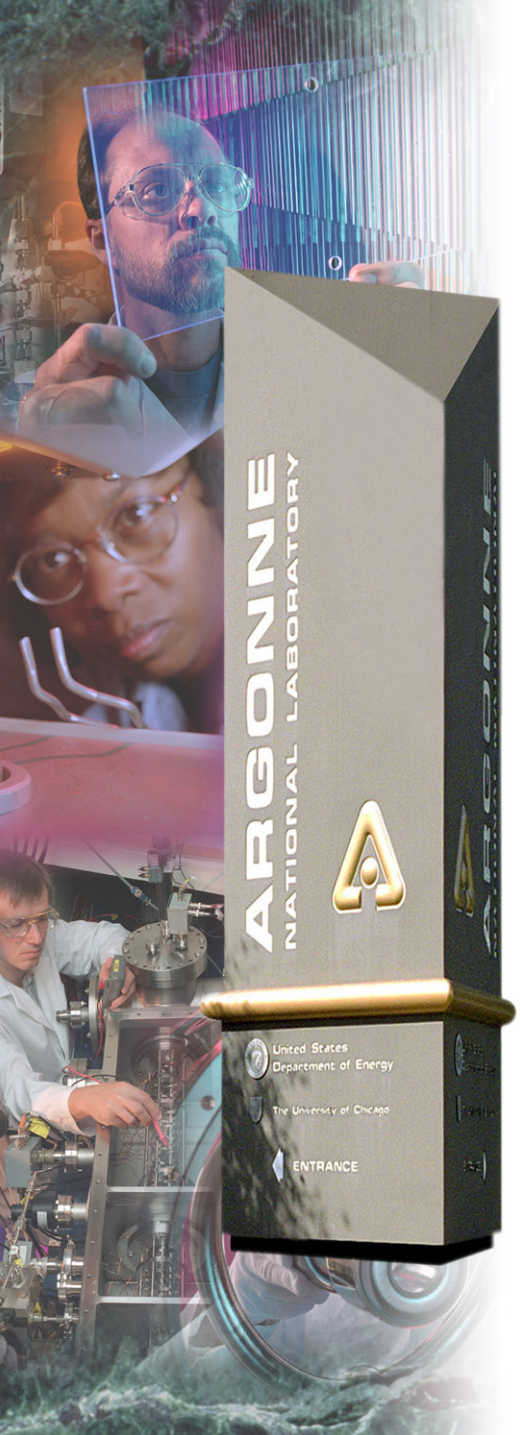

ITMC Code Analysis of Mixed-Material Surface Evolution and Sputtering

Plasma Facing Components (PFC) Meeting
November 17-20, Oakbrook, IL

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Argonne National Laboratory

Office of Science
U.S. Department of Energy

A U.S. Department of Energy
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Outline

- **Objectives**
- **ITMC Code**
- **Kinetic Processes**
- **Modeling of Kinetic Processes**
- **Simplified Model for Mixing in W Divertor**

Objective

- **Detailed analyze of mixed material behavior under ion irradiation**

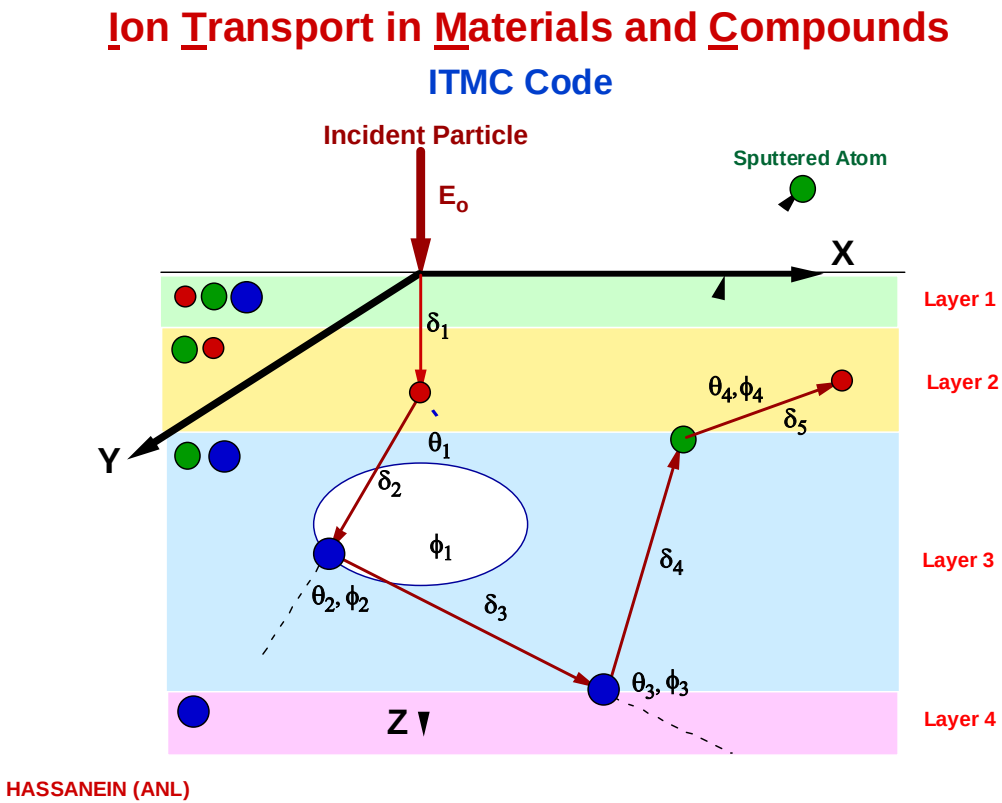
  - Combine Monte Carlo ion transport calculations with kinetic models
    - *Inclusion of possible thermally activated processes will enable the study of the temperature dependence of the mixed materials under ion irradiation*

    - *Study the dynamic evolution of the near surface region of a material bombarded with multiple fluxes with the possibilities of oxide or precipitate layer formation*

ITMC Code

- **ITMC code (Ion Transport in Materials & Compounds – Part of HEIGHTS Package).**
  - 3-D Monte Carlo simulation of charged particles transport in solid materials.
  - Material can be an alloy with a number of layers, each has a different composition
  - Sputtering, backscattering, implantation, range, spatial composition, and defect profiles are calculated.

ITMC Code



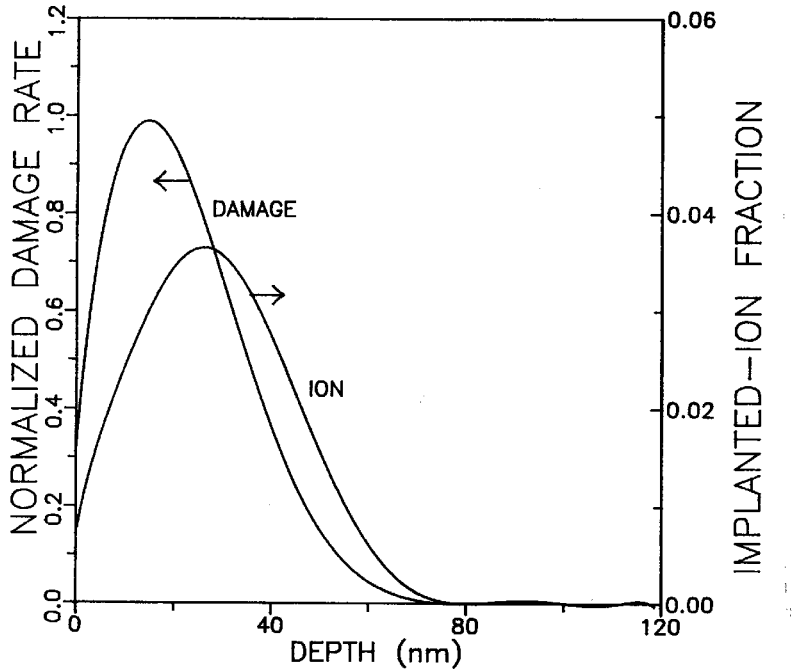
HASSANEIN (ANL)

Kinetic Processes

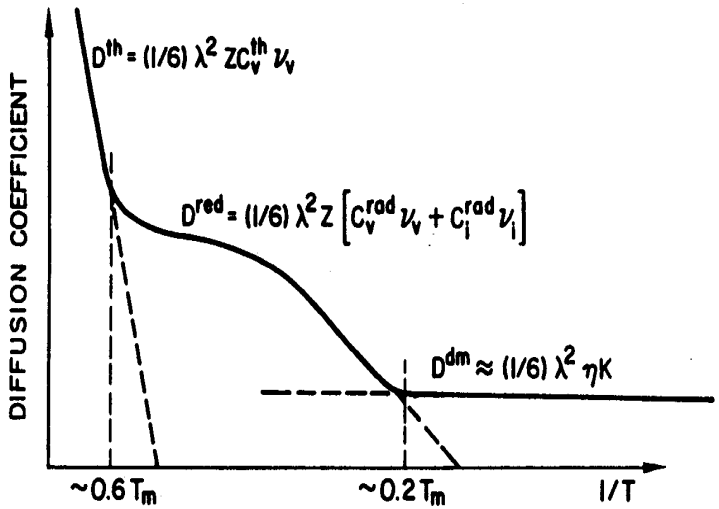
- **Kinetic Processes**
  - Preferential sputtering
  - Displacement mixing
  - Radiation induced segregation
  - Radiation-enhanced diffusion
  - Gibbsian adsorption

- **Kinetics of ion implantation and near surface precipitation**
  - Dynamic behavior of the implant profile
  - Temperature and dose effects
  - Development of the oxide or precipitate layers

Kinetic Processes



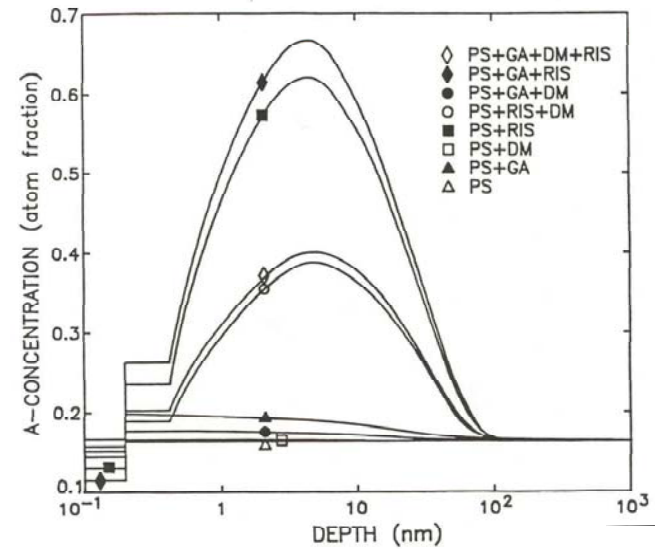
Damage and Implant Profiles



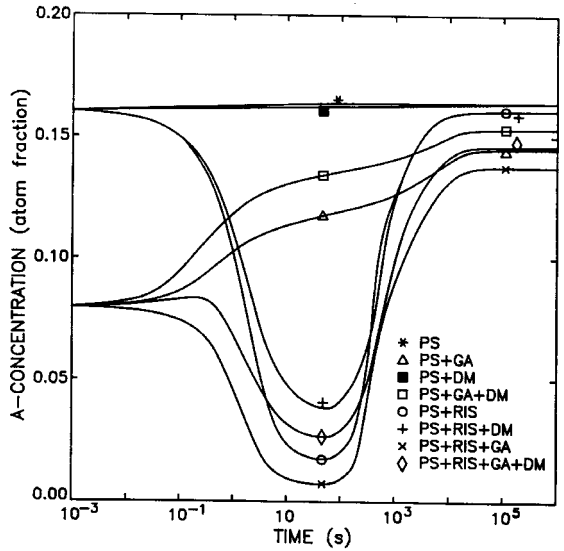
Temperature Regimes for Diffusional Processes

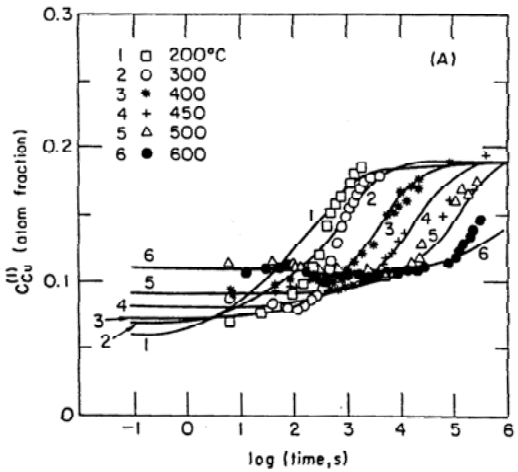
D^{th} = Thermal Diffusion
D^{red} = Radiation Enhanced Diffusion
D^{dm} = Displacement Mixing

Kinetic Processes



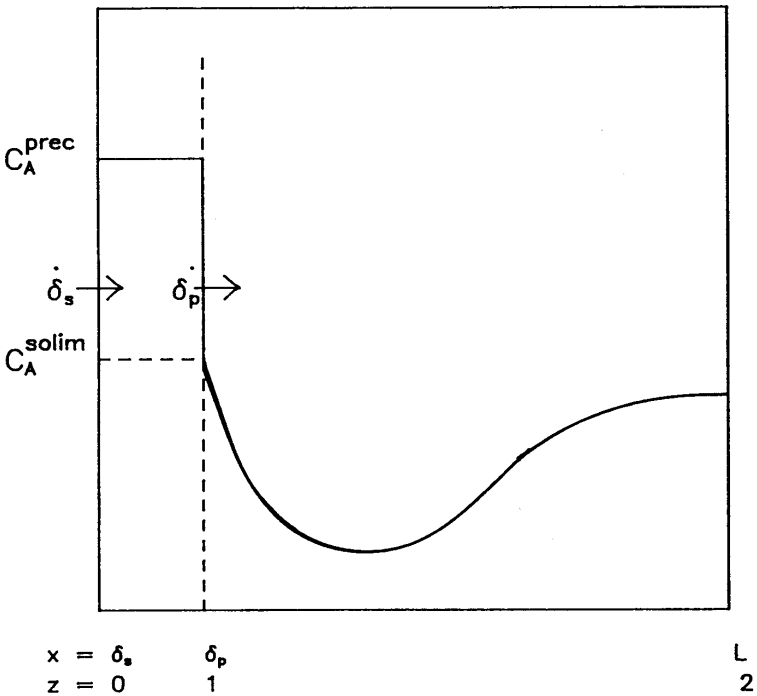
PS = Preferential Sputtering
GA = Gibbsian Adsorption
DM = Displacement Mixing
RED = Radiation Enhanced Diffusion
RIS = Radiation Induced Segregation

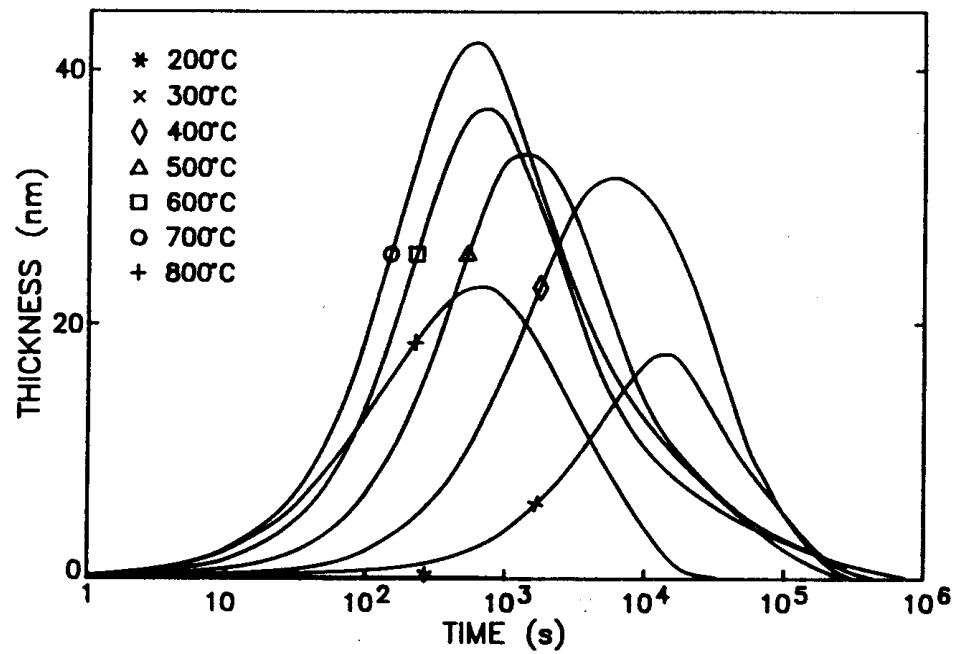




Comparison to Experiment

Kinetic Processes





Precipitate or Oxide Layer Dynamic Evolution

Modeling of Kinetic Processes

- **General Kinetics Equation**

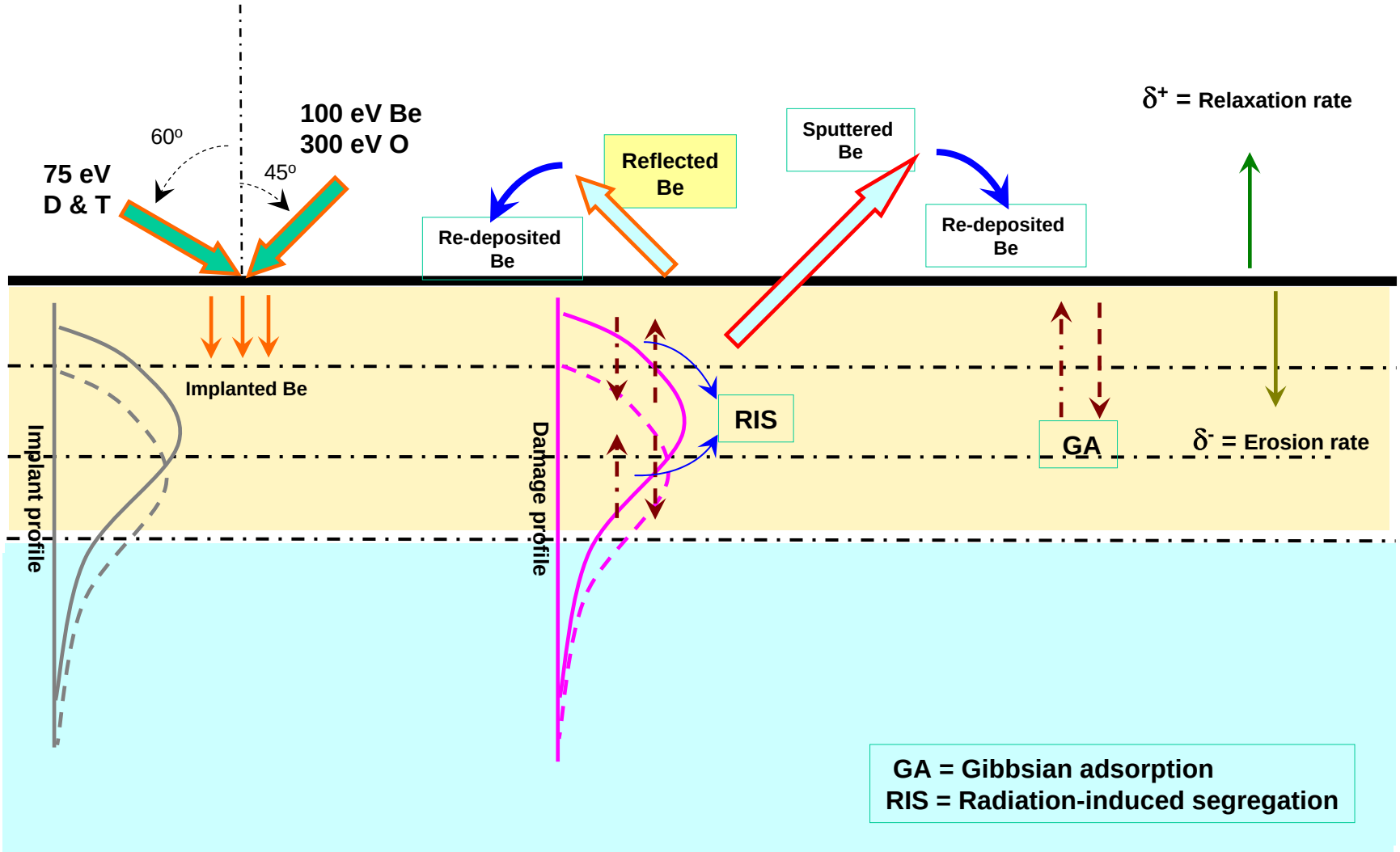
$$\frac{\partial C_k}{\partial t} = \nabla \cdot \left\{ G_j^k \nabla C_j^k \right\} + F_k$$

- ***K, j = interstitials, vacancies, implanted ions or target components***
- ***G's* are functions of the species concentrations and diffusion coefficients.**
- ***F_k* = source/sink terms that include local rates of production and loss of point defects by various mechanisms, production of the species through implantation into the tungsten, and losses through sputtering.**

Simplified Mixing Model in W Divertor

- **Tungsten divertor is bombarded with 0.1 keV Be, 0.3 keV O, 75 eV D and T at different angles**
  - First 3 mono-layers are considered
    - *Sputtered Be and W*
    - *Reflected Be*
    - *Implanted Be*
    - *Re-deposition of reflected and sputtered Be*

Simplified Mixing Model in W Divertor



Simplified Mixing Model in W Divertor

	W	Be	T	D	O
atomic number (z)	74	4	1	1	8
mass number (m)	183.9	9	3	2	16
component density (g/cm3)	19.3	1.85	.....	....	.....
bulk binding energy (ev)	4	3	0	0	0
surface binding energy (ev)	11.1	3.4	0	0	0
cutoff energy (ev)	4	3	3	3	3
displacement energy (ev)	20	20	.....	....	.....
Flux, #/m^{2}s	……	5.443×10^{20} *	1.4×10^{24}	1.4×10^{24}	1.4×10^{21}
Energy, eV	……	100	75	75	300
Angle of incedence	……	45	60	60	45

*** With convection term:**

Inner Divertor: $\Phi_{Be} = 5.443 \times 10^{20}$ #/m^{2}s ($J_{Be} = 2.15 \times 10^{21}$ s^{-1}, Area = 3.95 m^2)

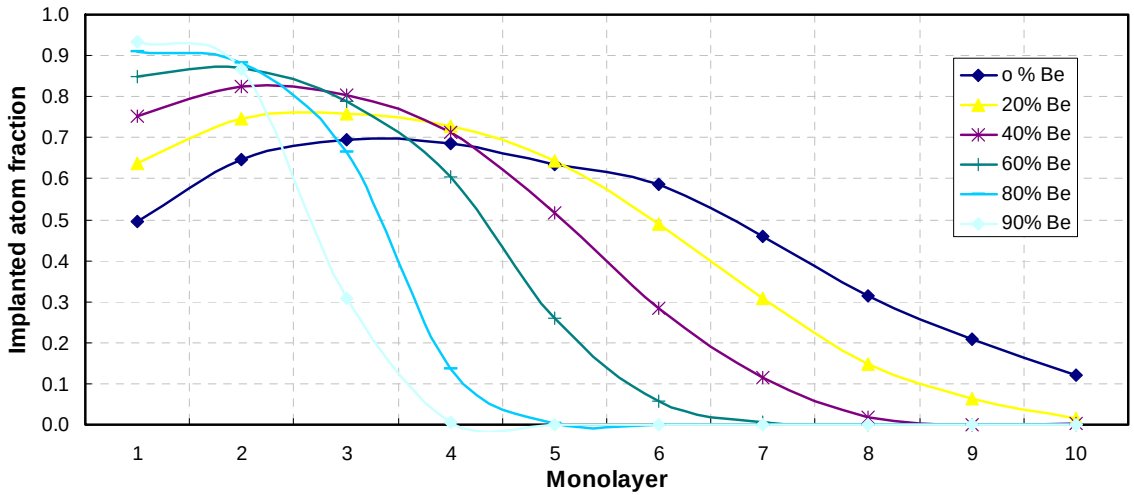
Outer Divertor: $\Phi_{Be} = 3.021 \times 10^{20}$ #/m^{2}s ($J_{Be} = 1.55 \times 10^{21}$ s^{-1}, Area = 5.13 m^2)

Without convection term:

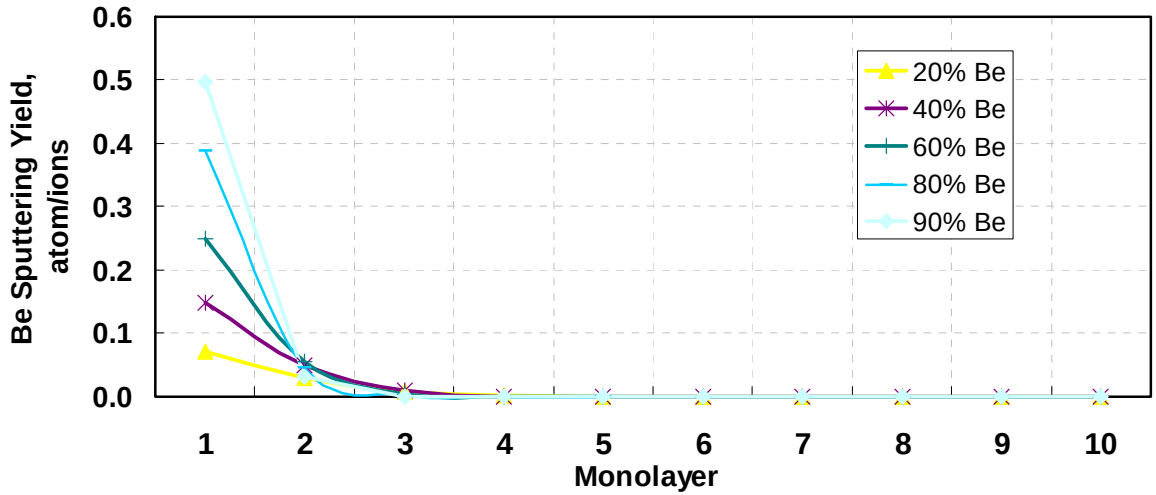
Inner Divertor: $\Phi_{Be} = 4.785 \times 1019$ #/m^{2}s ($J_{Be} = 1.89 \times 10^{20}$ s^{-1}, Area = 3.95 m^2)

Outer Divertor: $\Phi_{Be} = 1.633 \times 1019$ #/m^{2}s ($J_{Be} = 8.38 \times 1019$ s^{-1}, Area = 5.13 m^2)

Simplified Mixing Model in W Divertor



Be Sputtering Yield from the Different Mono-Layers for 0.1 keV Be Flux on in W-xBe



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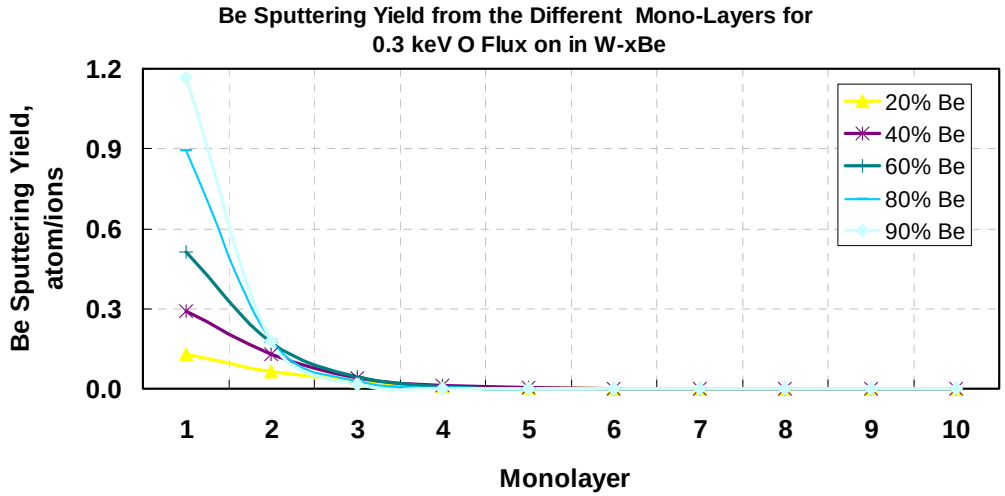

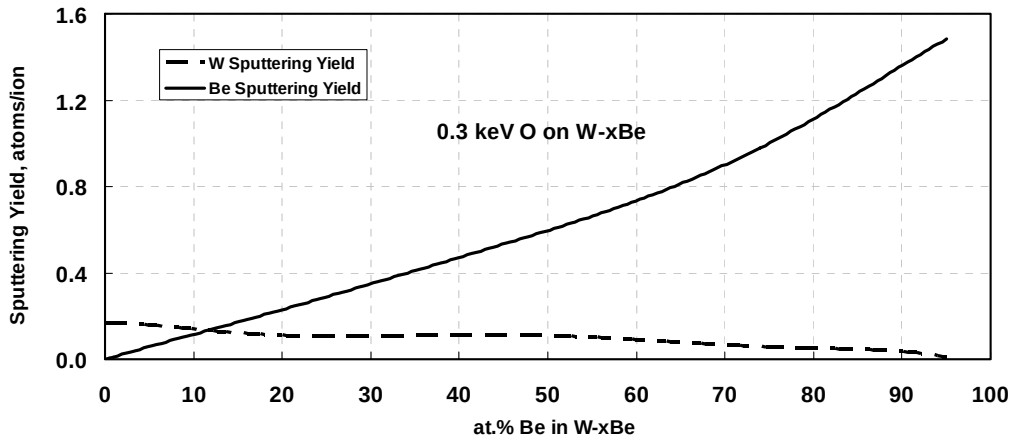

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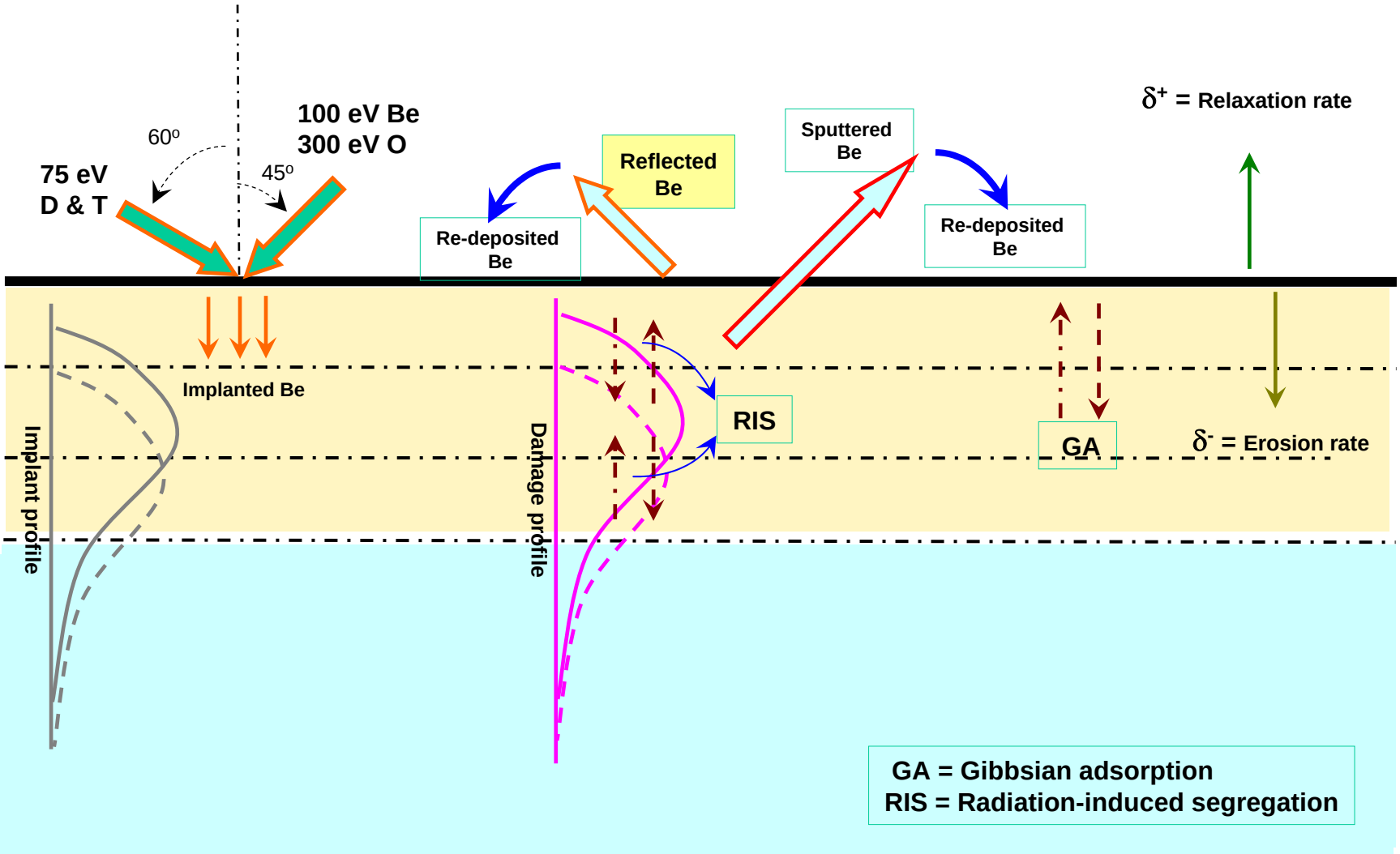
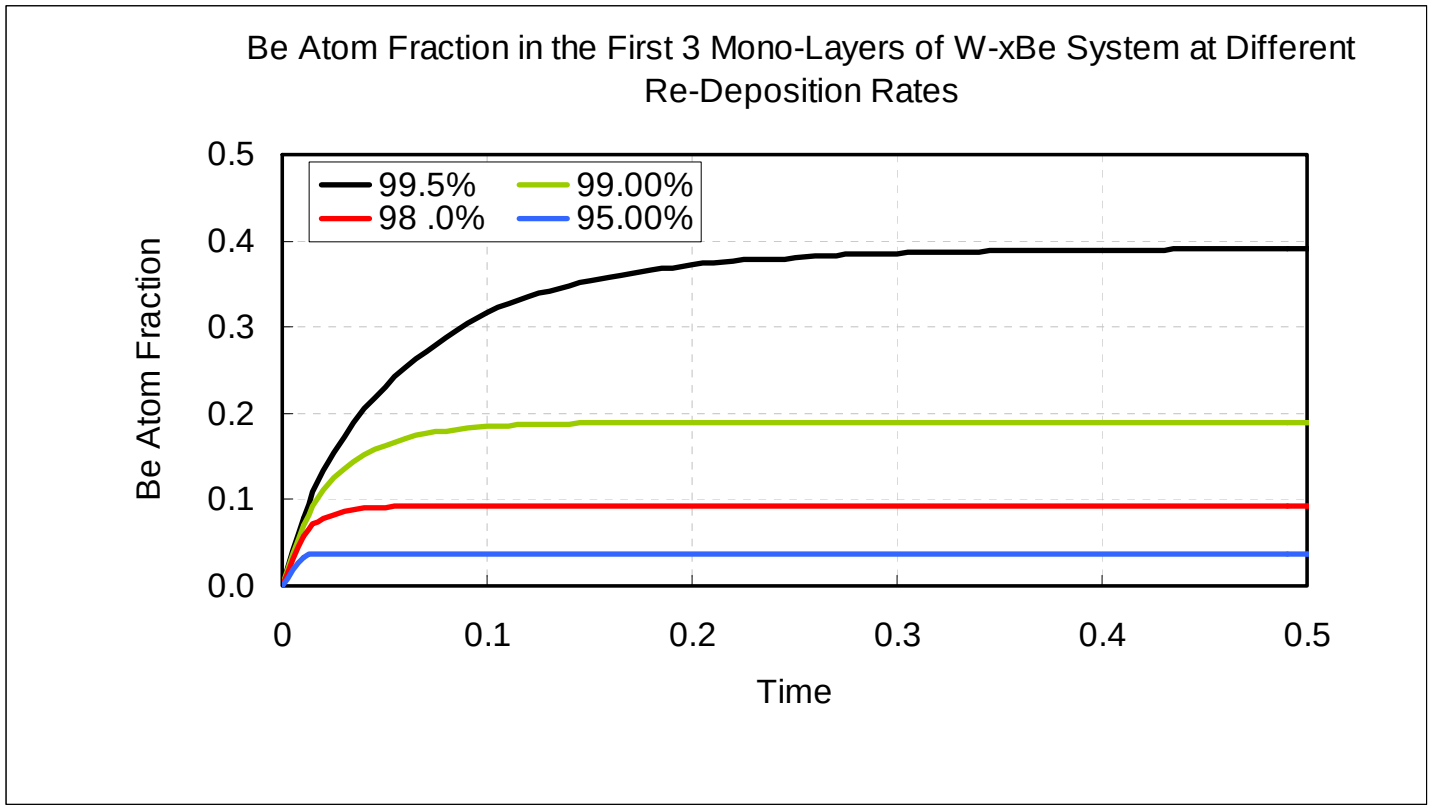
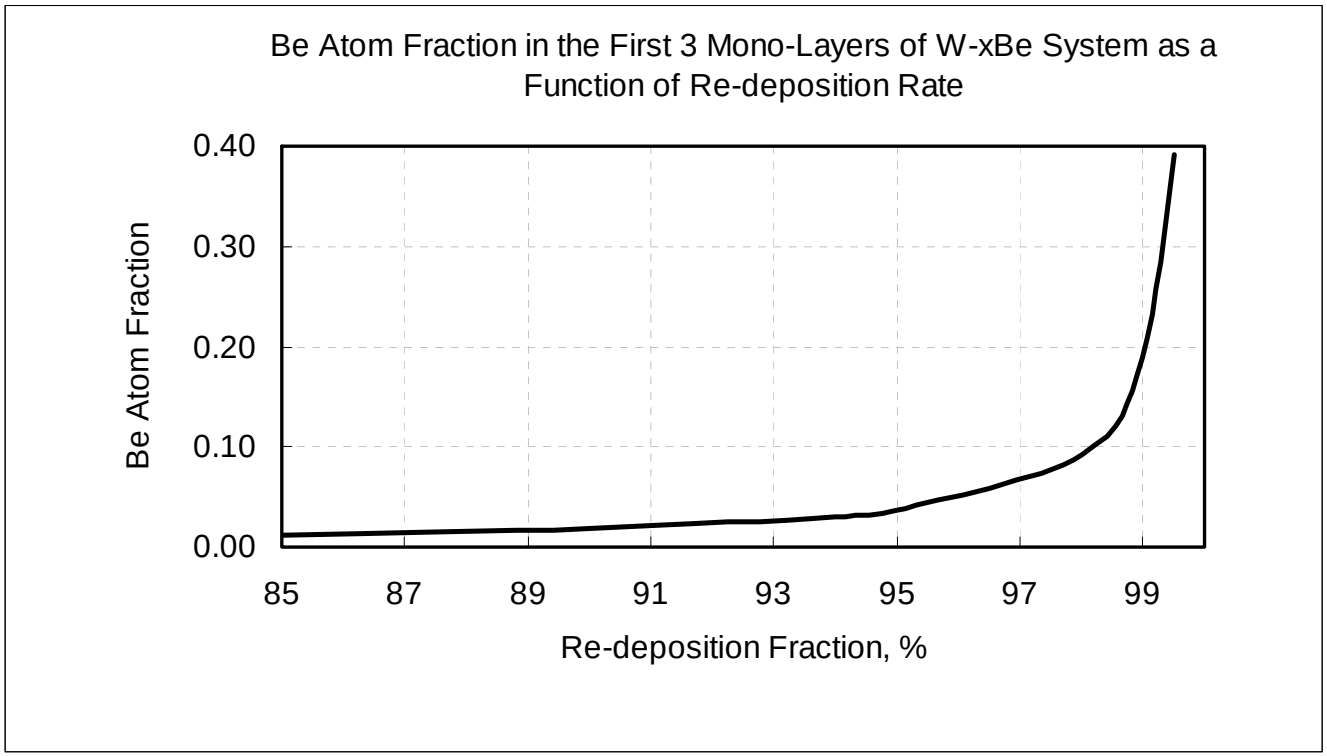


Simplified Mixing Model in W Divertor



Simplified Mixing Model in W Divertor