

# Plasma-surface interaction modeling work at the UIUC

J.P. Allain, D.A. Alman,  
M. Nieto and D.N. Ruzic

*University of Illinois, Urbana-Champaign  
Department of Nuclear, Plasma and Radiological  
Engineering*

Plasma-Material Interaction Group

ALPS/APEX Meeting, Del Mar, CA  
April 15-17, 2002

# Outline of Talk

- Molecular Dynamics simulations of hydrocarbon plasma-material interaction
- Molecular Dynamics simulations of liquid lithium plasma-material interaction
- Low-energy reflection and reflected charge state of lithium self-bombardment
- FIRE modeling of plasma-material interactions at the first wall and divertor regions
- Future PMI modeling work at the UIUC

# Introduction

- Reflection coefficients calculated using Molecular dynamics (MD) code
  - Incident species ultimately to include:
    - C, H, CH to CH<sub>4</sub>, C<sub>2</sub>H to C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H to C<sub>3</sub>H<sub>6</sub>
  - Low incident energies relevant to fusion
    - 0.0259 eV (room temperature) to ~10 eV
  - Also can vary angle of incidence, surface & projectile temperatures
- Key results
  - Reflection coefficient
  - Energy and angular distribution of reflected particles
- Results can be included in codes for erosion/redeposition modeling
  - WBC – Jeffrey Brooks' analysis of JET tritium codeposition on inner louver surfaces

# Molecular Dynamics Code

- MolDyn code used as starting point
  - Originally written by Keith Beardmore at Loughborough University (UK)
  - Modified to some extent by Karsten Albe while at the University of Illinois in R. Averback's group
  - Uses the Brenner hydrocarbon potential (specifically parameter set II) <sup>1</sup>
  - Temperature control by velocity scaling method of Berendsen <sup>2</sup>
  - Integrator: Beeman method (third order, fixed timestep) <sup>3</sup>
- Many modifications made to suit the problem at hand

Lattices other than pure graphite

Smart termination of the simulation

Random impact locations on the surface

Graphical user interface (GUI)

Molecule detector

Customized output (including graphics)

Hydrocarbon molecules incident

Distributed computing

<sup>1</sup> D. W. Brenner, Empirical potential for hydrocarbons for use in simulating the chemical vapor deposition of diamond films. Physical Review B, 1990. 42(15): p. 9458-9471.

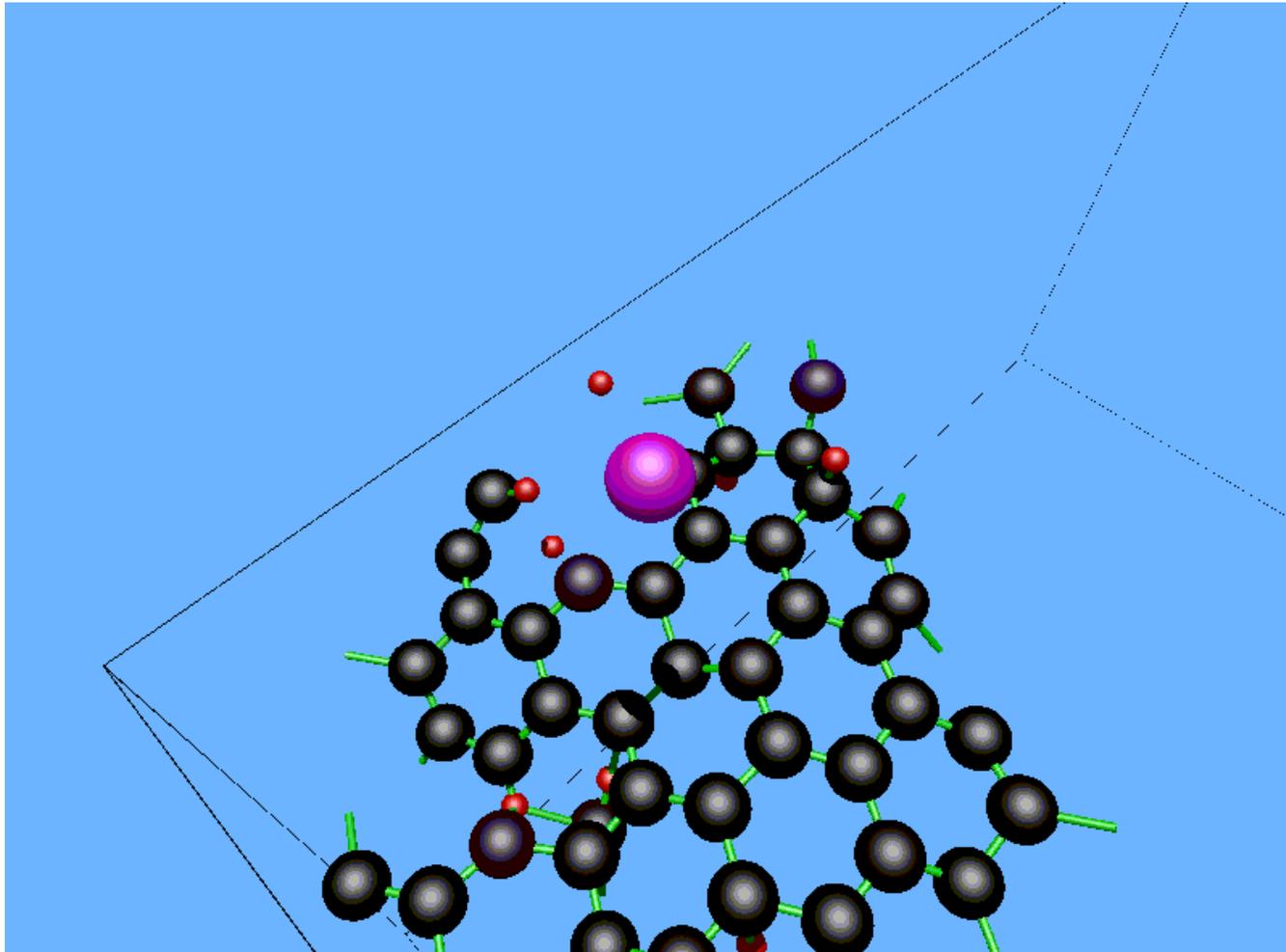
<sup>2</sup> H. J. C. Berendsen, J. P. M. Postman, W. F. v. Gunsteren, et al., Journal of Chemical Physics, 1984. 81: p. 3684.

<sup>3</sup> D. Beeman, Some multistep methods for use in molecular dynamics calculations. J. Comp. Phys., 1976. 20: p. 130-139.

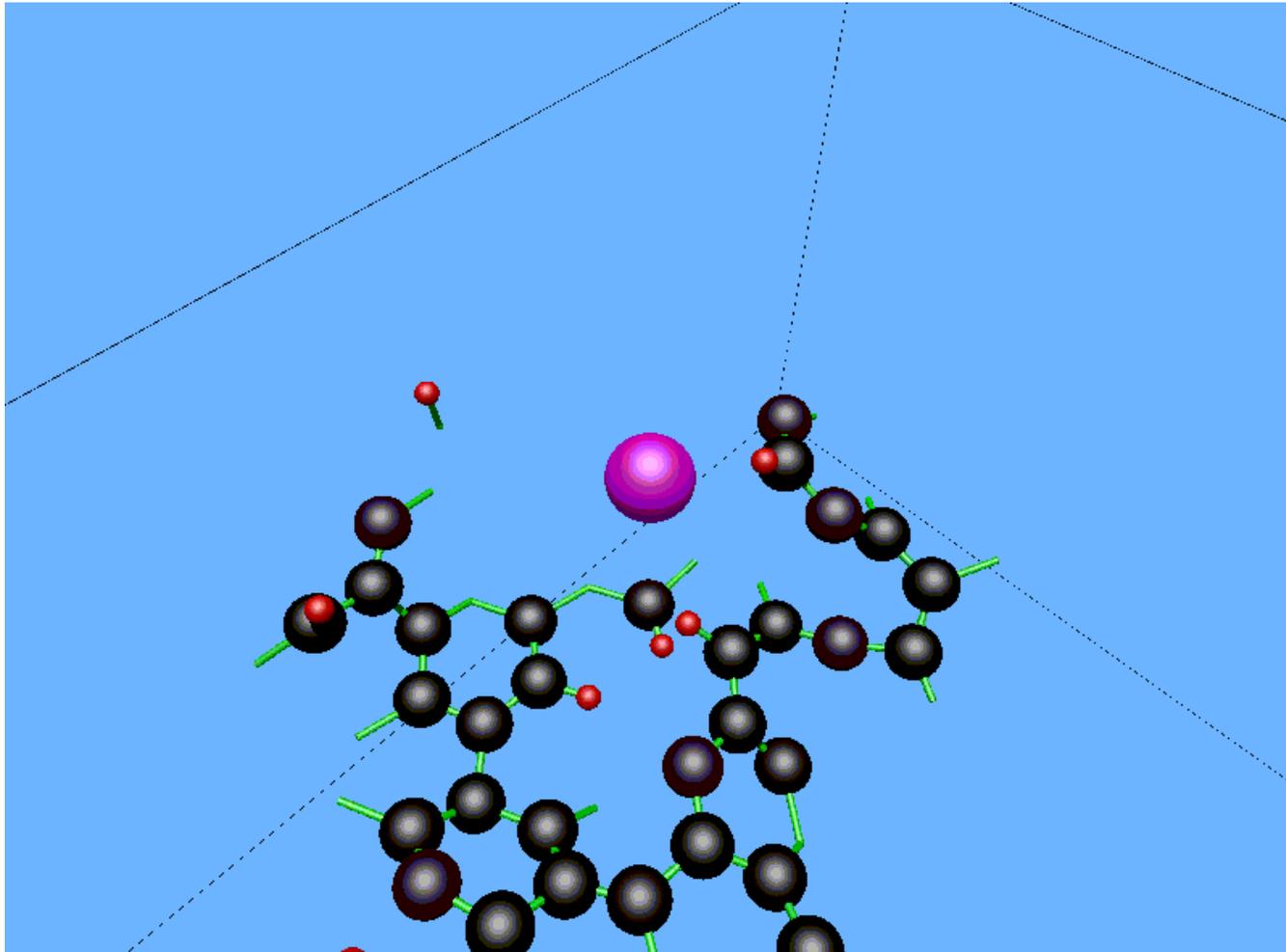
# How it works

- Pure graphite lattice bombarded by thousands of 20 eV hydrogen atoms
- Resulting saturated ( $\sim 0.4$  H:C) surface used in subsequent simulations
- Multiple separate flights launched, each at a random impact location on the surface
- Reflection coefficient, reflected species, energy and angular distributions tallied

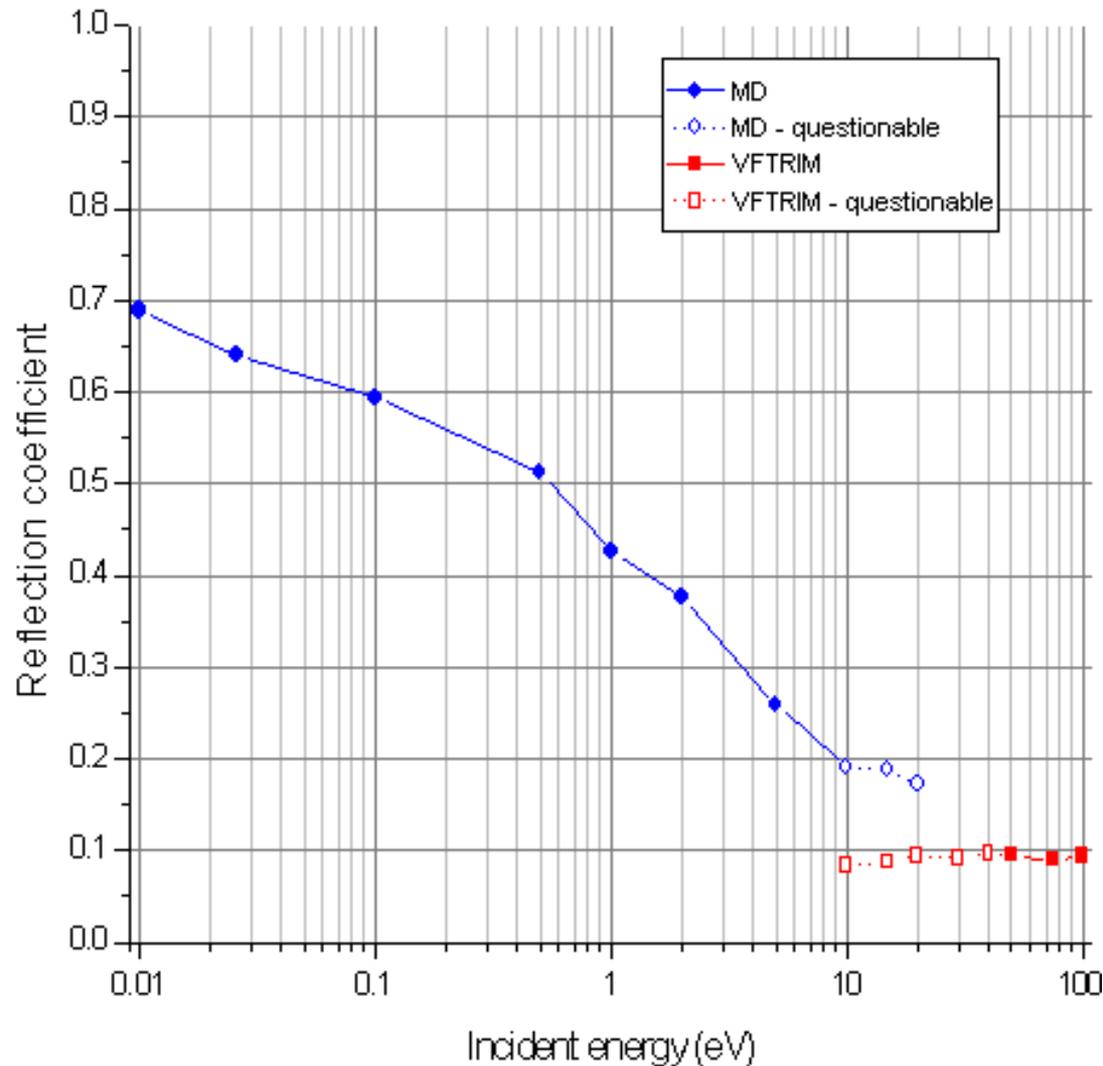
# Carbon incident at 5 eV and 45 degrees – Reflection



# Carbon incident at 5 eV and 45 degrees – Sticking

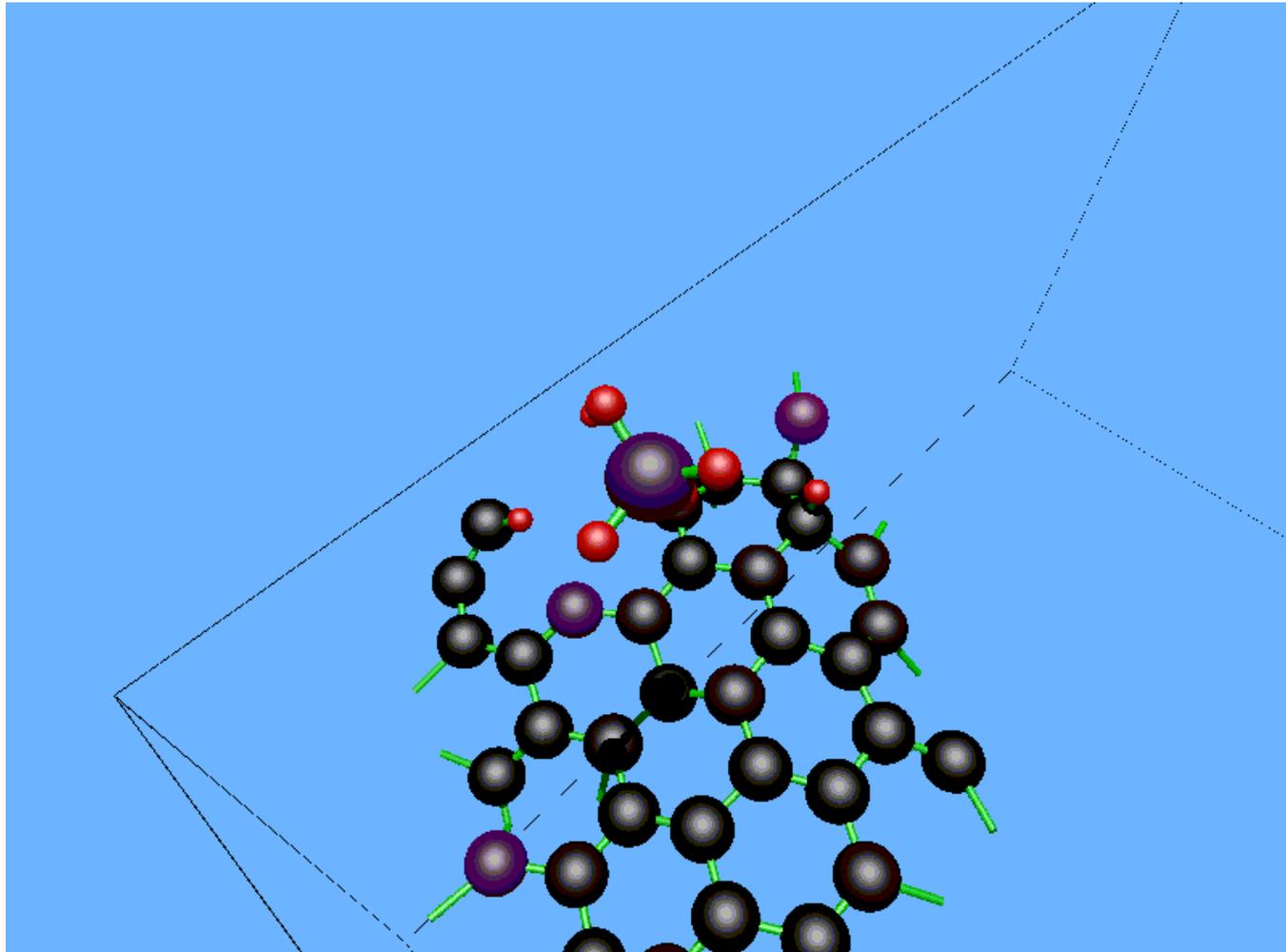


# Comparison with VFTRIM at upper end of energy range

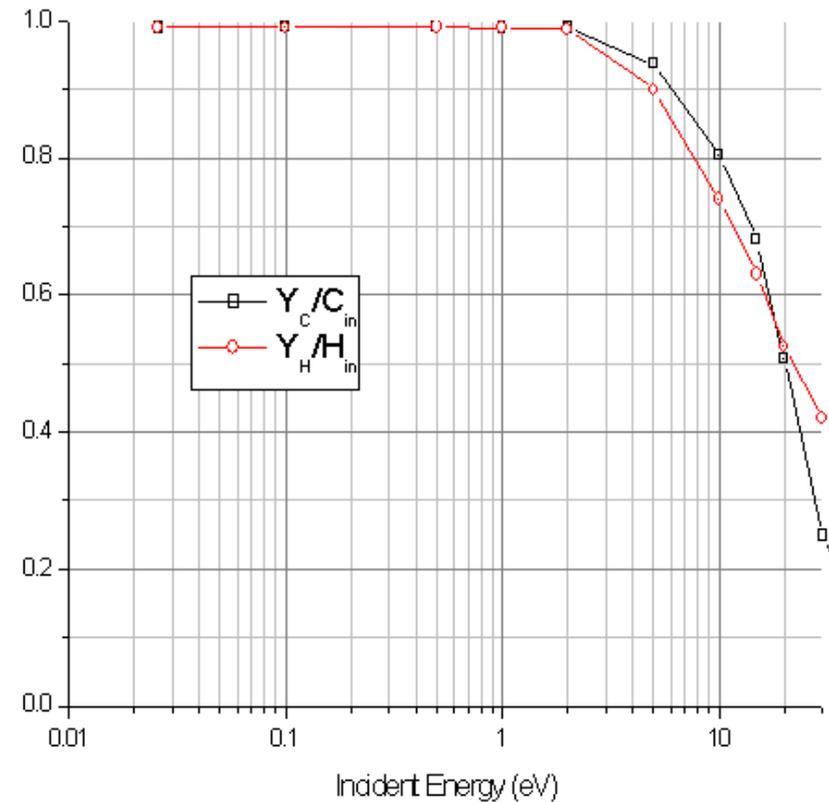
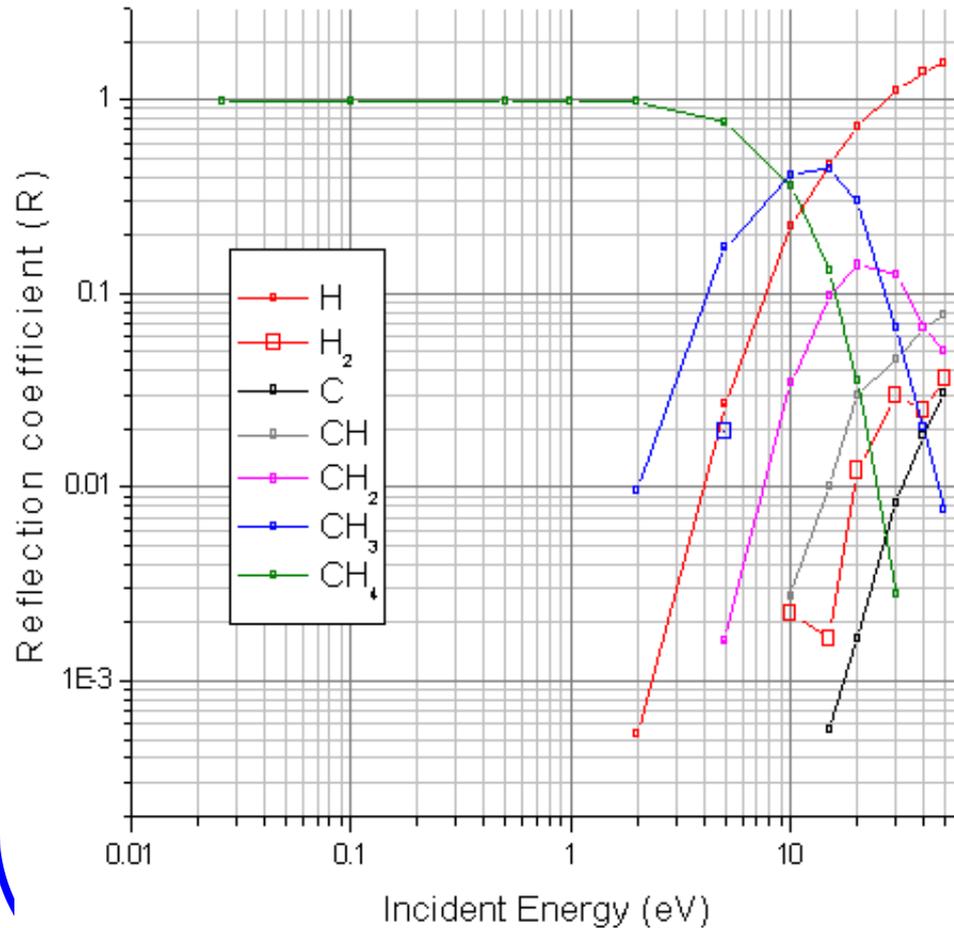


Reflection of  
carbon on C:H at  
45 degrees

# Methane incident at 5 eV and 45 degrees – Breakup



# CH<sub>4</sub> at 45° on C:H results



# Sticking coefficients of thermal hydrocarbon species

The surface loss probability ( $b$ ) is the upper limit of the sticking coefficient, defined as  $b = s + g$ , where  $g$  is the probability of the molecule to react at the surface, forming a non-reactive volatile molecule. The sum of reflection and  $b$  is  $r + s + g = 1$ .



Species	Surface Loss Probability	Sticking Coefficient	Method	Ref.
CH <sub>2</sub>	0.025-0.028		Decay in the afterglow	1
	<10 <sup>-3</sup>		Decay in the afterglow	1
	10 <sup>-3</sup> -0.014		Decay in the afterglow	2
CH <sub>3</sub>	<0.014	0.006	Modeling of ITMS result measured with diff. Pumped HIDDEN MS	3
		10 <sup>-4</sup> -10 <sup>-2</sup>	Radical beam experiments	4
C <sub>2</sub> H	0.92		Cavity experiment	5
C <sub>2</sub> H <sub>3</sub>	0.35		Cavity experiment	6
C <sub>2</sub> H <sub>5</sub>	10 <sup>-3</sup>		Cavity experiment	7

<sup>1</sup> H. Toyoda, H. Kojima, H. Sugai, Appl. Phys. Lett. **54**, 1507 (1989)

<sup>2</sup> M. Shirantani, J. Jolly, H. Videlot, J. Perrin, Jap. J. Appl. Phys. **36**, 4752 (1997)

<sup>3</sup> P. Kae-Nune, Plasma Sources Sci. Technol. **4**, 250 (1995)

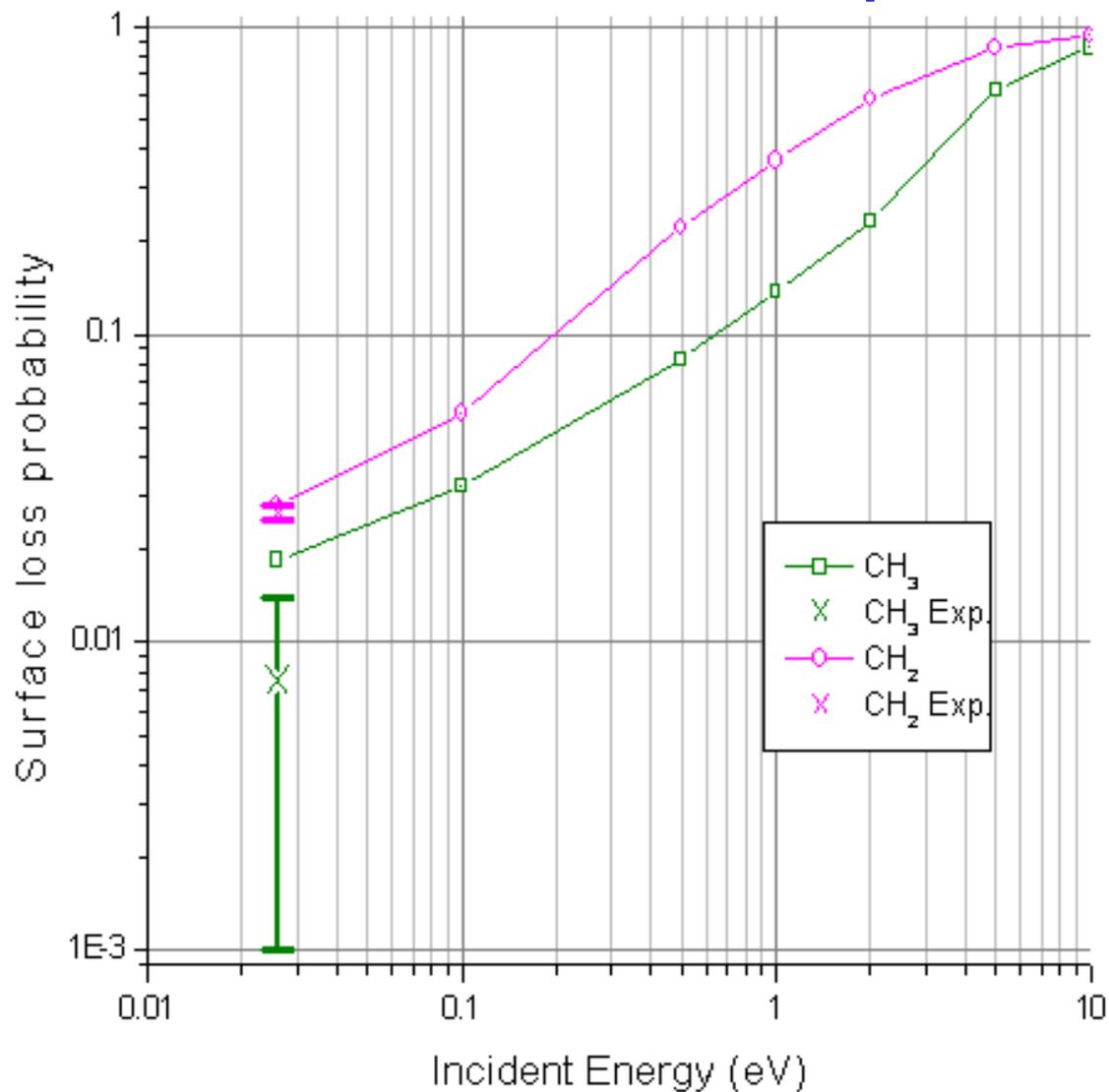
<sup>4</sup> A. von Keudell, T. Schwarz-Selinger, M. Meier, W. Jacob, Appl. Phys. Letters **76**, 676 (2000)

<sup>5</sup> C. Hopf, K. Letoumeur, T. Schwarz-Selinger, W. Jacob, A. von Keudell, Appl. Phys. Lett. **74**, 3800 (1999)

<sup>6</sup> A. von Keudell, C. Hopf, T. Schwarz-Sellinger, W. Jacob, Nucl. Fusion **39**, 1451 (1999)

<sup>7</sup> C. Hopf, T. Schwarz-Sellinger, W. Jacob, A. von Keudell, J. Appl. Phys. **87**, 2719 (2000)

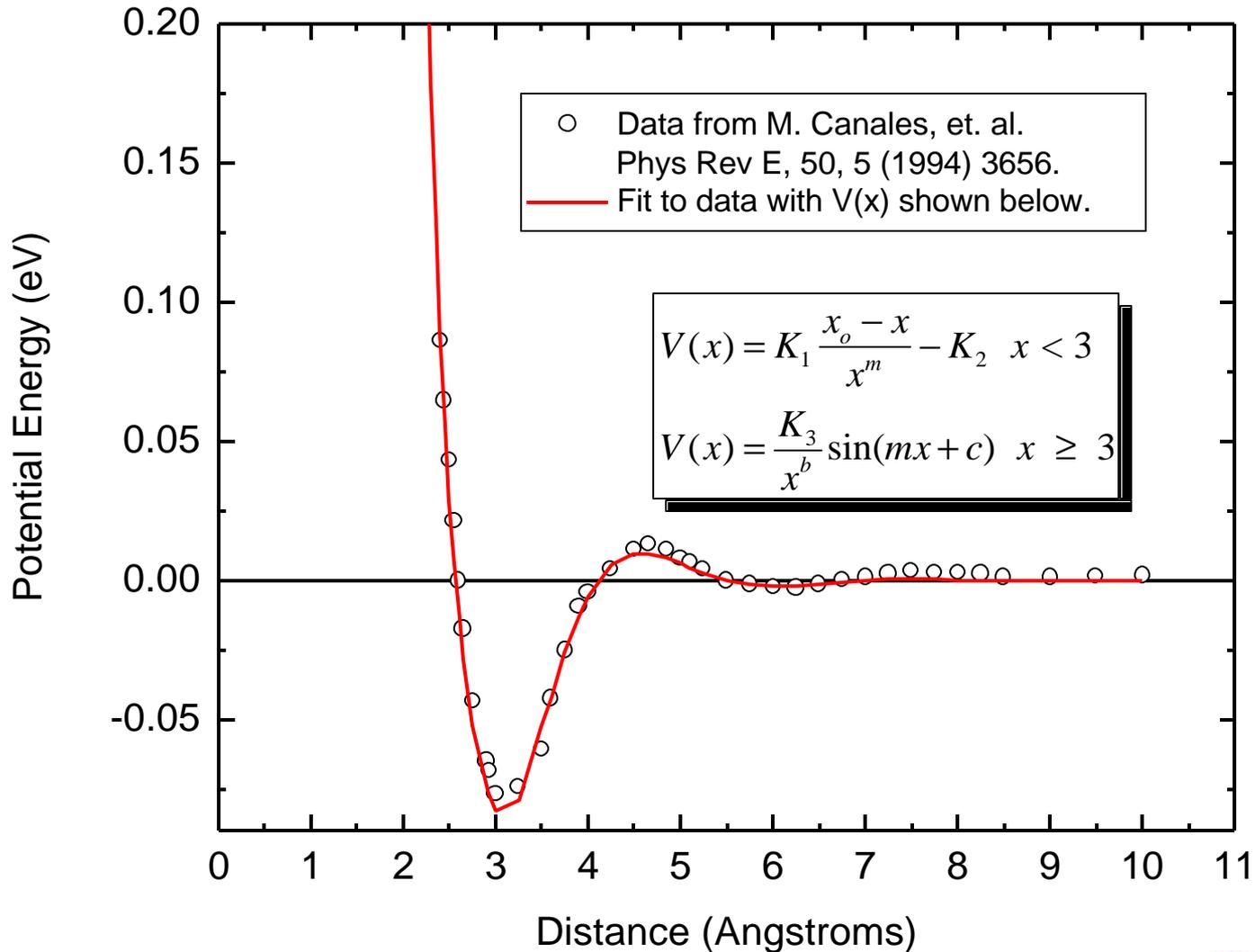
# Comparison of MD results to experimental surface loss probabilities



# MD Simulation of liquid lithium ion-surface interactions

- MoDyn code modified to study Li
  - Effective Li-Li pair potential at 473 K added, replaces Brenner hydrocarbon potential
  - Other adjustments required & completed
- Construction of a liquid lithium surface
  - Started with BCC Li at room temperature
  - Heated above the melting point, equilibrated at 473 K for 2 ps
  - Total number of atoms used: 2,733

# Liquid lithium interatomic potential

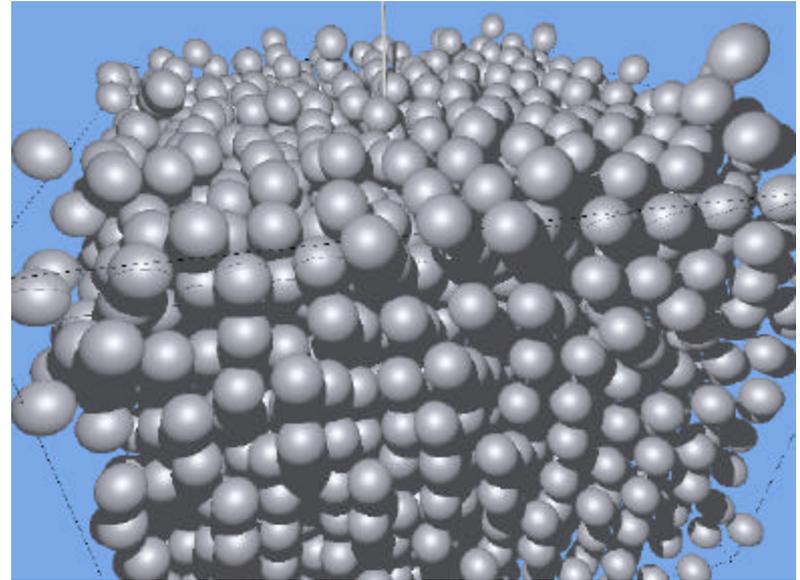
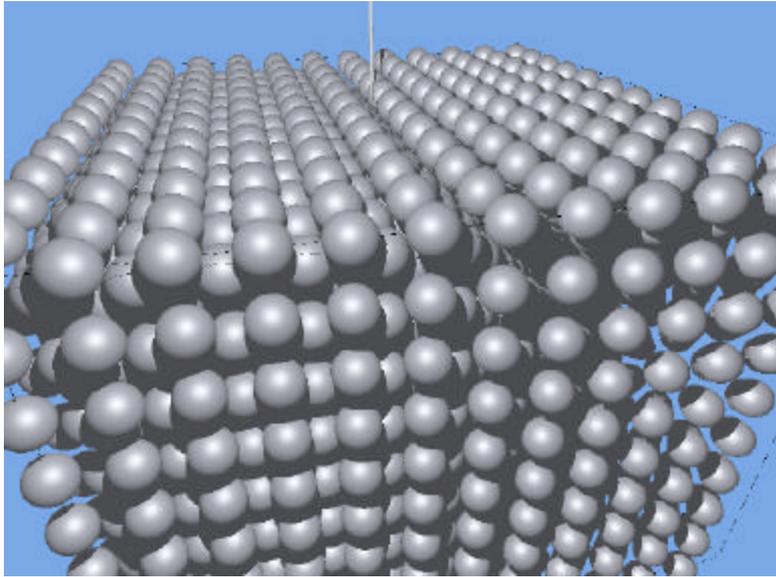


# Interatomic potentials for Liquid Li

Reference	Method	Well depth (eV)	Well Position (Å)
Canales et al	NPA/LDA	0.0767	3
Chihara	HNC/LFC	0.0935	3.18
Morimoto et al	Aschcroft	0.043	3.1

- Attractive well depth variations among different models
- All models coincide on the minimum potential location
- However, NPA and HNC models are more sophisticated and widely used
- Analytical fit to the potential by Canales was used for liquid Li MD simulations

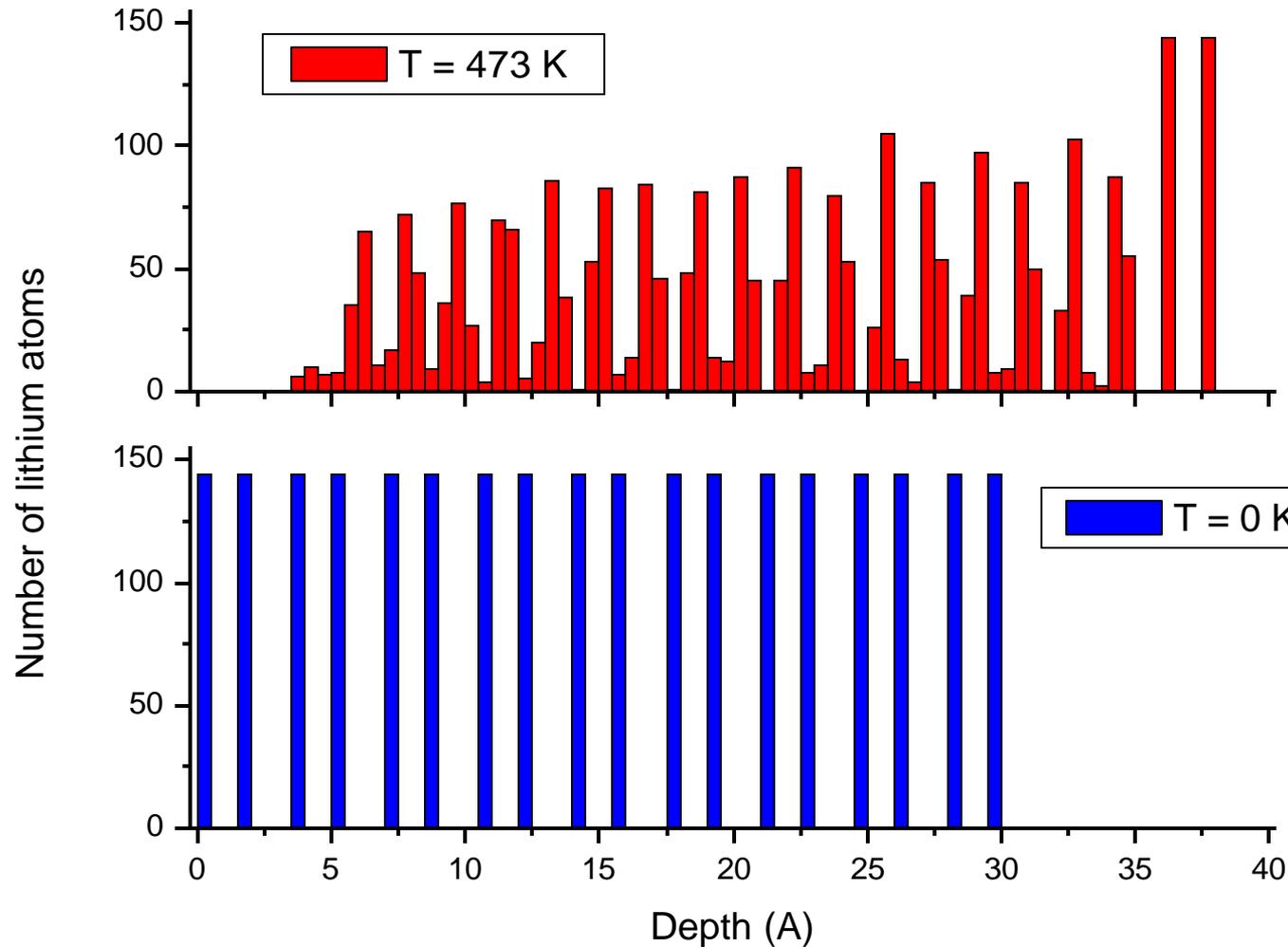
# Liquid lithium simulation setup



- Temperature control is achieved by using a simple velocity scaling technique at each time step<sup>1-3</sup> to maintain the desired temperature at the edges of the surface.
- The resulting target surface is an amorphous liquid lithium surface 42.2 by 42.2 Å and 34.2 Å deep.

1. L. V. Woodcock, Chem. Phys. Lett. **10**, 257 (1970).
2. D. J. Evans, Mol. Phys. **37**, 1745 (1979).
3. T. Schneider and E. Stoll, Phys. Rev. B **13**, 1216 (1976).

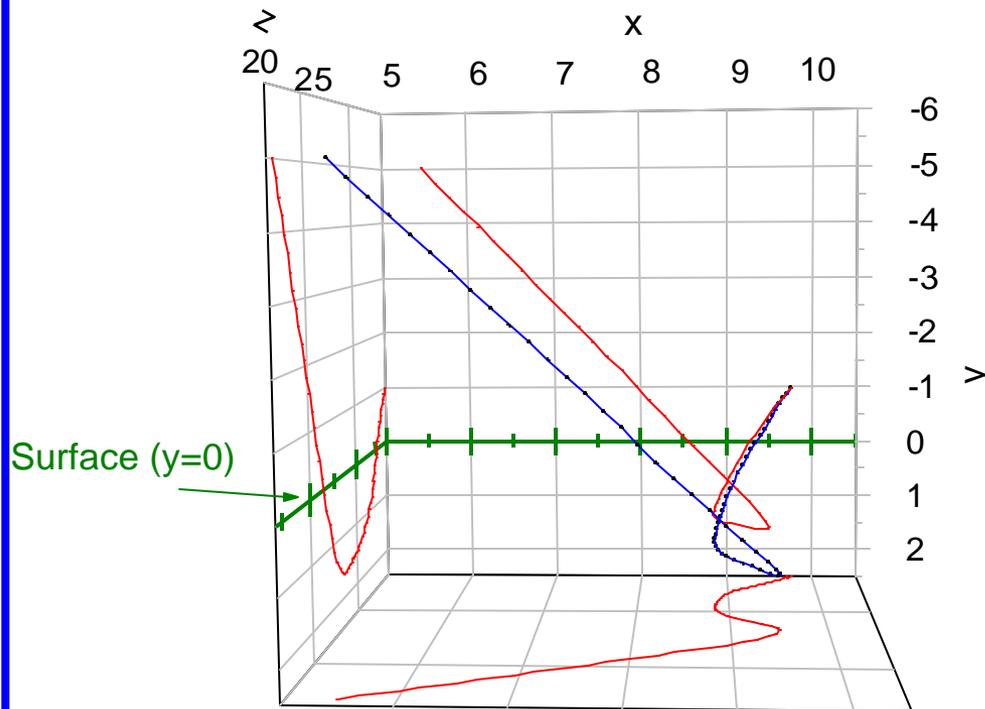
# Order of lithium atoms near the surface



# Study of low energy lithium self-bombardment reflection

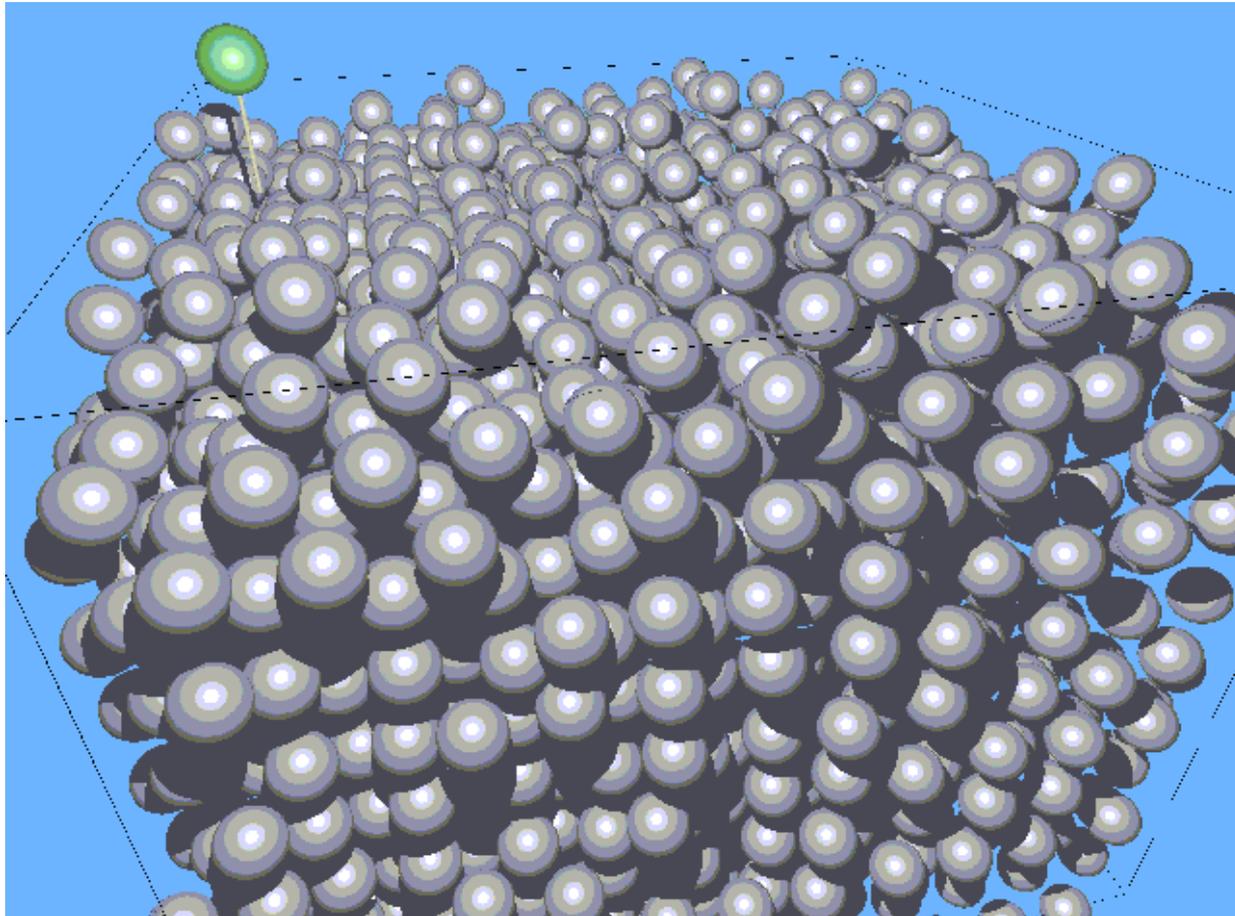
- Sputtered lithium particles leave with a peak energy between 1-2 eV for incident particle energies ranging from 200-700 eV.
- Neutral sputtered particles are ionized very close to the lithium surface and return with nearly the same energy.
- Need to determine lithium self-particle reflection coefficient and an estimate of its charge state at these energies.
- BCA methods are limited at energies below 50-100 eV, therefore MD simulations are conducted.

# Reflected Li from liquid Li surface

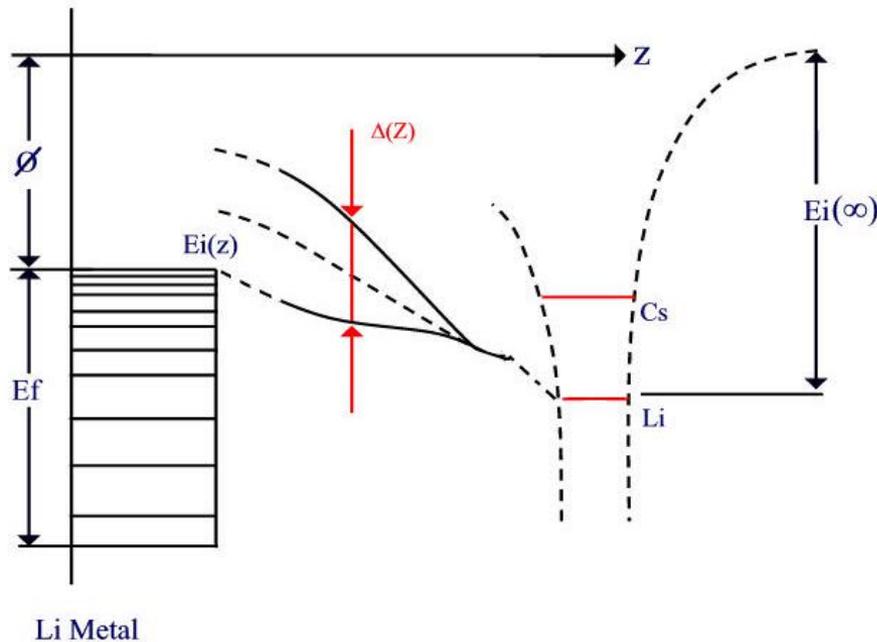


- Criteria for counting reflected particles
  - Final position of lithium atom after 1 ps
  - If position was inconclusive, velocity of particle was considered
    - A particle moving steadily away from the surface could have reflected given more time
  - The potential energy of the atom – whether the atom is bound to the surface or not
    - Atoms with large negative potential energy won't escape

# Lithium at 2 eV, 45 degrees on liquid lithium



# Charge state of lithium reflected particles at low energy



$$P^+(z) = \exp\left(\frac{-2\Delta(z)}{av_p}\right)$$

- Estimate is based on a model developed by R. Brako and D.M. Newns<sup>1</sup> for the charge state of backscattered alkali atoms from metals.
- The model assumes that a single spinless atomic orbital participates in the charge transfer and uses the Newns-Anderson Hamiltonian to model the coupling of the atomic state of the particle to that of the metal.

# Results of low energy lithium self-bombardment reflection from liquid lithium

- Self particle reflection coefficient for lithium atoms at 473 K is  **$0.39 \pm 0.037$** .
- The average energy of reflected lithium atoms is 0.354 eV with a standard deviation of 0.325 eV
- This case is for 45-degree incidence and 2 eV incident particle energy
- The charge state of reflected particles can range from **75-80%** consistent with previous secondary ion sputtered fraction results and results in the literature<sup>1,2</sup>

1. A.J. Algra, E.v. Loenen, E.P. Th. M. Suurmeijer and A.L. Boers, Rad. Effects, **60**, 173 (1982)
2. R. Brako and D.M. Newns, Surf. Science **108**, 253 (1981).

# Future MD simulations of liquid lithium

- Study liquid lithium enhanced erosion phenomena at low energies
- Reflection and sputtering from liquid lithium under fusion-relevant conditions
- Develop interatomic potentials for the lithium-hydride system
- Determine effect on D-treatment on lithium sputtering from MD simulations

# NSO/FIRE Modeling

- Current focus - beryllium/tungsten mixed material erosion issues
- Beryllium from first wall is sputtered, and transported to the divertor
- Result is a Be/W mixture on the divertor surface
- Erosion behavior of this mixed material is critical to FIRE divertor performance
- Collaborative modeling effort, combining several computer codes
  - UEDGE, DEGAS2, VFTRIM, WBC, ITMC

From M. Rensink and T. Rognlien

UEDGE

Data file

Our UEDGE data  
reader/writer

(see screen shots in  
following viewgraph)

Modified UEDGE data file with mesh extended to  
real wall and new ion currents at walls added

DEGAS2 (with  
several  
modifications)

Neutral flux, energy spectrum,  
angular spectrum to first wall

VFTRIM (in a special  
mode to match the  
energy & angle bins  
from DEGAS2)

Sputtered  
beryllium  
from wall

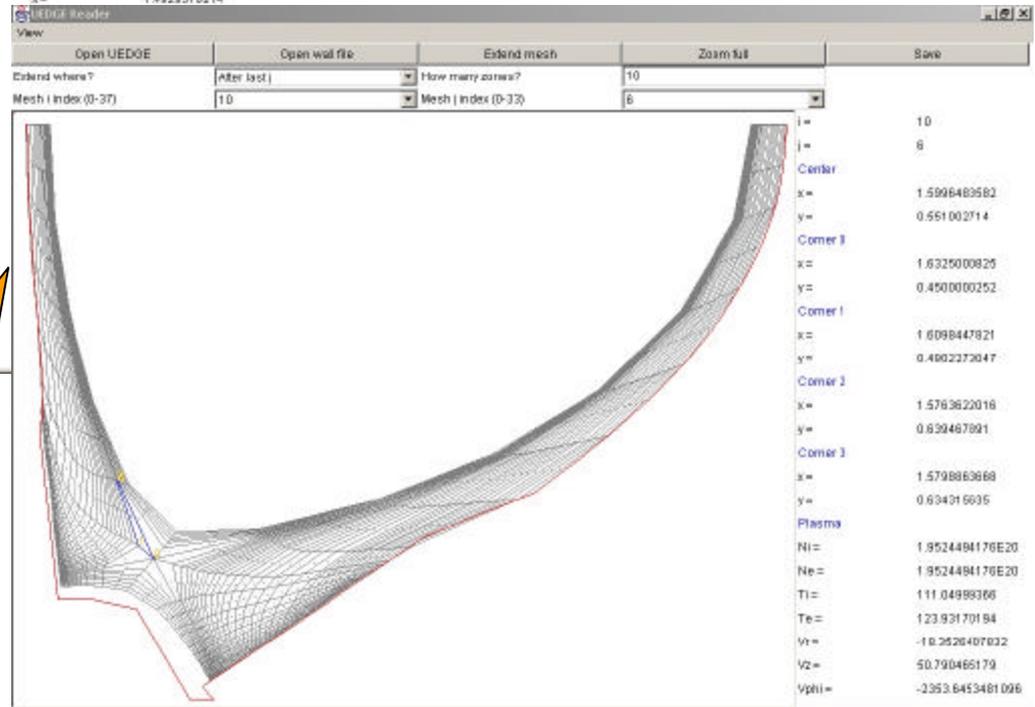
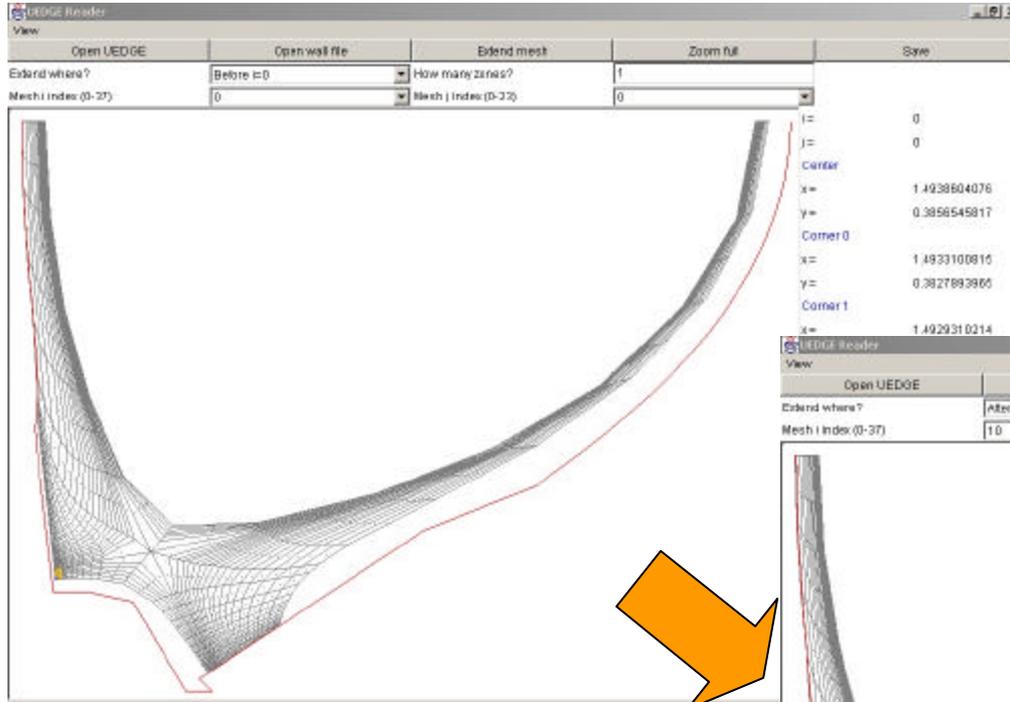
WBC+

Transport  
of Be to  
divertor

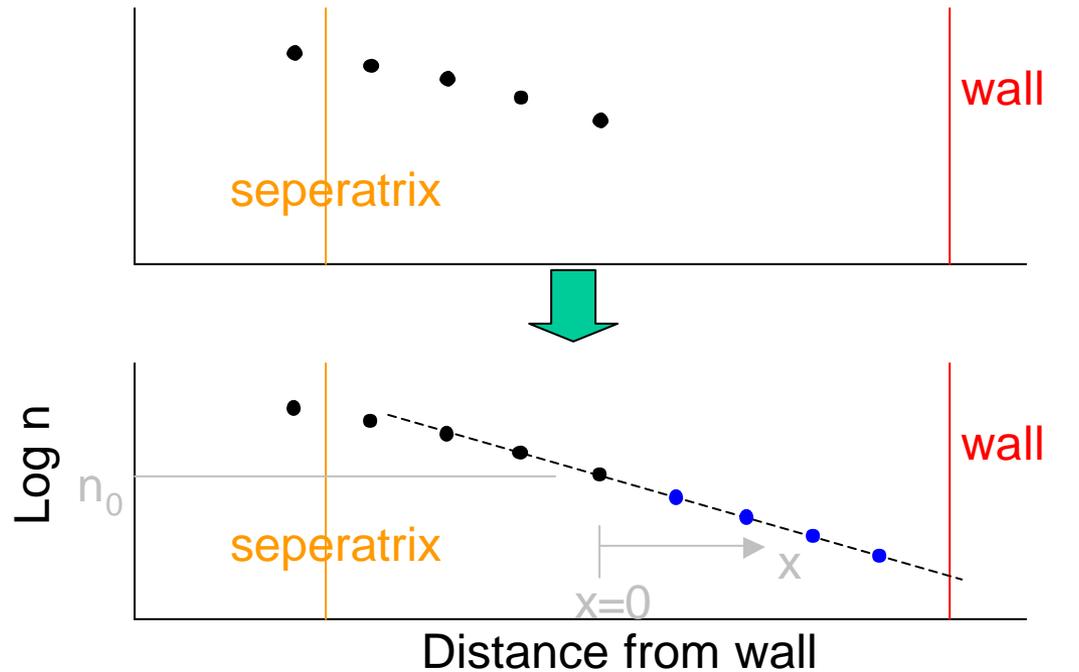
J. Brooks,  
A. Hassanein  
Be/W divertor  
erosion /  
redeposition  
analysis

3-D ITMC  
WBC

# Extrapolation of UEDGE mesh to realistic wall location



# Extrapolation of plasma parameters out to real wall

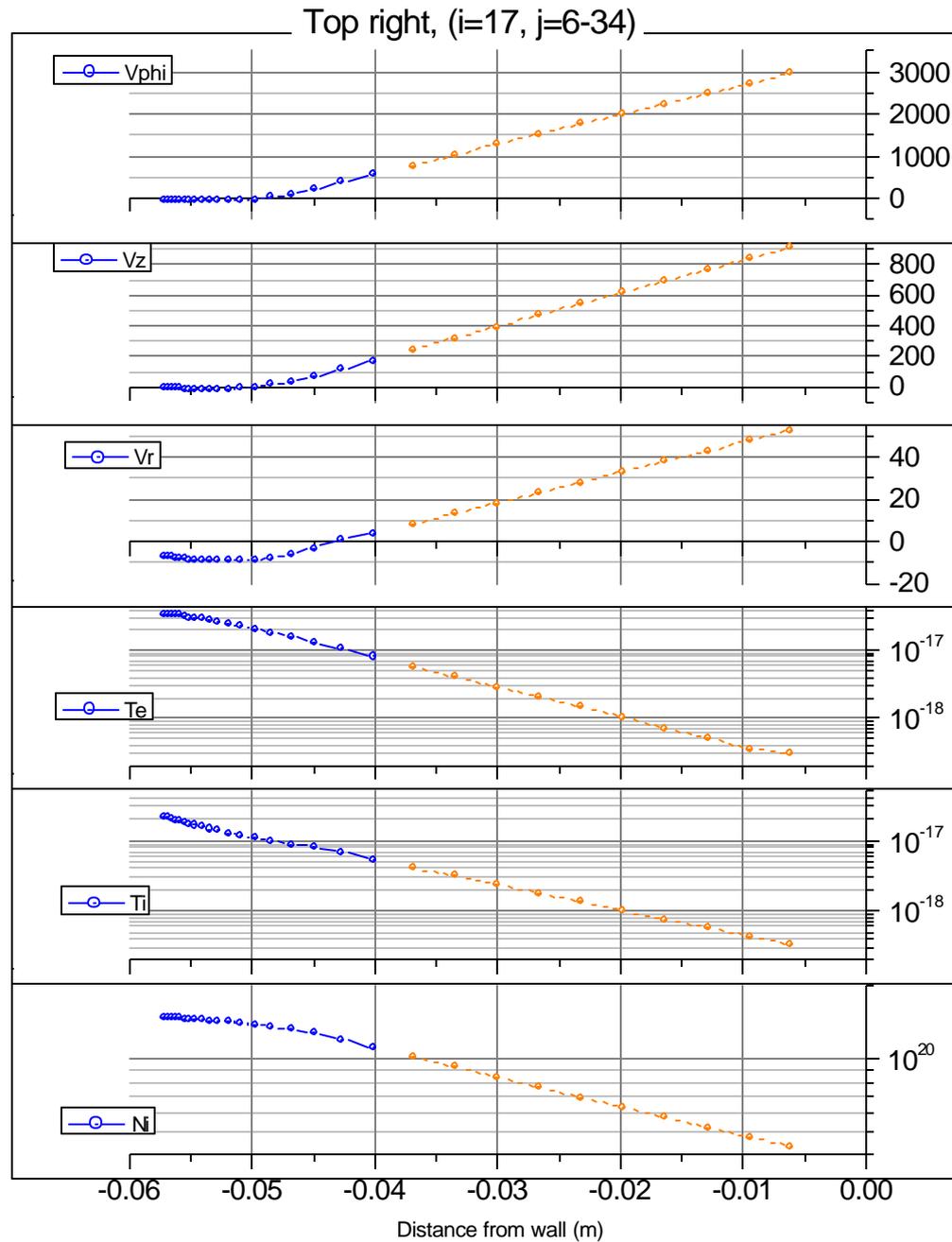


Plasma parameters are calculated from some scrape-off length, as in

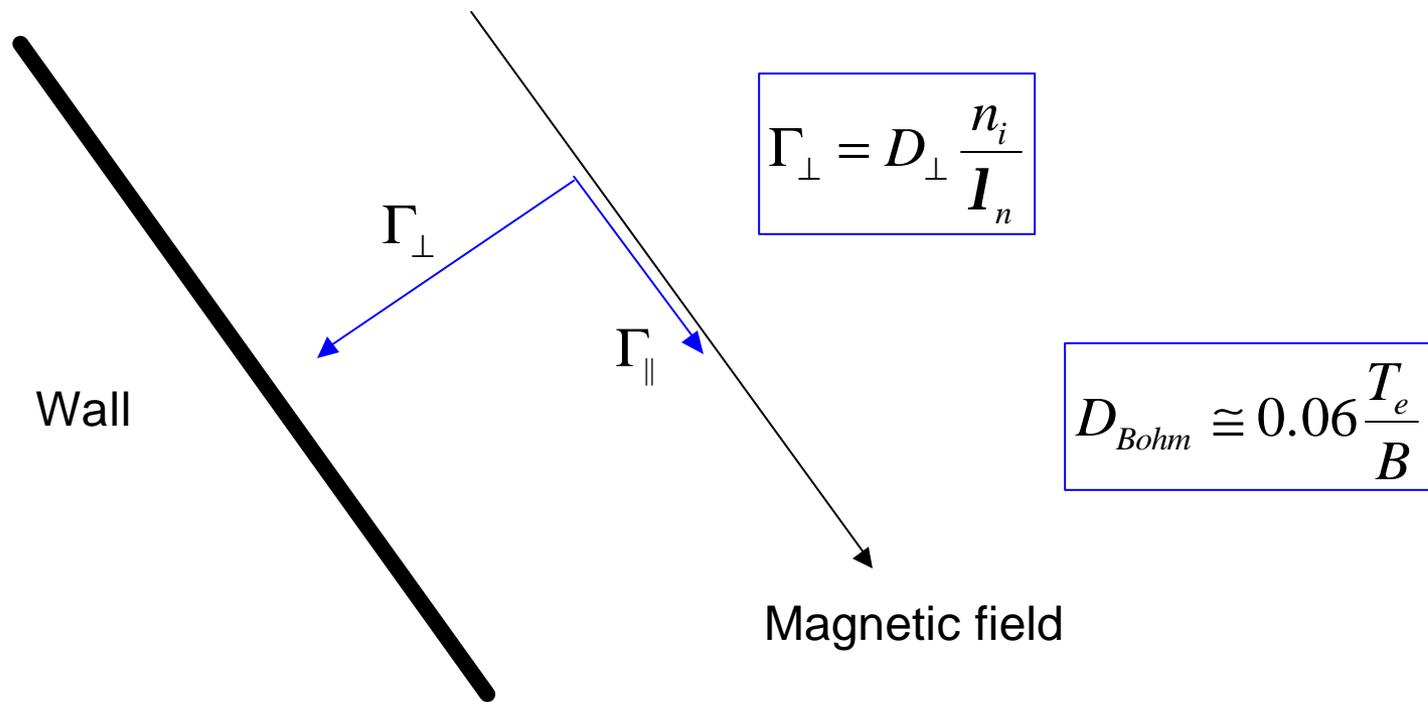
$$n(x) = n_0 \exp\left(\frac{-x}{l_i}\right)$$

where  $l_i$  is calculated to fit the outermost zones in each i row.

An example of the fits and extrapolation

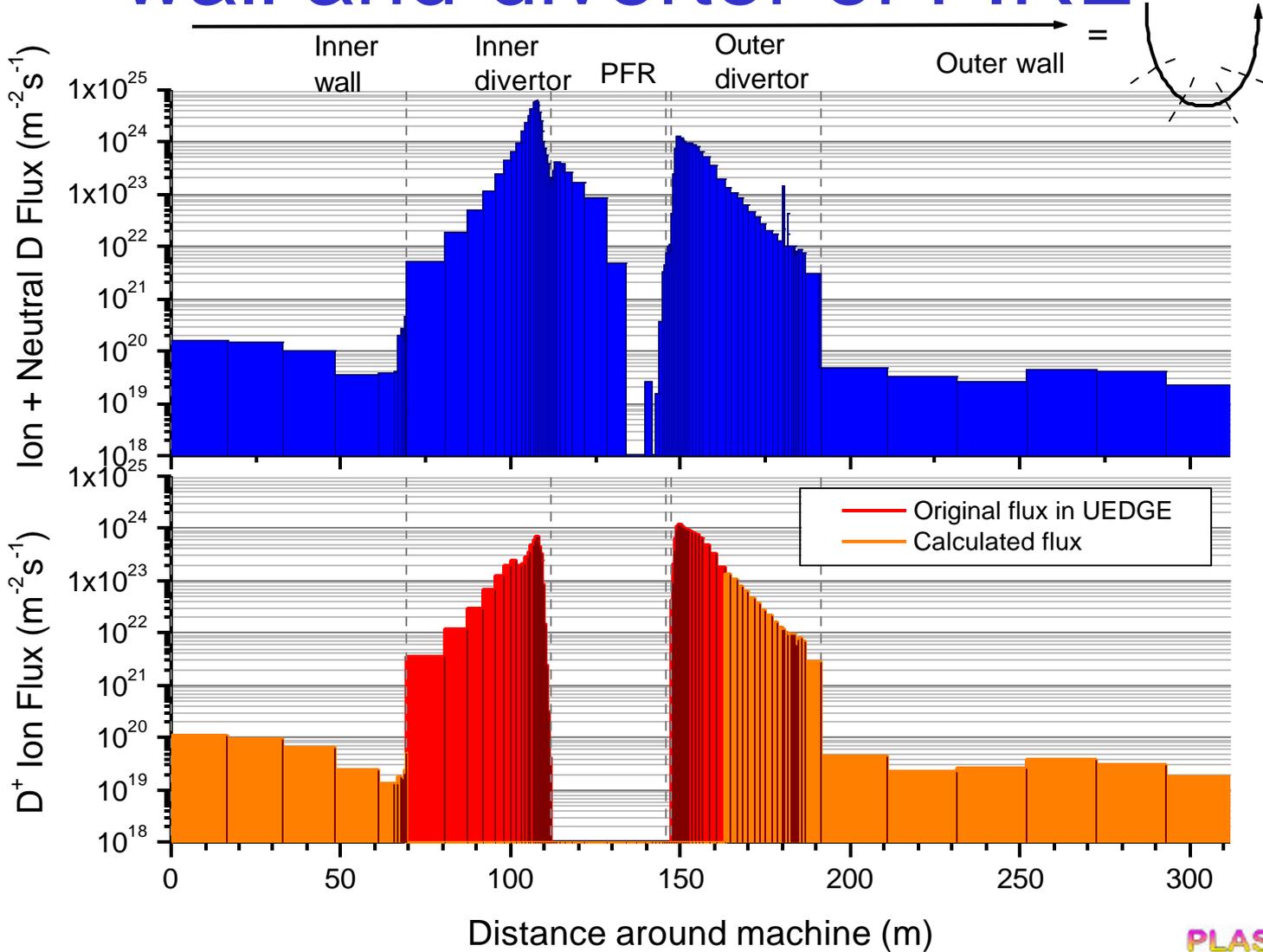


# Model for ion flux to wall

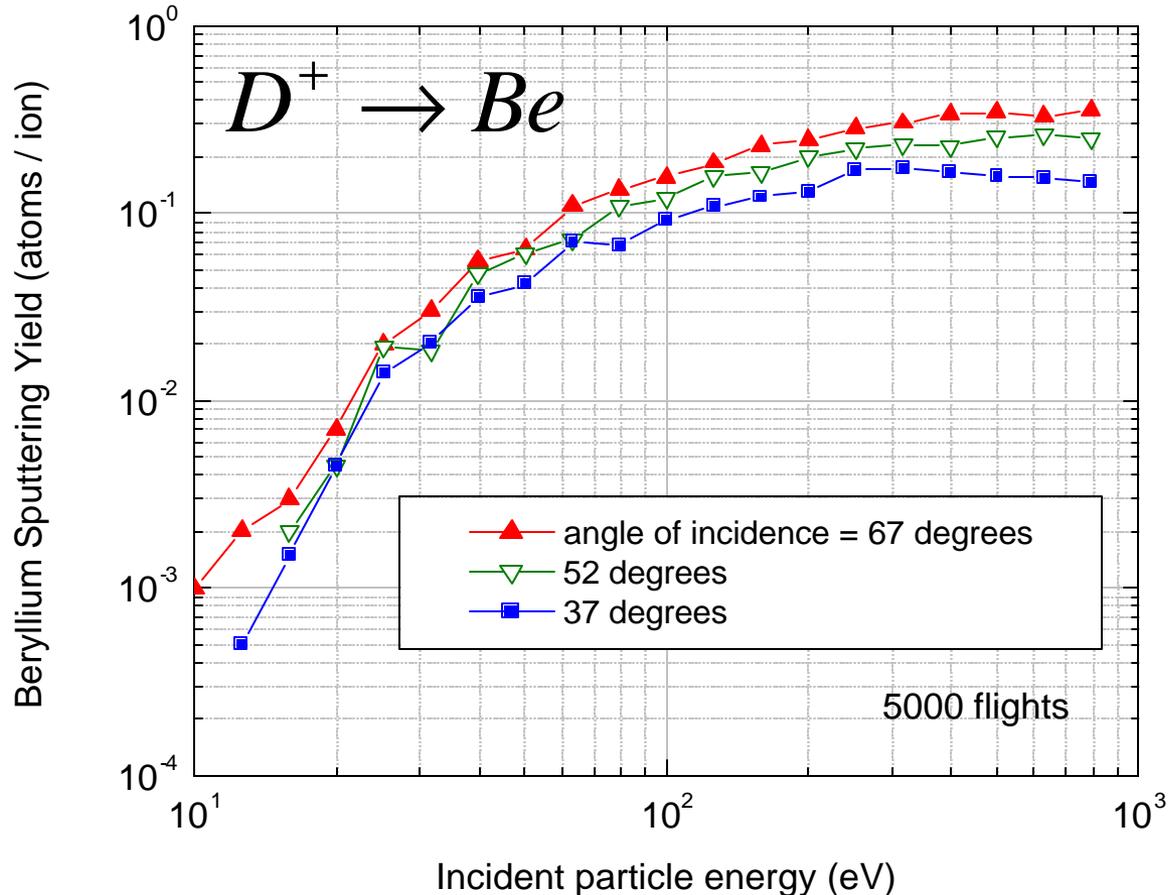


- Since the wall is tangent to the magnetic field, the flux comes from cross-field diffusion
- The perpendicular diffusion coefficient is estimated as the Bohm diffusion coefficient
- The density scrapeoff length was calculated previously (see previous two slides)

# Ion and neutral fluxes to the first wall and divertor of FIRE

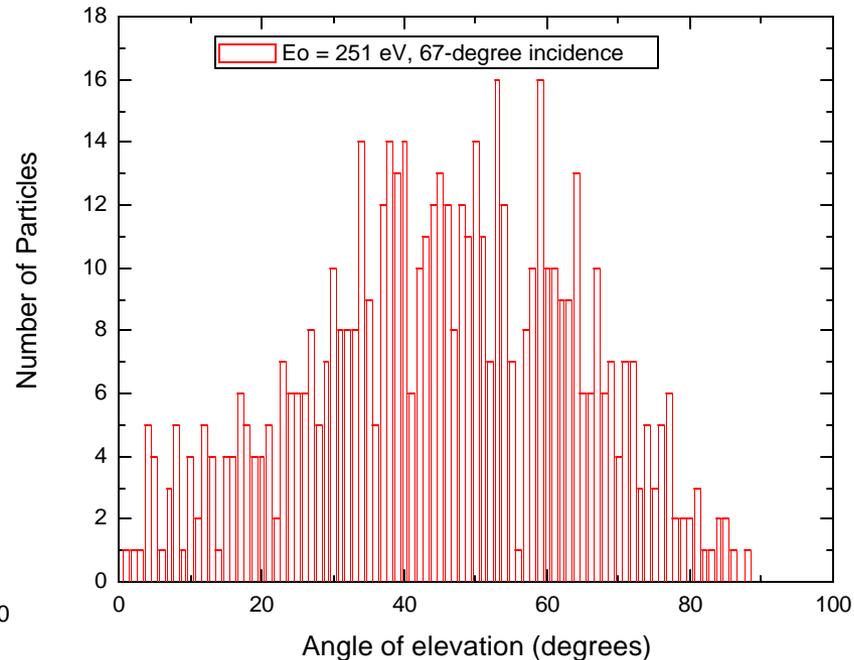
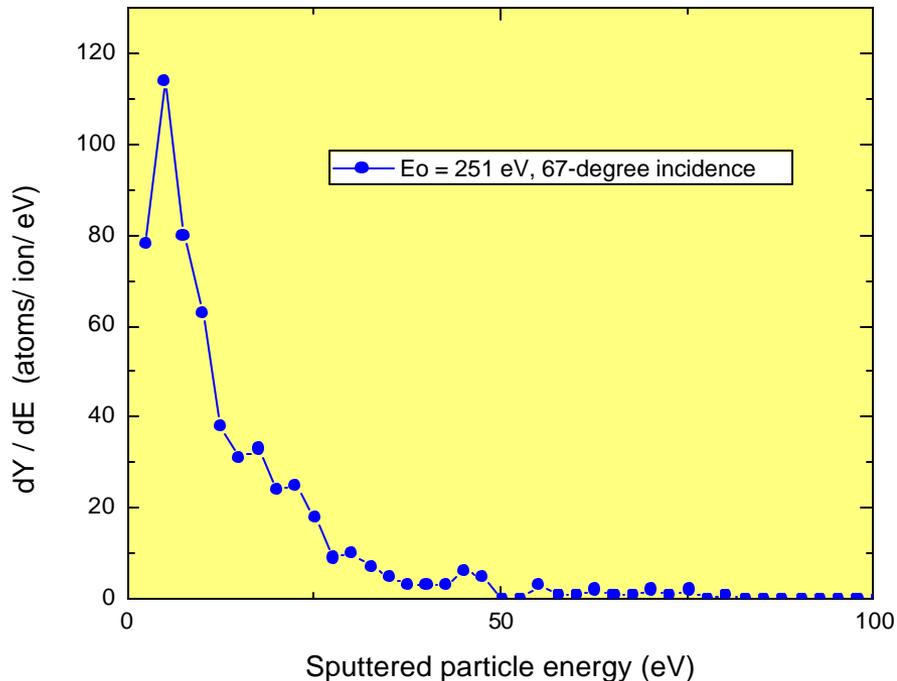


# VFTRIM-3D on Be results



- Fractal dimension  $D = 2.05$ , Surface binding energy = 3.38 eV.
- Binary collision based on the Kr-C interaction potential and classical scattering kinematics.
- Electronic inelastic energy loss model uses an equipartition between the local Oen-Robinson model and non-local Lindhard-Sharff model.

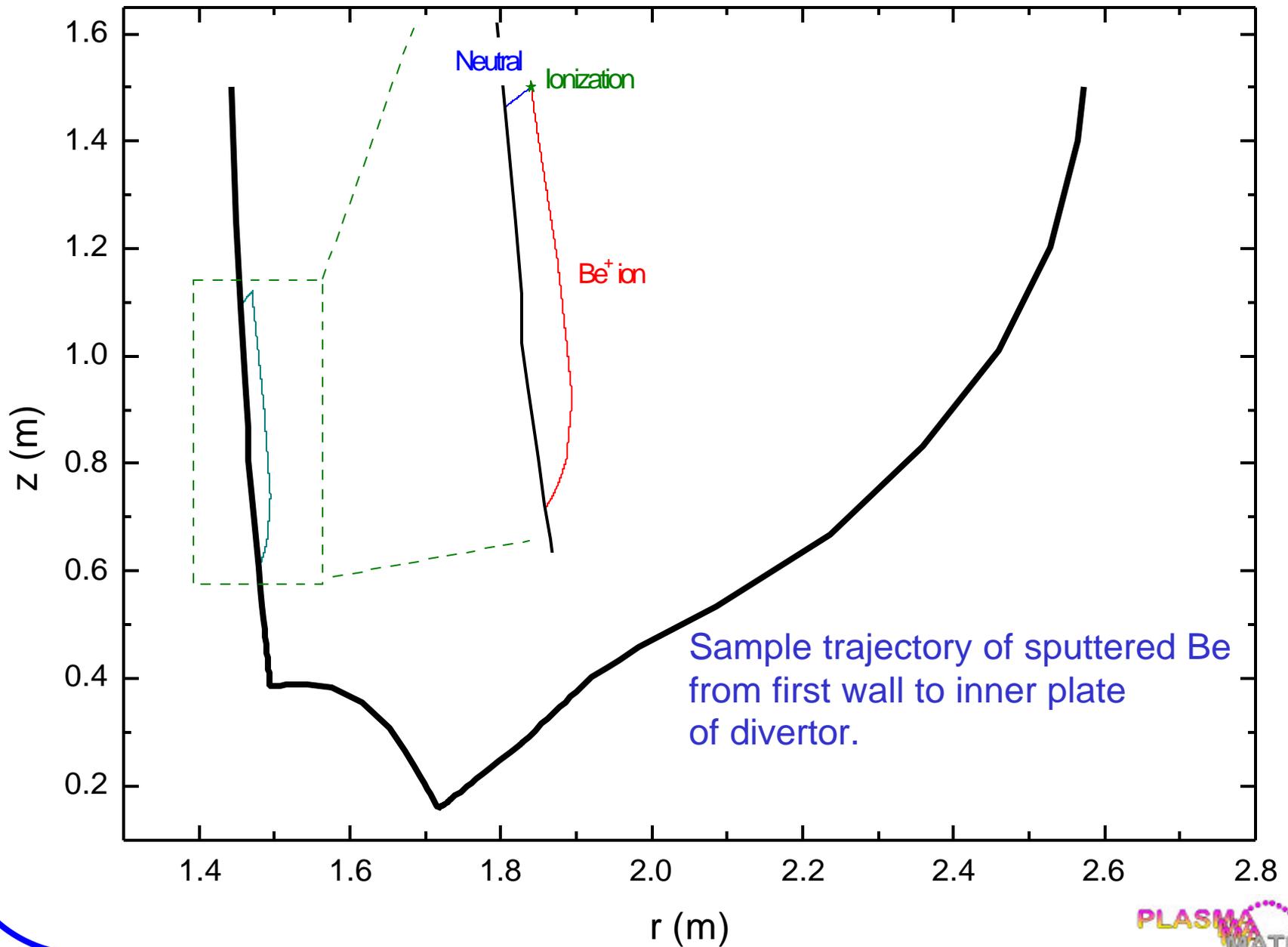
# VFTRIM D on Be results (cont.)



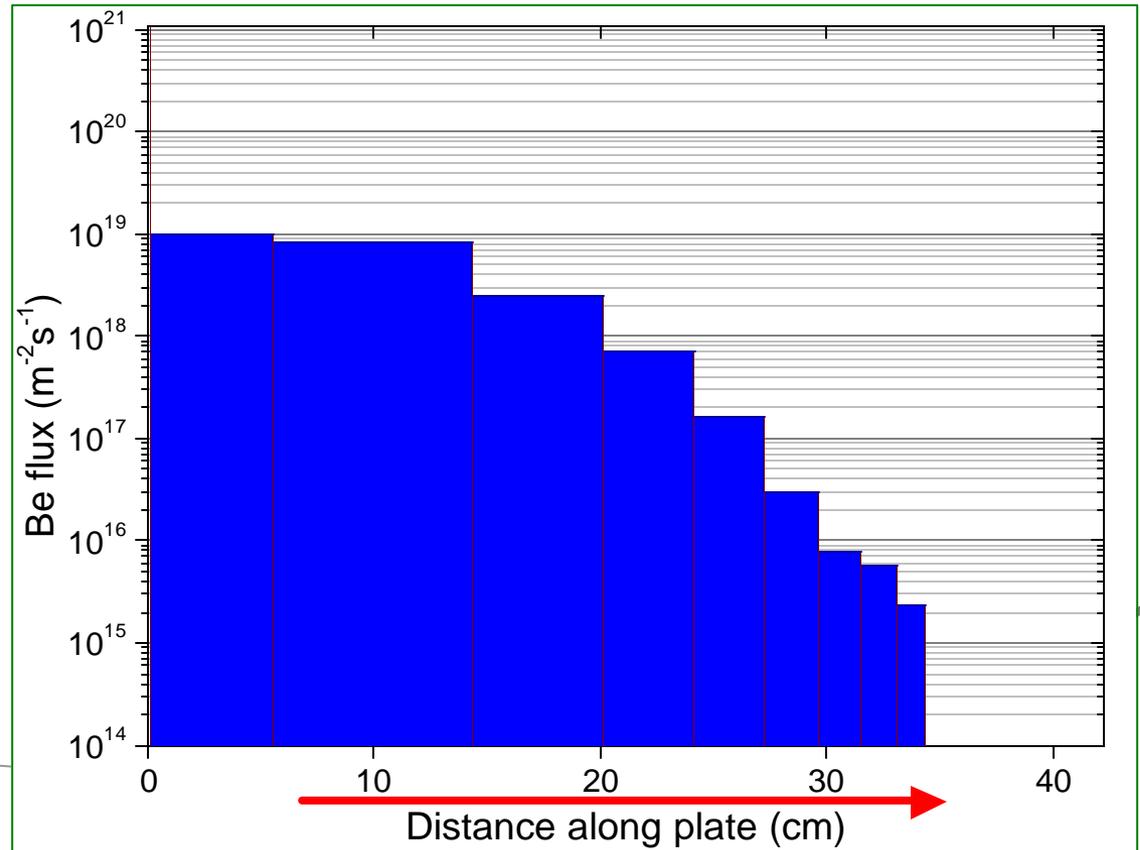
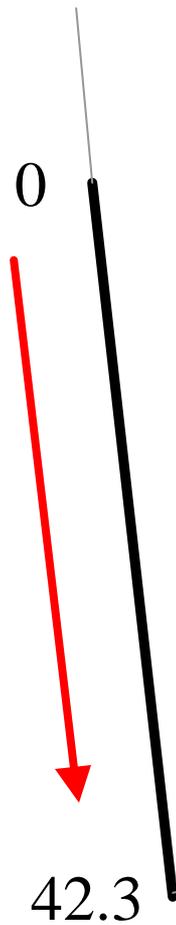
- Energy and angular distributions of sputtered particles from VFTRIM-3D are used with fluxes from DEGAS2 along with UEDGE data as inputs to WBC+ to calculate fluxes to the tungsten divertor.

# Summary of WBC+ code

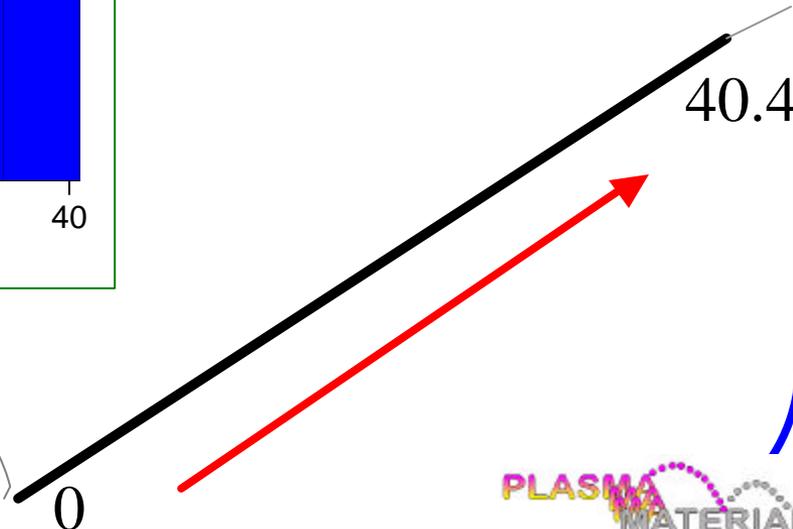
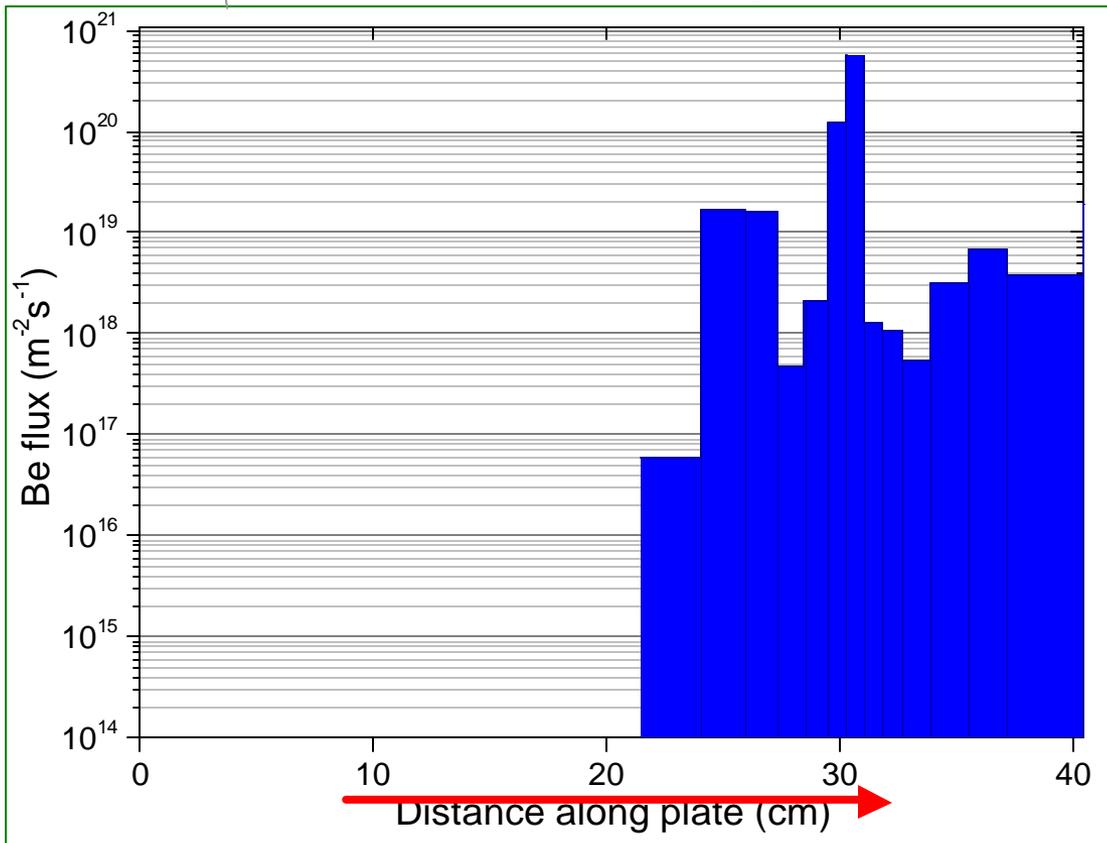
- Impurity transport code obtained from J. Brooks
- Determines the flux of Be from the wall arriving on the divertor
- Inputs to WBC+
  - FIRE Geometry & plasma background from modified UEDGE data
  - Results of DEGAS2/VFTRIM calculations
    - Flux of sputtered Be from the walls
    - Energy & angular distributions of sputtered Be
- Method
  - Particles are launched randomly by sampling the Be sputtering distributions above
  - Neutrals move in straight line until ionized
  - Once ionized, they follow the magnetic field lines
  - Particles tracked until they hit a surface



# Beryllium flux to inner divertor plate



# Beryllium flux to outer divertor plate



# Future Work Plan for Modeling Effort at the UIUC

- Continue study of hydrocarbon reflection from “soft” and “hard” graphite surfaces.
- Continued study of low energy liquid lithium reflection and sputtering under fusion-relevant conditions.
- Study of deuterium treatment on liquid lithium erosion and study of enhanced sputtering with molecular dynamics modeling of liquid lithium.
- FIRE runs on first wall/ divertor mixing problem.
- Modeling plans on variation of energy deposition mechanisms in VFTRIM-3D.

# Acknowledgements

- ALPS/DOE Subcontract from ANL
- J.N. Brooks, A. Hassanein, M. Rensink, T. Rognlien and D. Stotler for helpful discussions
- R. Averback, for MolDyn code
- Undergraduate student: Andy Simnick
- Image rendering done with POV-Ray software