the equilibrium concentrations***.

  - The expression for the equilibrium concentration of vacancies in the vicinity of a bubble* is:

$$C_v^{eq} = exp\left[-\frac{(\epsilon_v - s_v T)}{kT} - \frac{\Omega}{kT}(P_b - \gamma_b \kappa)\right]$$

- The diffusion of point defects (vacancies) and crystal atoms follow the Fick's law

- 5-point difference scheme is adopted for space discretization in 2-D

- Explicit Scheme with forward difference in time is used for time discretization

- After the diffusion step, the bubbles are updated with their new volumes and the new centers (as the center of voids)

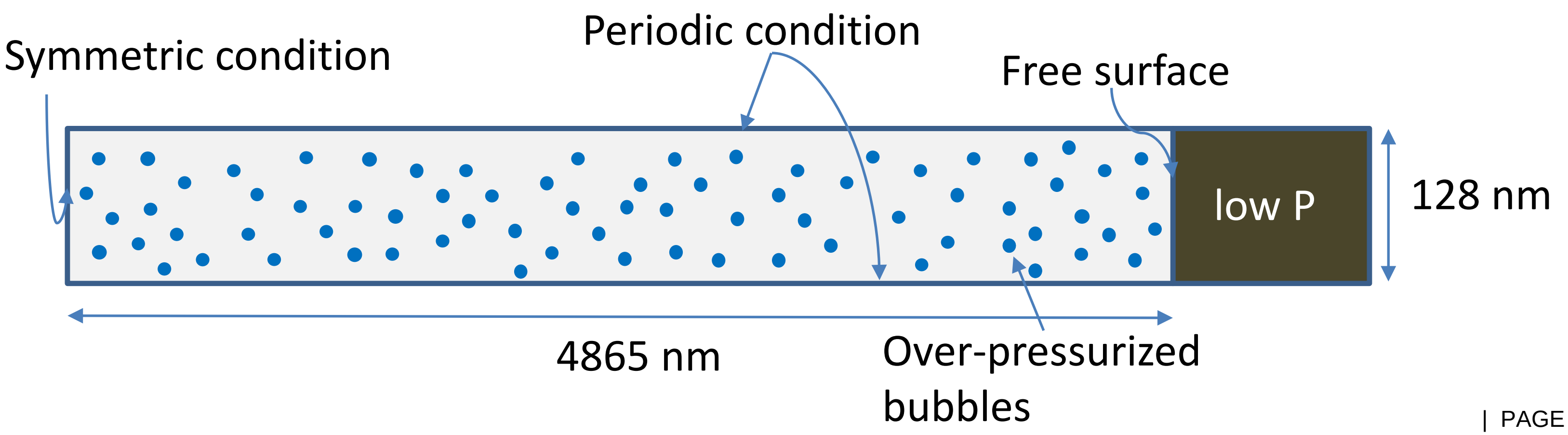
* *L. Noirot, A method to calculate equilibrium concentrations of gas and defects in the vicinity of an over-pressured bubble in UO_2, J. Nucl. Mater. 447 (2014) 166-178.*

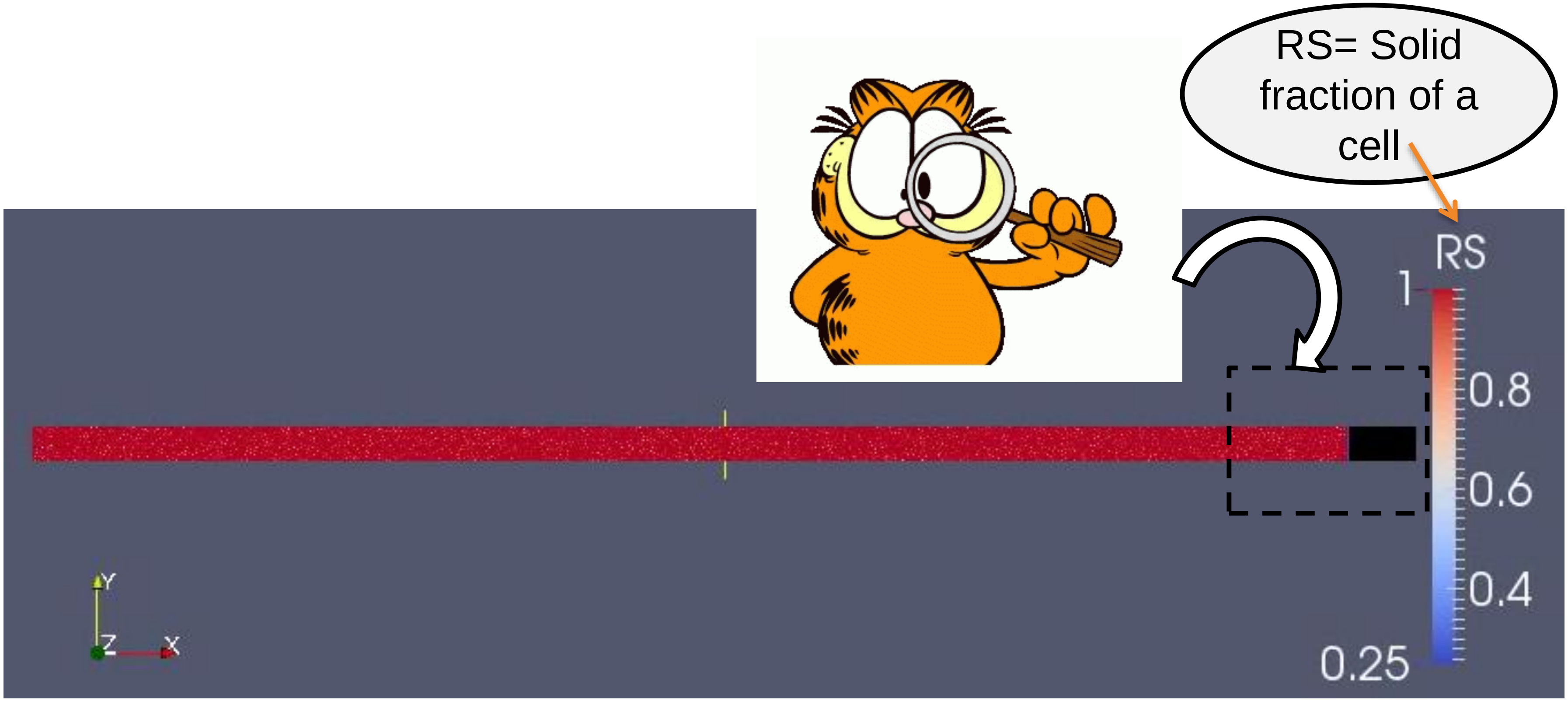
2-D Analysis

BEEP Model | **2-D Analysis** | Conclusions & Prospects

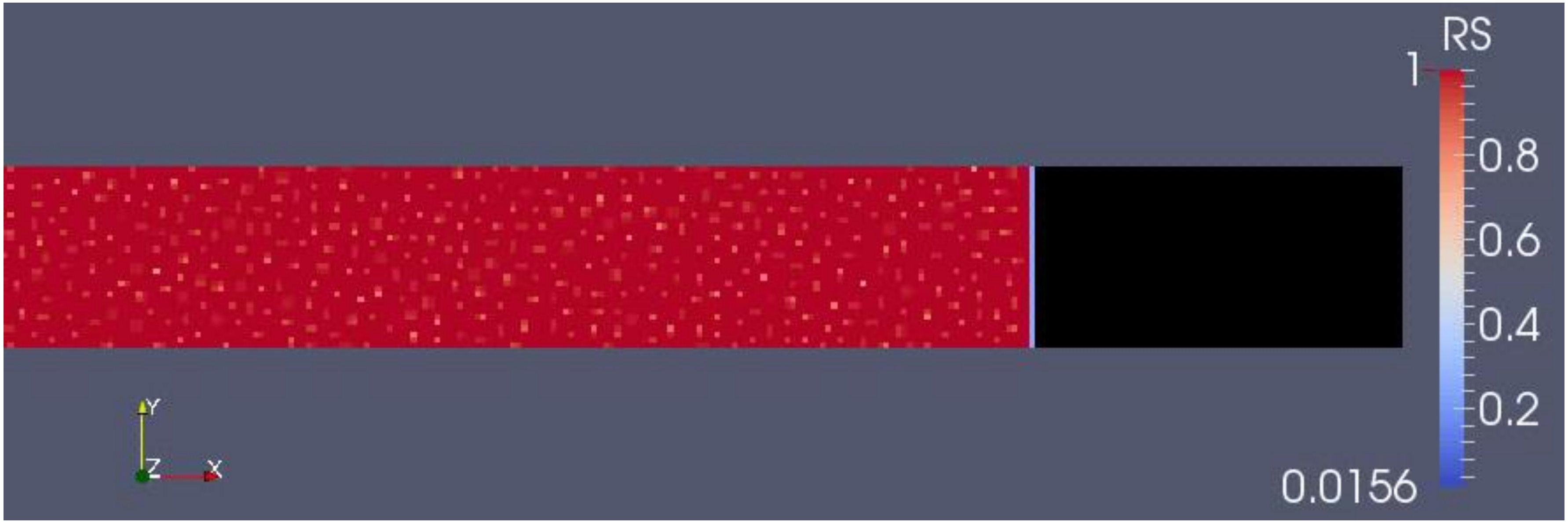
- We consider a domain of length equal to the radius of a grain with several pressurized bubbles contained in it.
- A vacancy concentration gradient exists between the pressurized bubbles and the exterior surface at lower pressure.

- Simulation domain = 1280 x 32
- Grid size = 4 nm
- Annealing temperature = 1800°C
- Simulated time = 77 hours





*U. Ayachit, The ParaView Guide: A Parallel Visualization Application, Kitware, 2015. ISBN 978-1930934306.


RS
1
0.8
0.6
0.4
0.2
0.0156
Y
Z
X

We observe that:

- The bubbles move towards the free surface, i.e, up the vacancy gradient
- They grow by trapping the vacancies emitted from the free surface
- Some bubbles coalesce with each other during the movement
- Bubbles at the vicinity of the free surface coalesce with the exterior
- The surface of the grain moves outward, indicating the swelling of the grain

- Fractional fission gas release

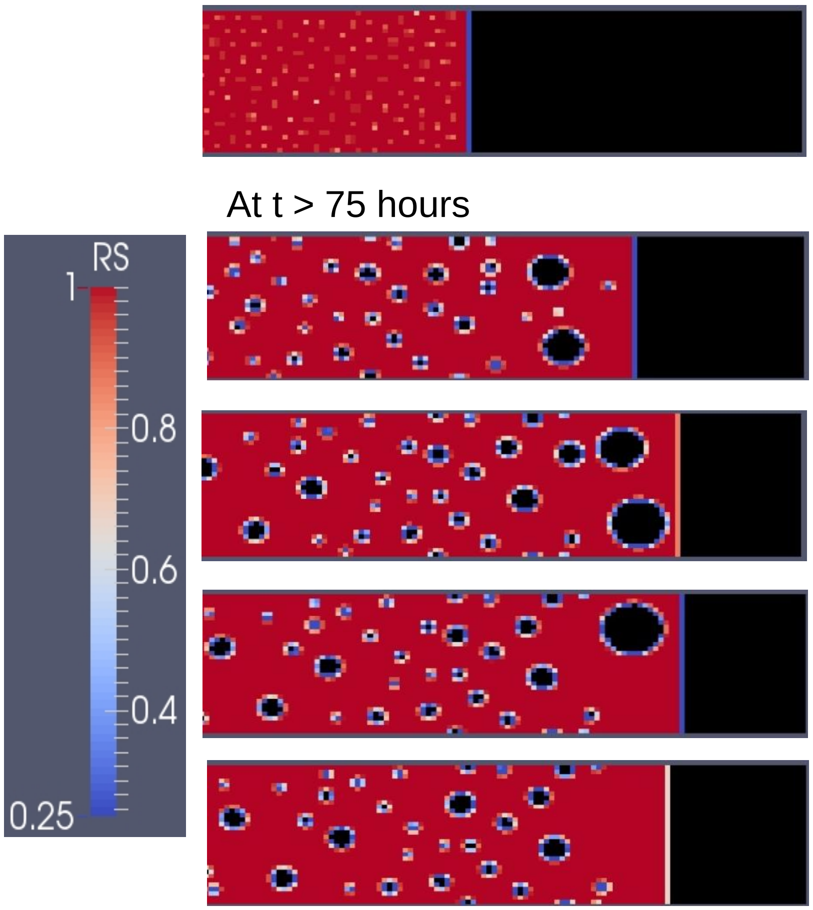
$$fFGR\ (\%) = \frac{N_x^{exterior}(t) - N_x^{exterior}(t=0)}{\sum_{bubbles\ \epsilon\ solid} N_x^{bubble}(t=0)} * 100\%$$

- Fractional swelling

$$\left(\frac{\Delta V}{V}\right) = \frac{V_f - V_0}{V_0} * 100\%$$

At t = 0

At t > 75 hours



- fFGR (%) = 4.94%
- $\left(\frac{\Delta V}{V}\right)$ = 3.16%

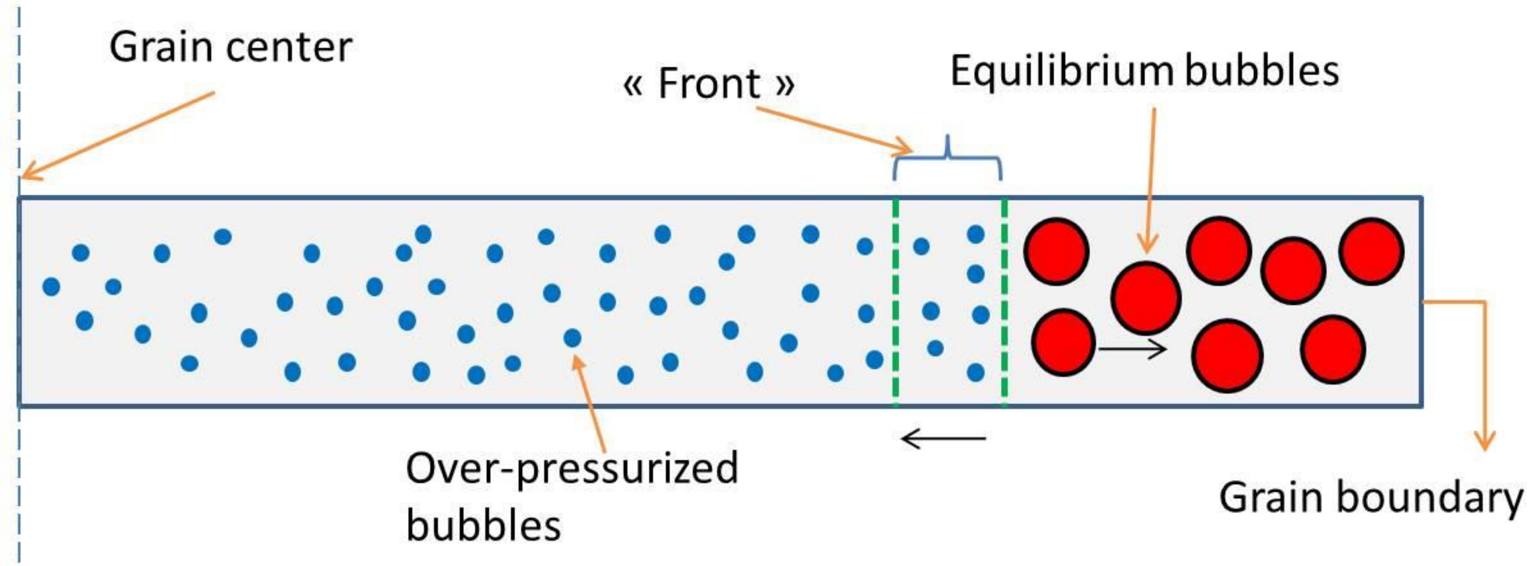
Experimental value
> 60% for 3h @ 1600°C

Conclusions & Prospects

- BEEP Model is able to simulate the bubble movement within the grain.
- The gas bubbles are observed to move up the vacancy gradient and out of the grain.
- The fractional fission gas release is found to be significantly lower than that obtained from experiments (upto ~60% gas release).
- **The gas bubble migration solely cannot account for the gas released during post irradiation annealing.**
- Random motion of bubbles is being incorporated to the model in addition to the directed motion in the vacancy concentration gradient.

Thank you for your attention

EVANS' MODEL

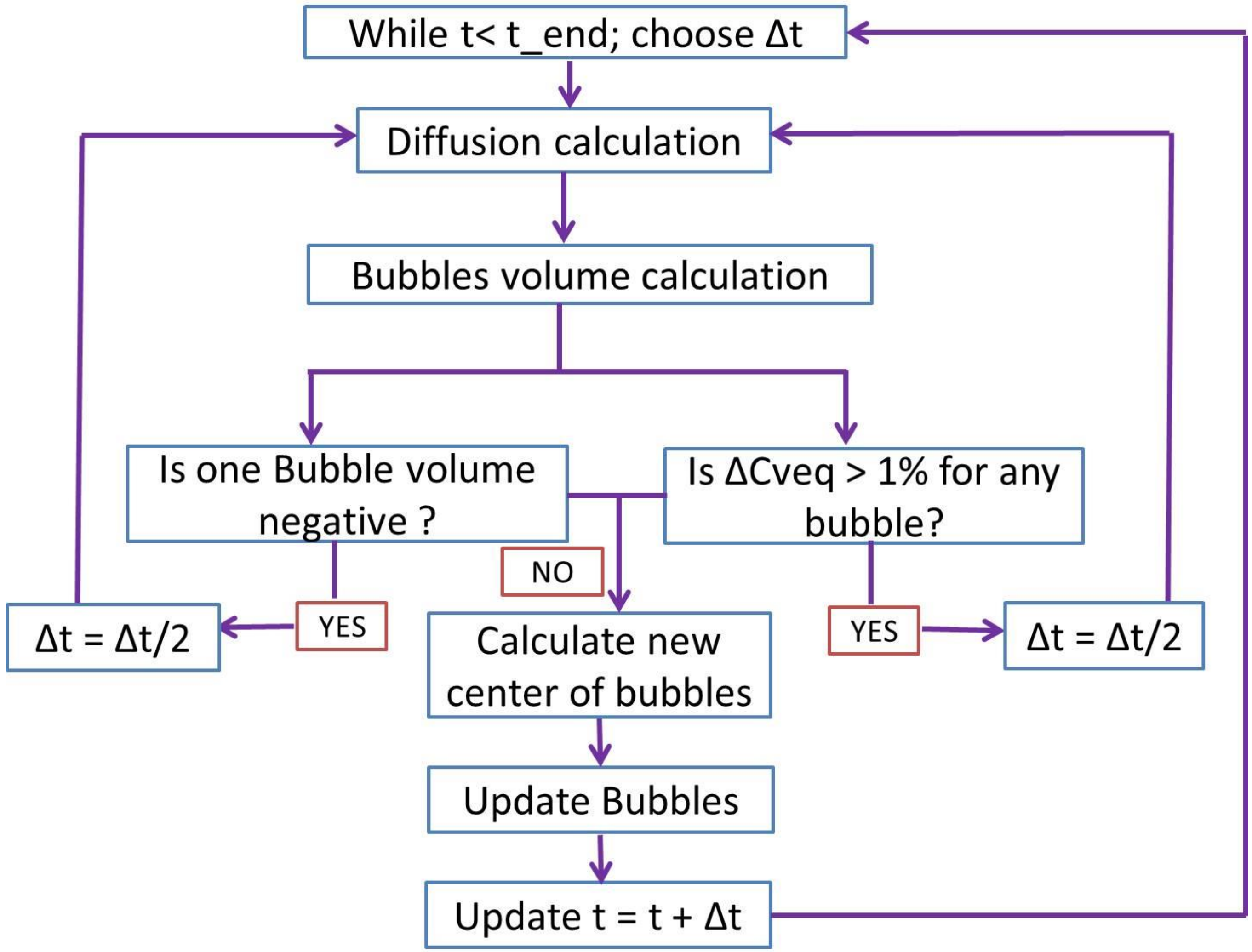


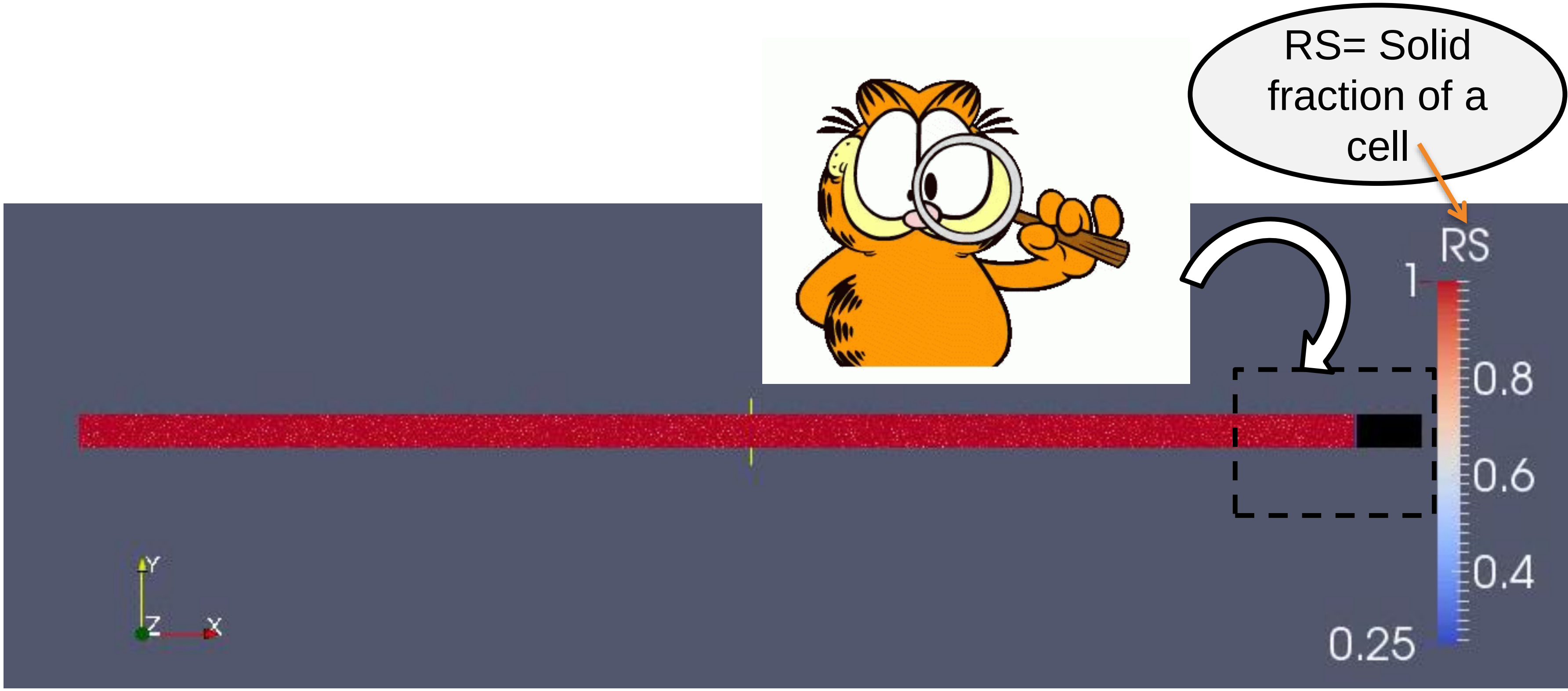
Equilibrium bubbles do not grow further but move in the vacancy gradient

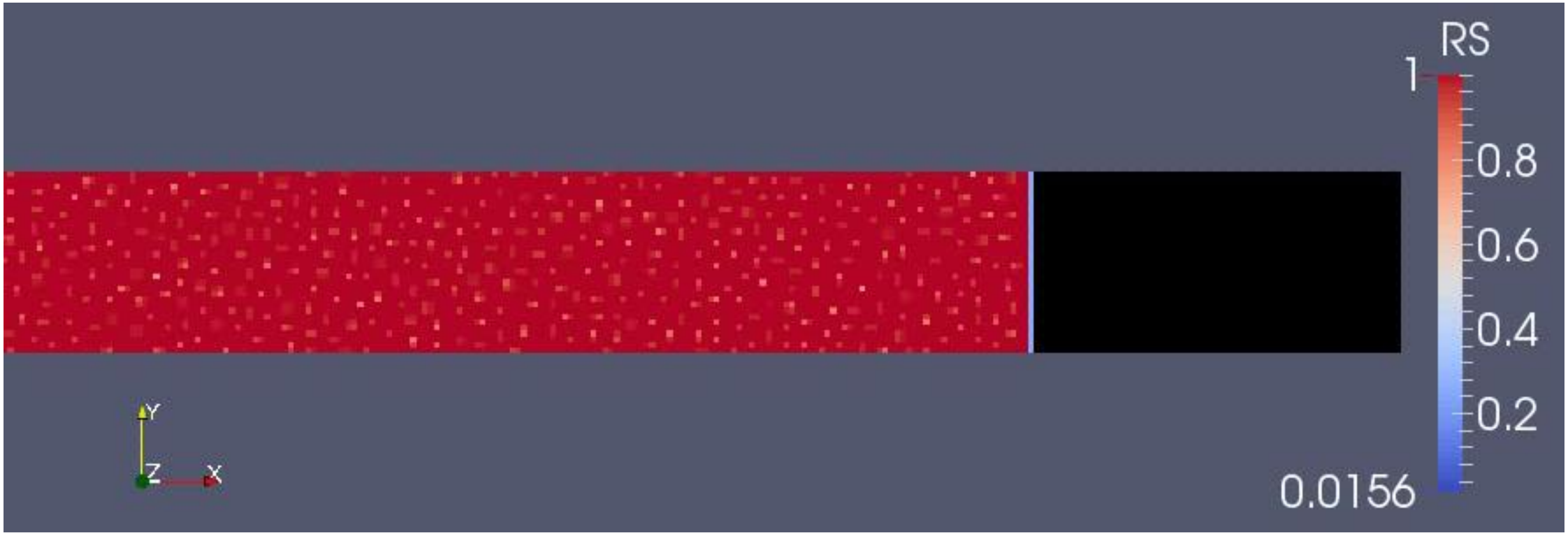
The bubbles within the front grow by trapping vacancies

The bubbles further inside the grain from the front are unaffected by the vacancy influx

General Algorithm




RS= Solid fraction of a cell
RS
1
0.8
0.6
0.4
0.25
Y
Z
X


RS
1
0.8
0.6
0.4
0.2
0.0156
Y
Z
X