AID – MD

Atomic Interaction and Diffusion Molecular Dynamics

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Motivation

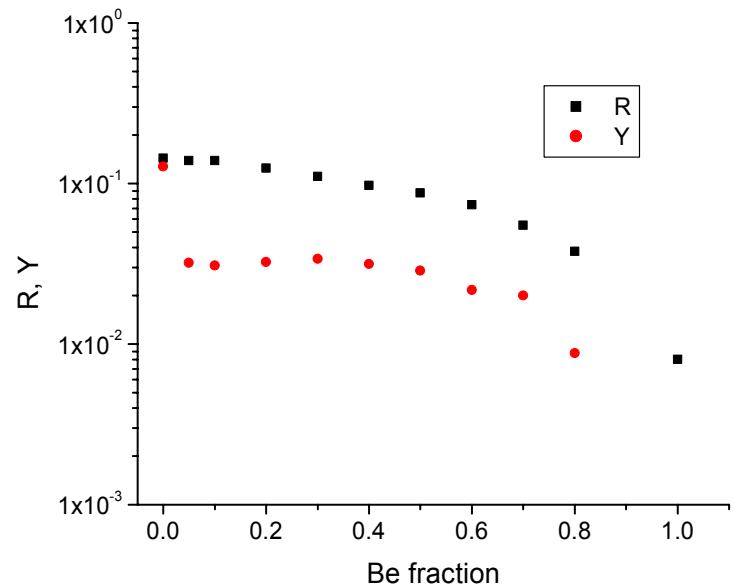
- The behavior of multi-component materials under energetic particle bombardment is of critical interest to PFC research
- For low energy interactions, molecular dynamic codes are the ones most suited.
- There needs to be a code that can predict sputtering and reflection **in liquids** as well as solids as a function of
  - Energy
  - Surface Roughness
  - Material Mixing
  - Temperature

Questions to Answer

- Does the surface get enriched with particular components?
- How important is the ion beam mixing effect?
- How do reflection, retention and sputtering coefficients change as composition in the target changes?
- Does re-deposited material tend to form a coating on the material or does it mix with the substrate material?
- Can depleted components get replenished in the surface by other mechanisms (i.e. surface segregation)?
- How do increases in temperature effect mixing, segregation, reflection, sputtering and retention?
- Are there components that get depleted faster by sputtering?

Effects of Mixed Materials

- Sputtering yield and reflection coefficient of W on W as a function of Be content
- Small Be fraction on surface dramatically reduces sputtering

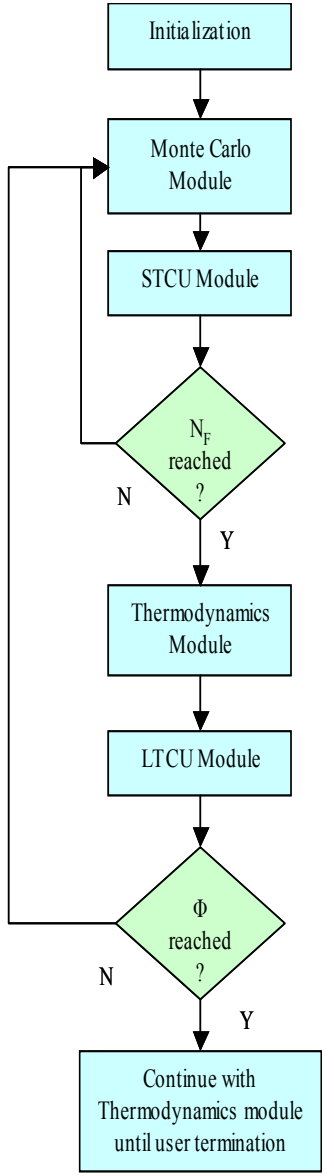


Current MAID code

- Analytic Monte-Carlo
- Object-oriented programming to facilitate code modifications and upgrades
- Multi-component beam definition, each with different energies or incidence angles if desired
- Up to 10 layers with different compositions and thicknesses in the target
- Dynamical target composition
- Thermodynamic target relaxation mechanisms (diffusion, segregation, etc.)

Flow Chart

- Monte Carlo module
- Short-term composition module updates after each history
- Thermodynamic modules calculates concentration gradients
- Long-term compositions module takes into account longer time scale phenomena



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Improvements

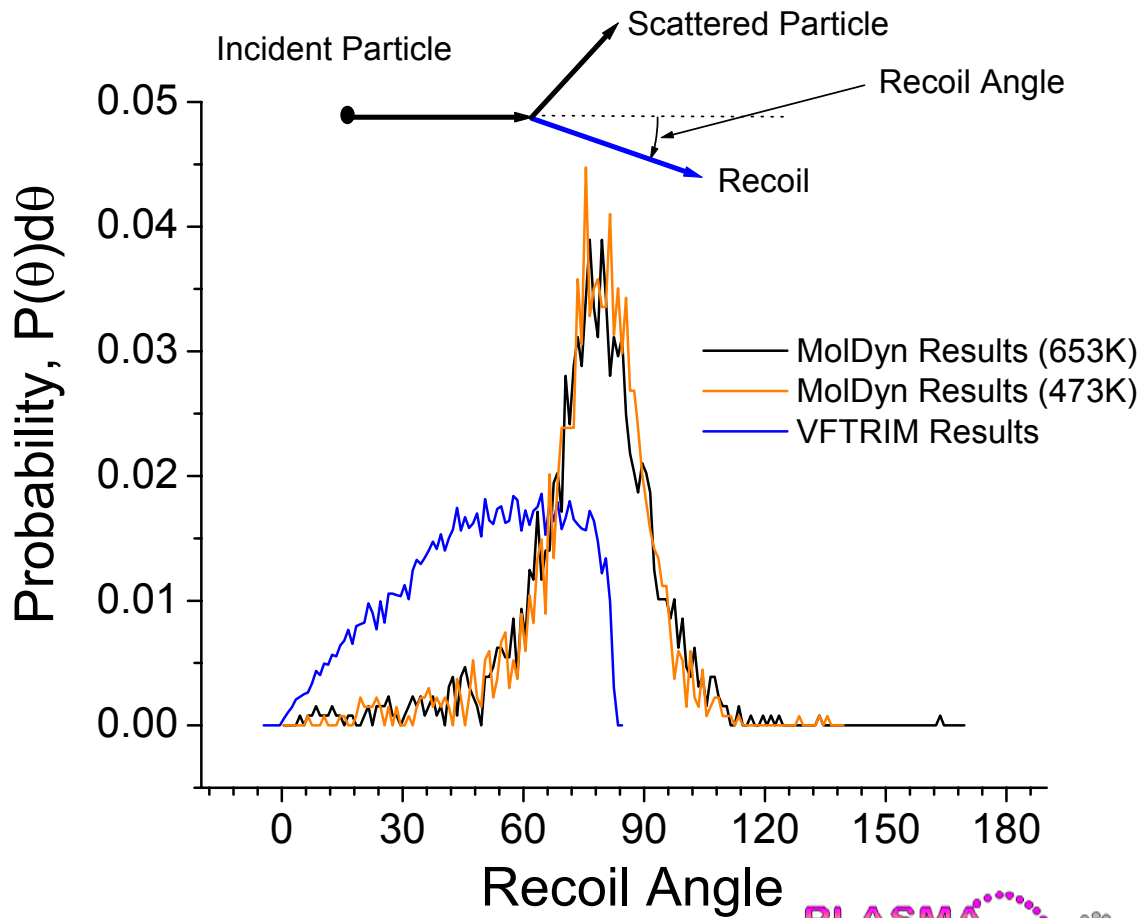
- Add fractal surfaces to account for roughness
  - VFTRIM-3D uses a geometrical grid
  - Change to fractal probabilities
- Add MD calculations to primary-knock-on cascades
  - MD-TRIM showed process and importance
  - Can account for temperature effect

MD-TRIM, an example of how to make a hybrid code

- Principle Objective: Develop model to explain temperature-enhanced sputtering in liquid metals
- For 473 and 653 K, 1000+ MD flights were performed to acquire sufficient PKA angular and energy distribution information (~ 1200 total PKA's)
- This information was then folded into VFTRIM to examine the impact of simulating the MD cascade dynamics near surface for a large number of flights

Recoil angular distribution from MD simulations

- VFTRIM uses BCA therefore, no recoil angles can exceed 90°
- In MD however, multi-body effects allow the *net* recoil angles to exceed 90°, recoils in general are along surface



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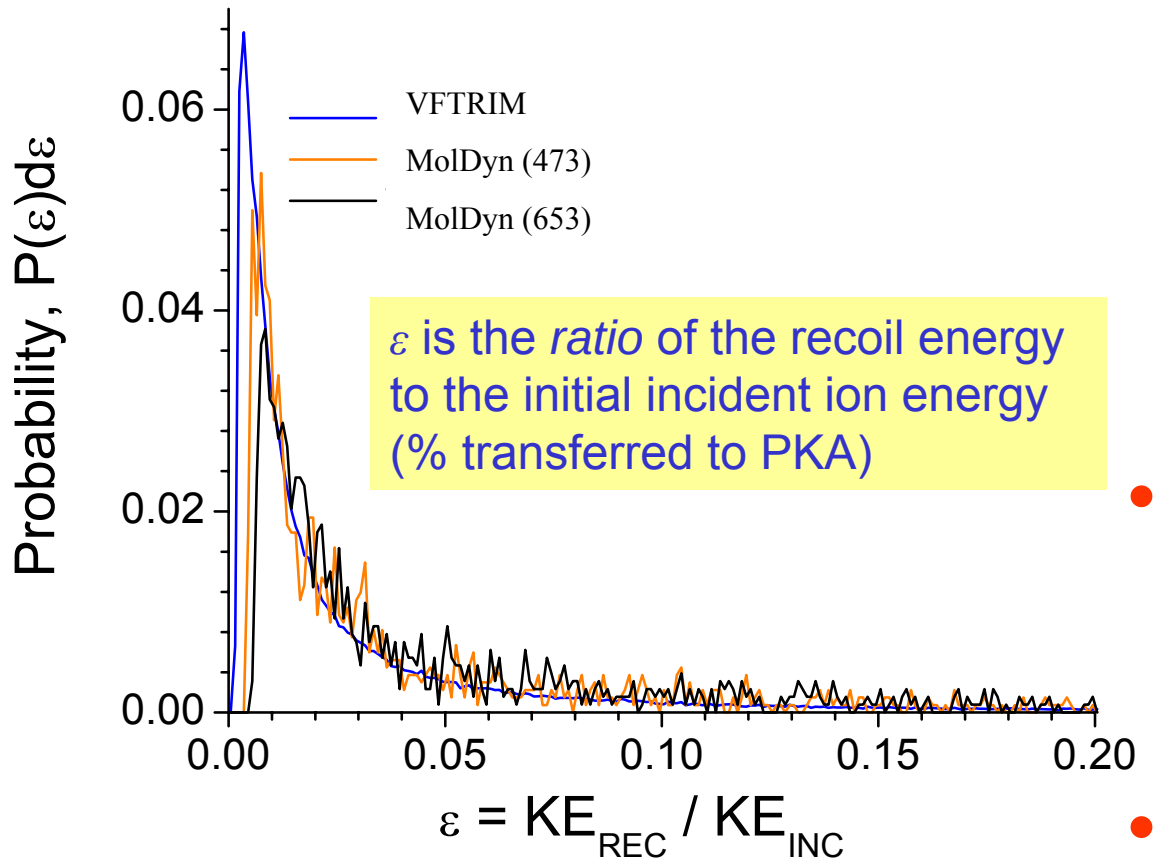
Recoil energy distribution from MD simulations



ε is the *ratio* of the recoil energy to the initial incident ion energy (% transferred to PKA)

- The key difference between the high temperature (653°K) MD run and both the low temp. (473°K) MD and the VFTRIM runs is the larger amount of energy transferred to PKA's
- As the temperature increases, an increasing amount of the incident ion energy is transferred to the PKA's
- Note: The x-axis values extend to unity

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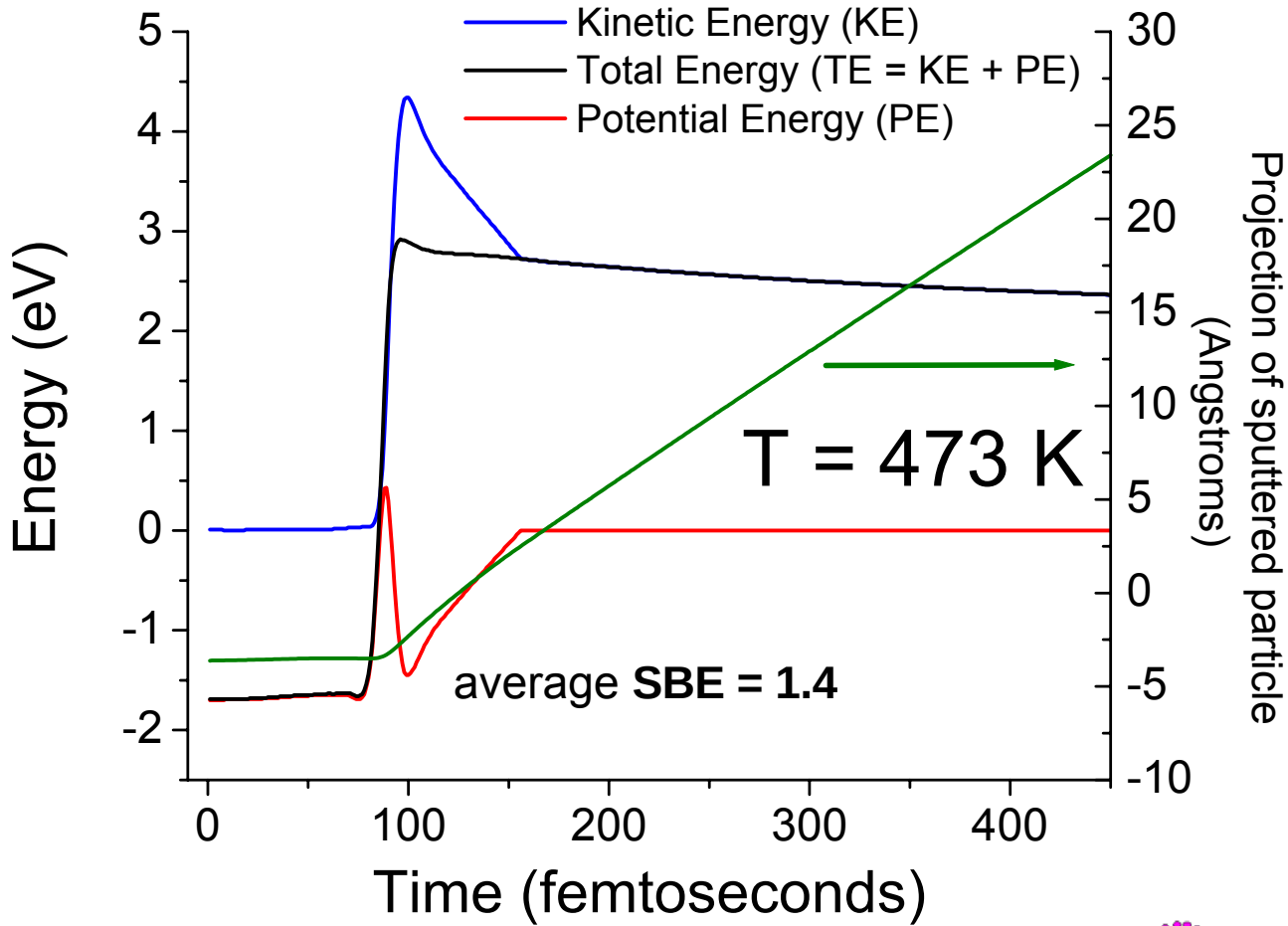
How surface binding energy is obtained from MD simulations (473 K)

- The sbe is obtained from the potential well of the sputtered atom's PE curve
- An average sbe is calculated from the sputtered atoms obtained from 100 MD flights



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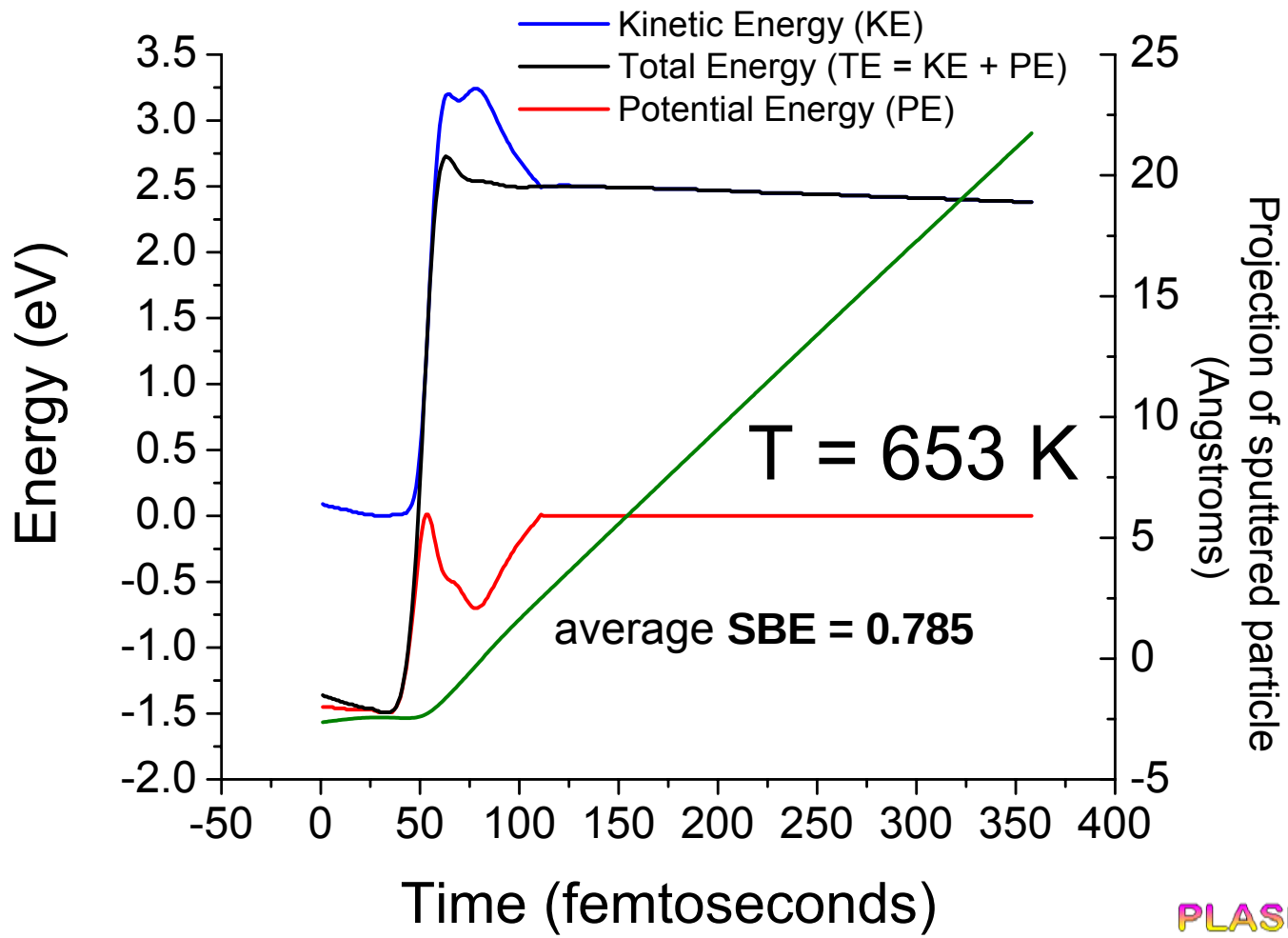
Surface binding energy from MD simulations at 653 K is lower !



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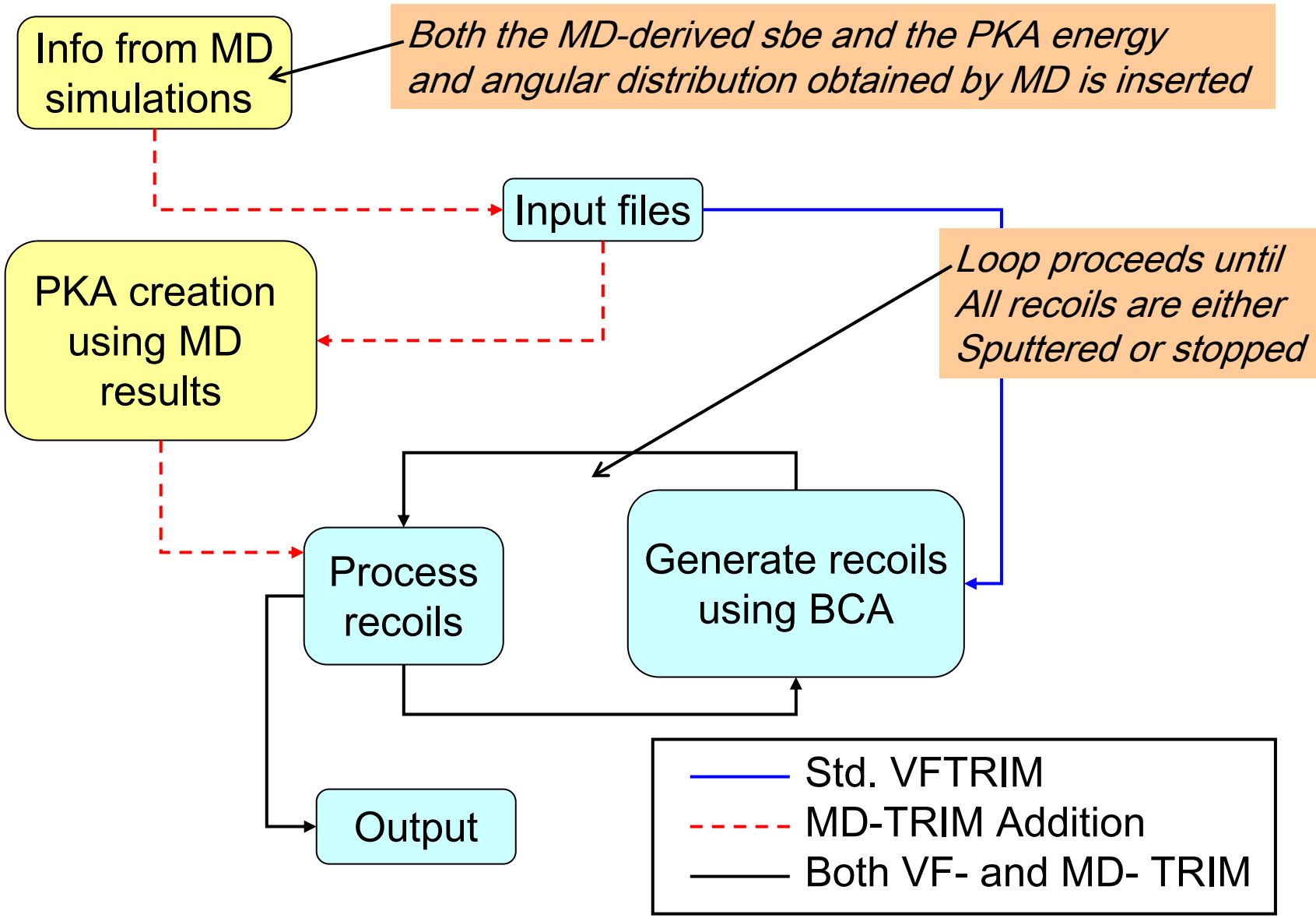
Info from MD simulations
Both the MD-derived sbe and the PKA energy and angular distribution obtained by MD is inserted
Input files
PKA creation using MD results
Loop proceeds until All recoils are either Sputtered or stopped
Process recoils
Generate recoils using BCA
Output
Std. VFTRIM
MD-TRIM Addition
Both VF- and MD- TRIM

Why University of Illinois ?

- Proven History of Code Development
  - First to introduce surface roughness (Fractal Trim, VFTRIM-3D)

Ruzic, D. N., "The Effects of Surface Roughness Characterized by Fractal Geometry on Sputtering," Nucl. Instr. Meth., B, 47, 118-125 (1990).

  - First to utilize MD (H on Ni, then H-C work, Li MD most recently) for PFC work

Ruzic, D. N. and H. K. Chiu, "Modeling of Particle-Surface Reflections Including Surface Roughness Characterized by Fractal Geometry," J. Nucl. Mater., 162-164, 904-909 (1989).

  - First to incorporate changing surface morphology among PFC ALPS community

Shaheen, M. A. and D. N. Ruzic, "Evolution of Atomic-Scale Surface Structures During Ion Bombardment: A Fractal Simulation," Vac. Sci. Technol., A, 11 , (1993).

Why University of Illinois ?

- Codes and expertise already exists in the group
  - MAIDS, VFTRIM-3D, MD-TRIM
- Close coupling with experiments
  - IIAX facility, EUV mirror experiments
- Ideal project for a PhD student
- Low incremental cost

Annual Budget

• Graduate Student (1 yr.)	$ 19,000
• Tuition and Fees	5,000
• Computer Upgrades	2,000
• Travel	2,000
• Indirect Costs	10,000
Total	**$ 38,000**

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