Molecular Dynamics Modeling of Hydrogen in Lithium

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Outline

- Theory background
  - H – Li inter-atomic potential
  - Li – Li NPA potential
- Simulation results
  - Pure lithium (Li)
    - Sputtering
    - Reflection
  - Hydrogenated lithium (LiH / LiD)
    - Hydride concentration
- Conclusion
- Future work

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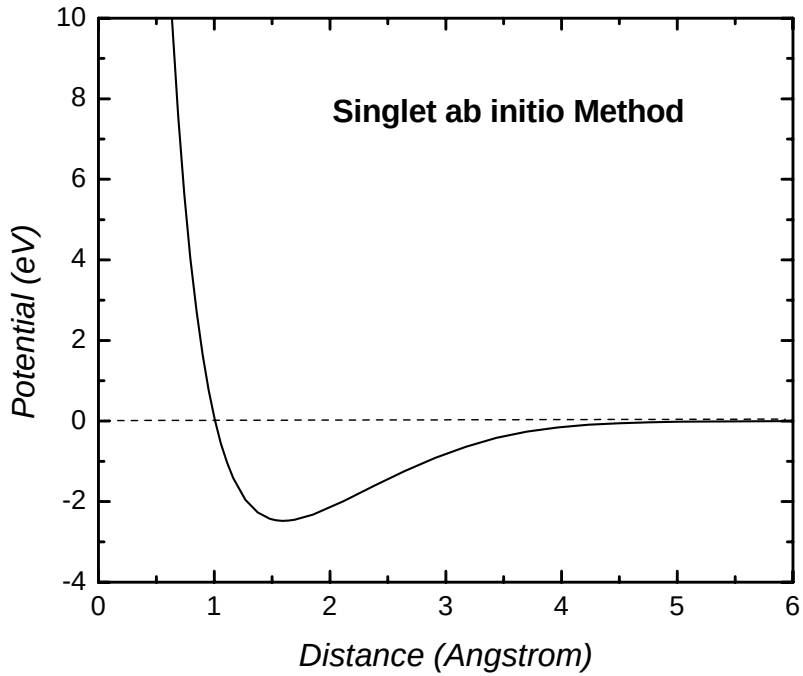
H-Li Inter-Atomic Potential

- Use singlet ab initio potential method[1]
  - Including dispersion forces and exchange interactions
  - Using a large scale configuration interaction method
- Split with universal potential at small distances



- Interaction Cutoff: 5 Angstrom
- Bond Min Distance:1.05 Angstrom
- Bond Max Distance: 3.60 Angstrom
- Bond Energy: 2.526 eV

[1] R. Cote, *et al.*, *Enhanced Cooling of Hydrogen Atoms by Lithium Atoms, Physical Review Letters*, 2000. **84**(13) p. 2806-2809.

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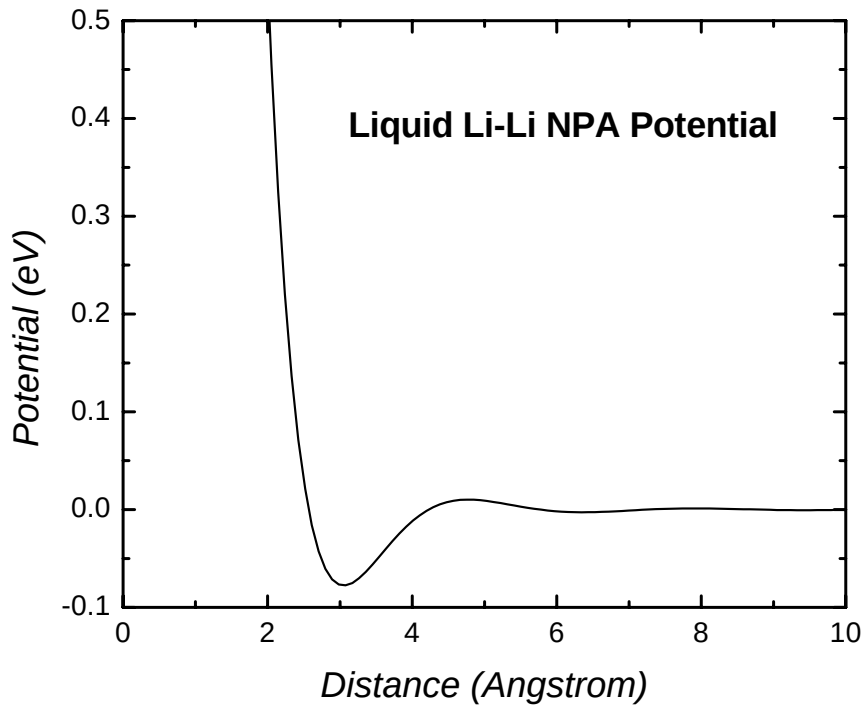
Why Trust This H-Li Potential?

- Calculated by MOLCAS program[2], a specific program used for molecular configuration-interaction calculations
- Enable accurate predictions to be made of the scattering of the alkali metal atoms by hydrogen atoms[1]
- The resulting interaction potential is available to public from AIP[3]

[2] K. Anderson, *et al*., *MOLCAS*, Version 4, 1997, Lund University, Sweden.
[3] American Institute of Physics (AIP), EPAPS
http://www.aip.org/pubservs/epaps.html

Liquid Li-Li NPA Potential

- Use Neutral Pseudoatom (NPA) method[4]
  - Involving structural and thermodynamic properties
  - Developed for liquid Lithium



- Interaction Cutoff: 5.75 Angstrom
- Bond Min Distance: 2.60 Angstrom
- Bond Max Distance: 4.13 Angstrom
- Bond Energy: 0.083 eV

[4] Manel Canales, L. E. Gonzalezt, *et al*., *Computer Simulation Study of Liquid Lithium at 470 and 843K, Physical Review E*, 1994. **50**(5) p. 3656-3669.

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Why Trust This Li-Li Potential?

- Calculated by a specific MD group for liquid Li of Spain[4]
- Involving both structural and thermodynamic properties for liquid Lithium
- Reasonable agreement with available experimental data[4]
- Effective for high temperature ranging 470K ~ 843K

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MolDyn Code

- Molecular Dynamics code
- Modified to handle lithium/hydrogen systems
- Code configurations
  - Time step: *0.2 fs*
  - Time scale: *2000 fs*
  - Lattice size: 2727 Li atoms initially
  - Periodical side boundary and fixed bottom
  - Cutoff: 5.75 angstrom/Li-Li & 5 angstrom/H-Li
- Creation of the Li lattice
  - Originally from BCC structure
  - Slowly heated to required temperature

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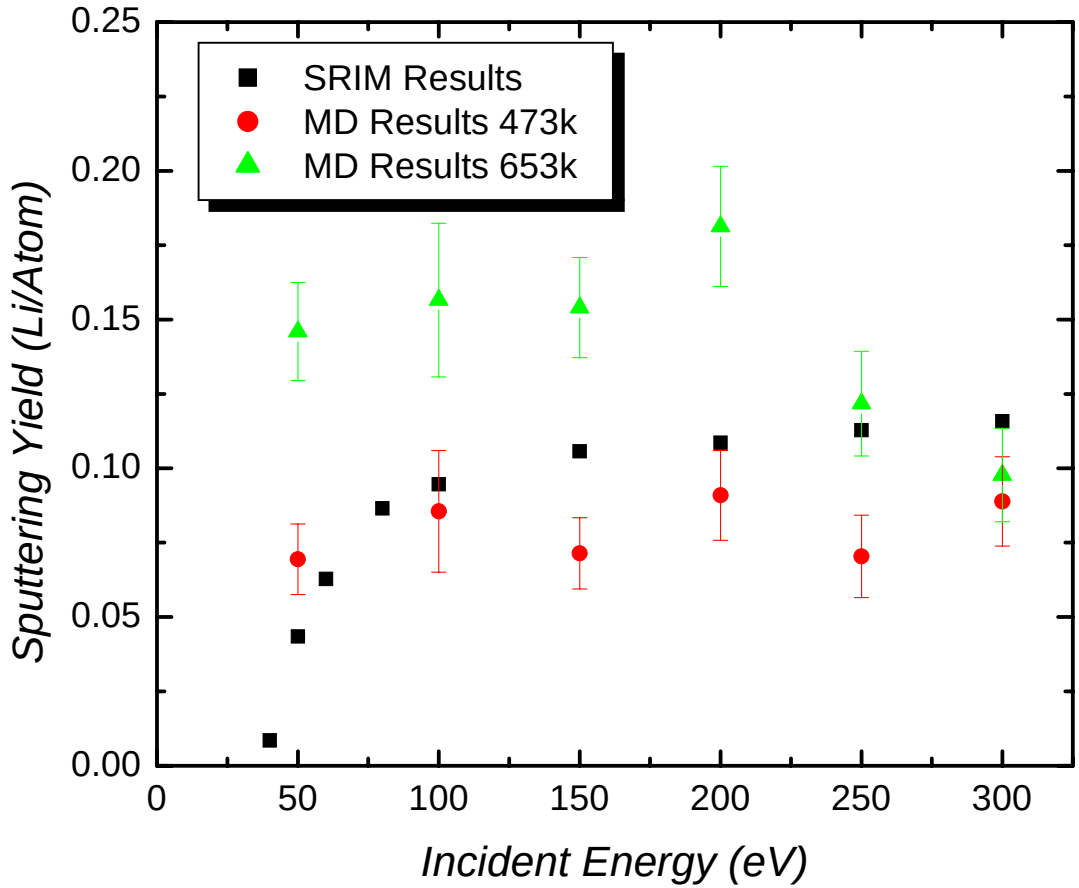
Deuterium incident at 45° for different temperature – Sputtering Yield

- MD and SRIM results converge at high incident energies



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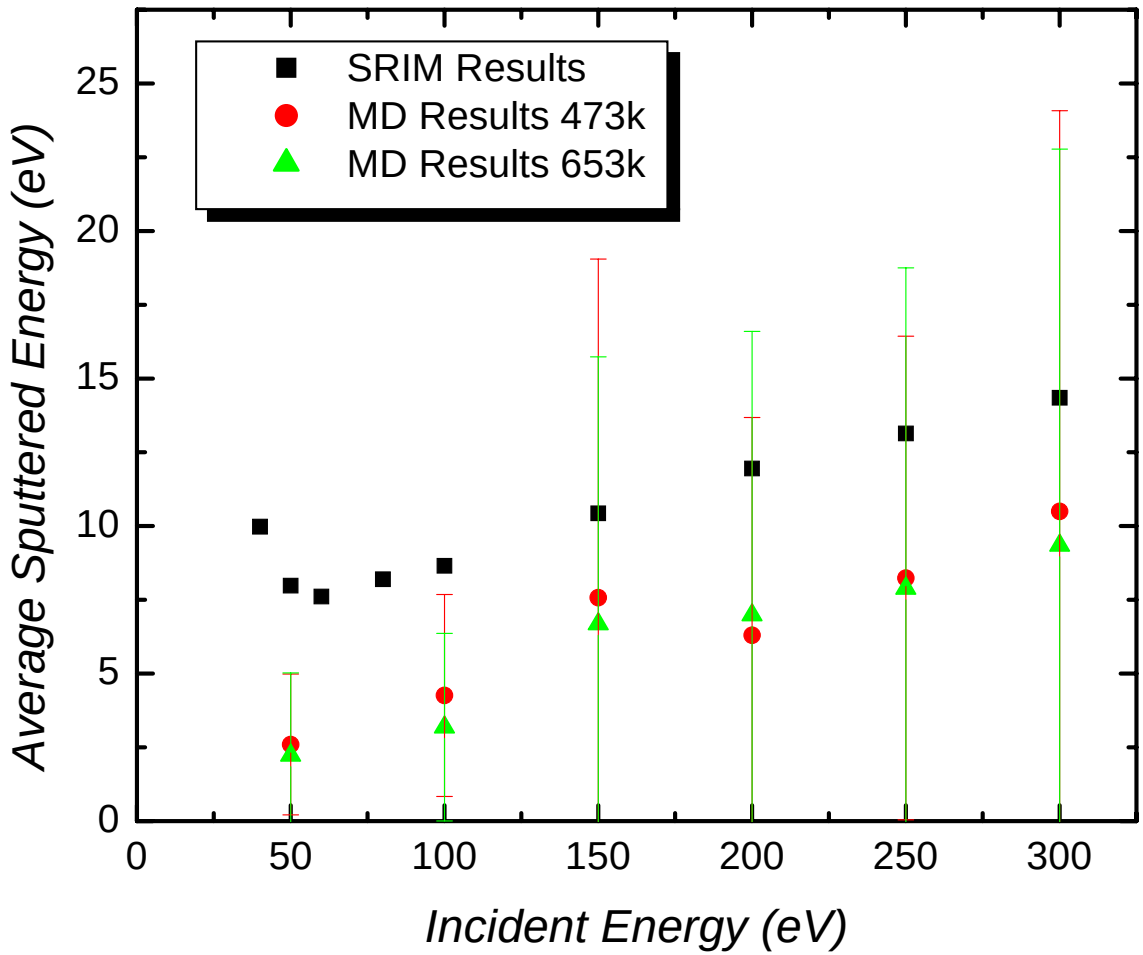
Deuterium incident at 45° for different temperature – Average Sputtered Energy



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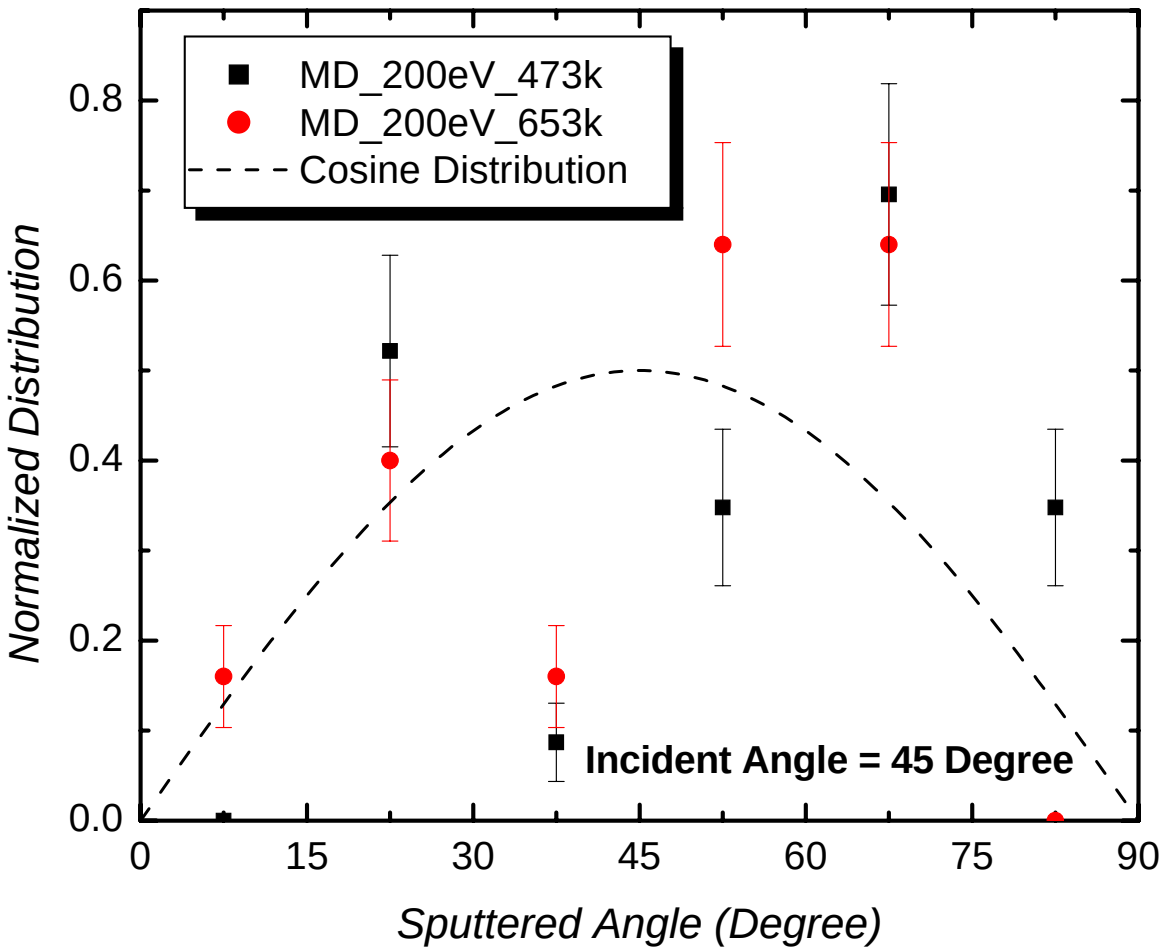
Deuterium incident at 45° for different temperature – Sputtered Angle



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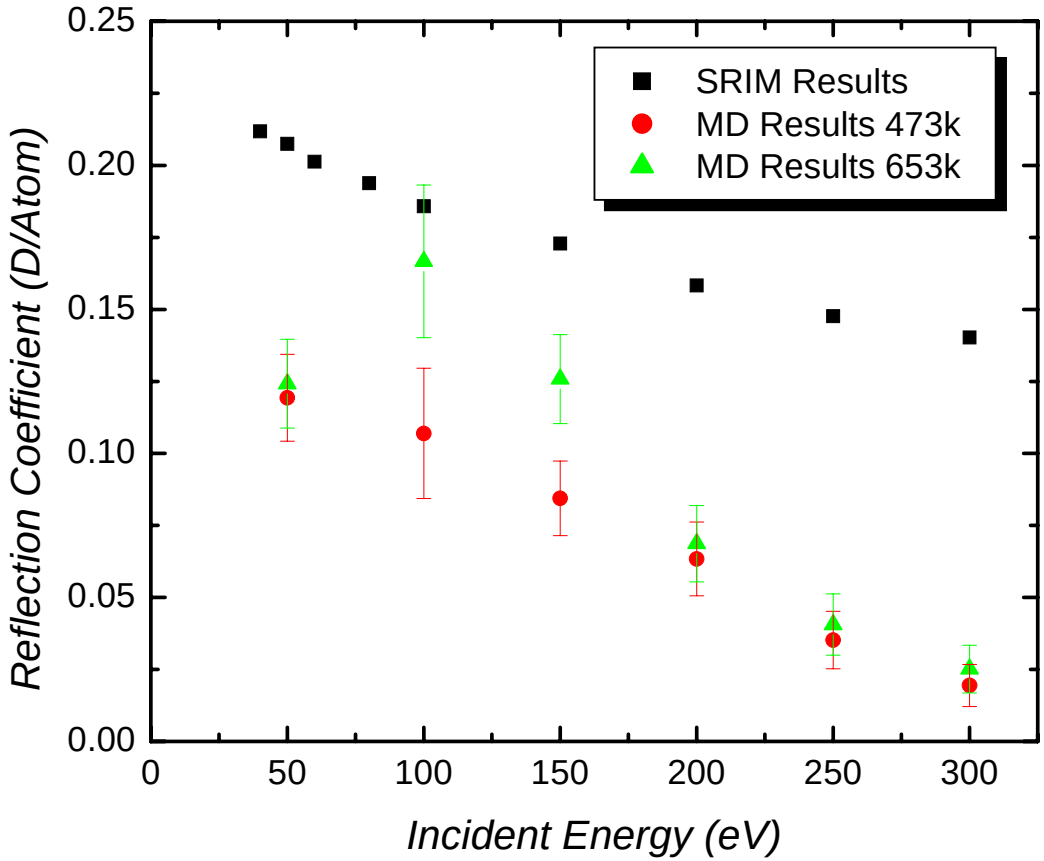
Deuterium incident at 45° for different temperature- Reflection Coefficient

- SRIM result (Solid Li) and MD result (Liquid Li)
- Reflection Coefficient decreases for liquid Li compared with solid Li lattice



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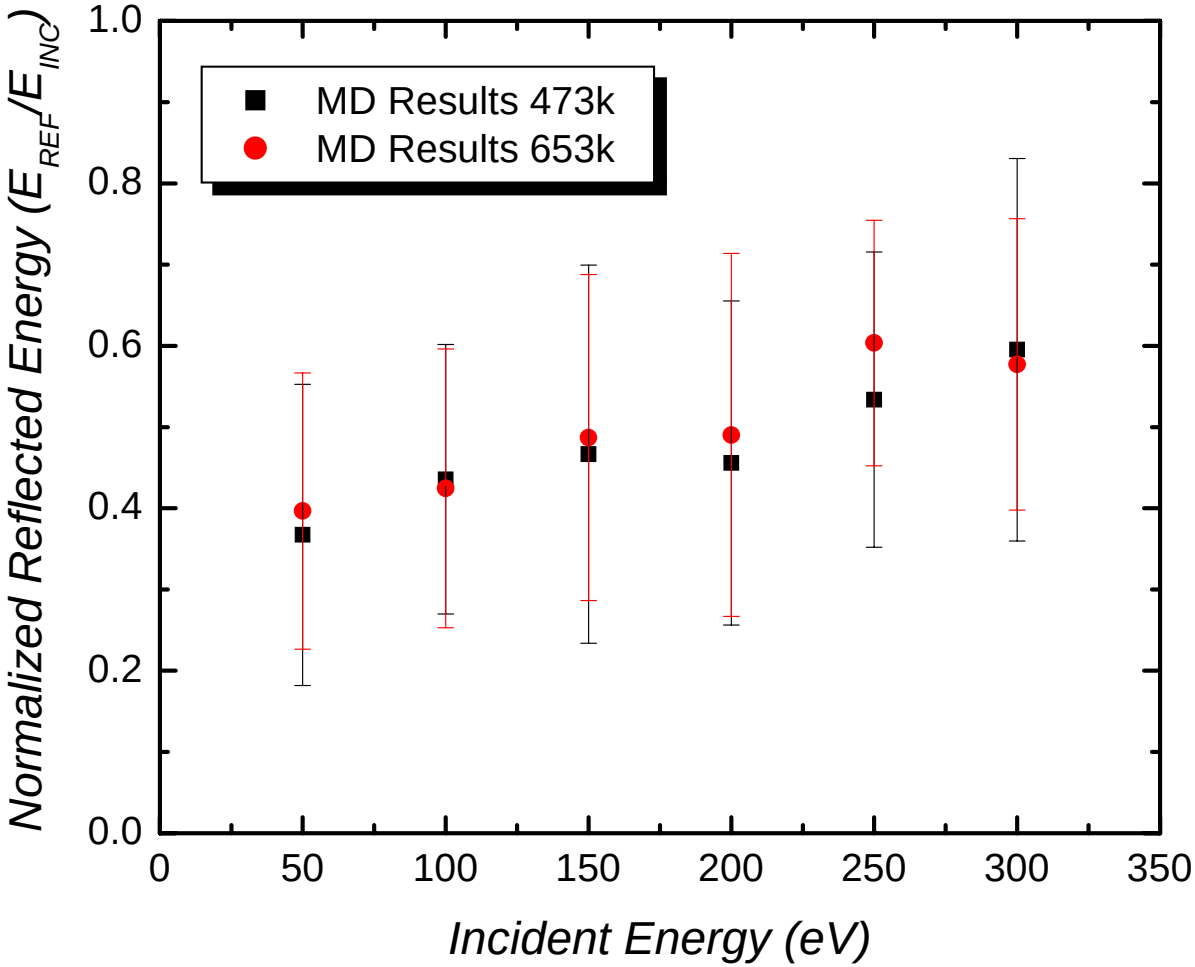
Deuterium incident at 45° for different temperature - Reflected Energy



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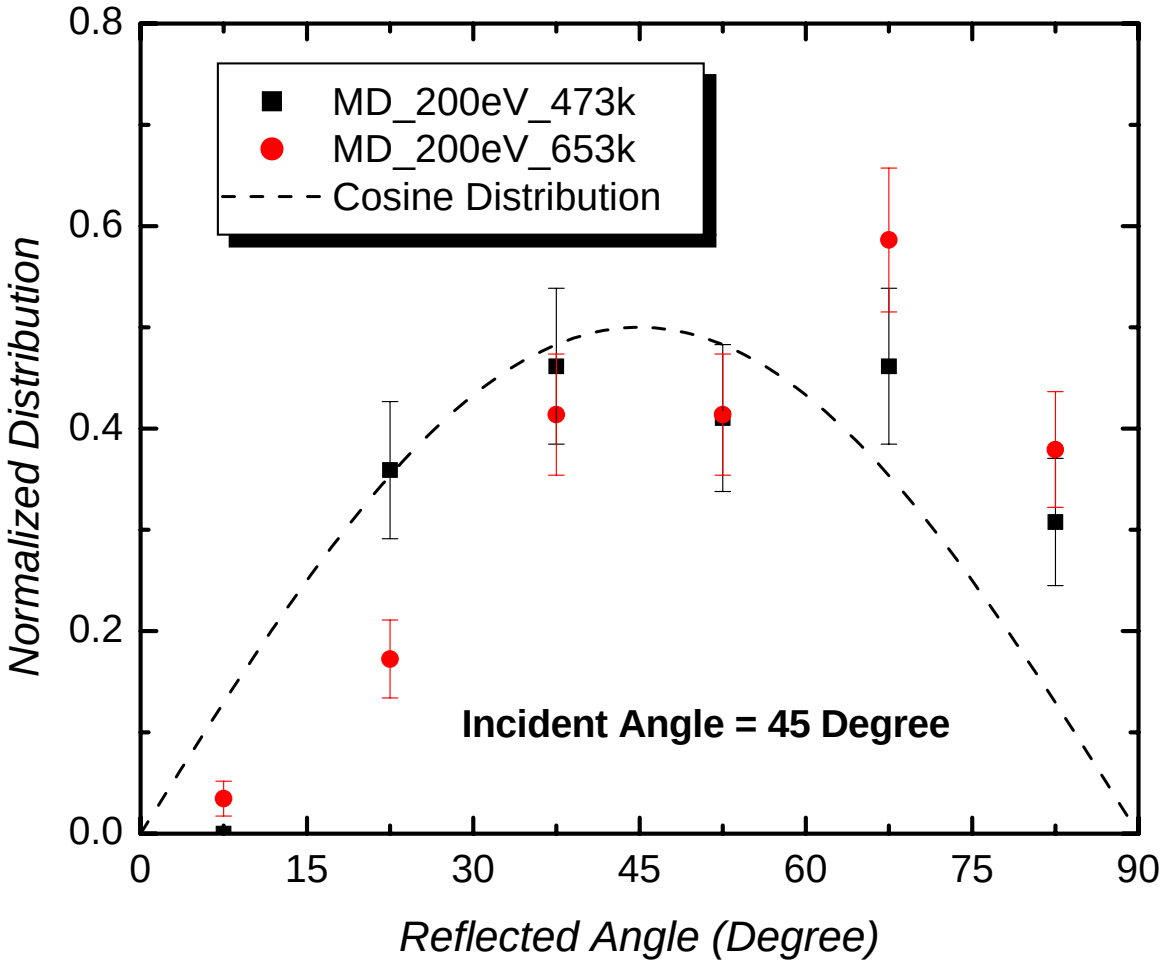

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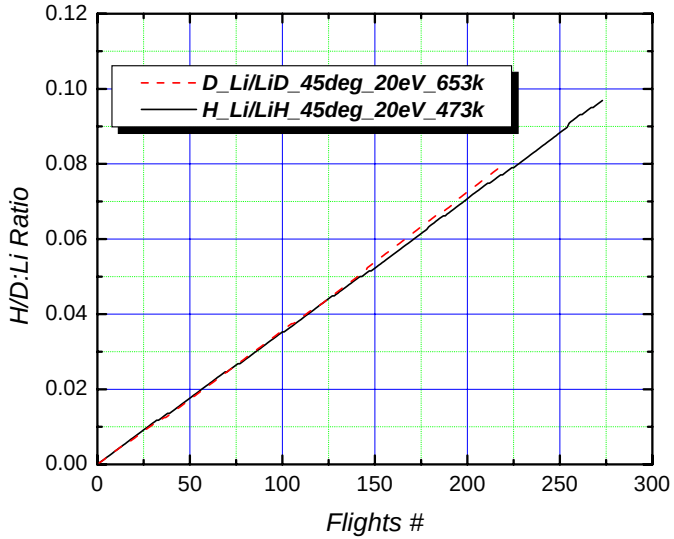
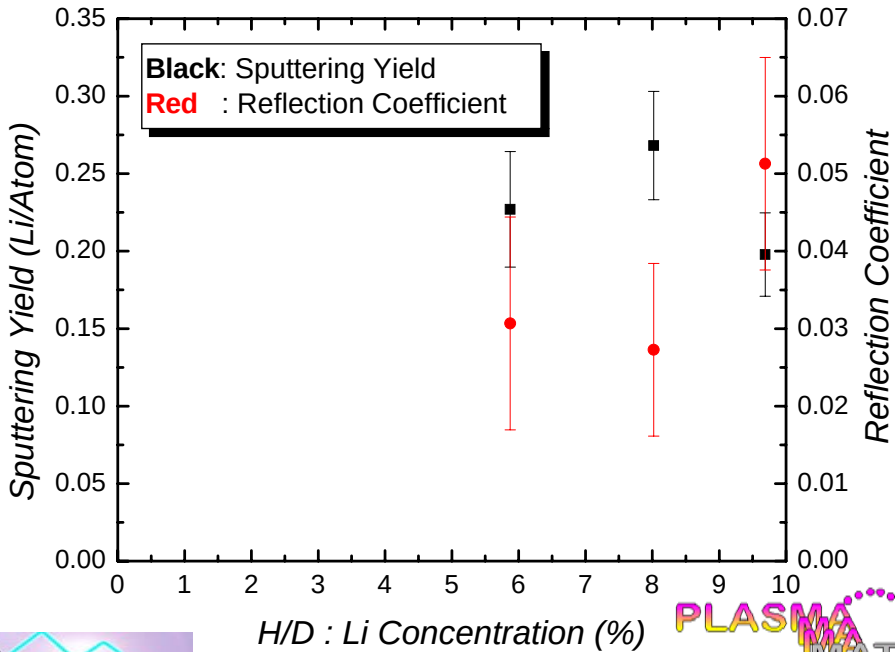
Lithium Hydride Concentration

- The curve shows the linear increase of sticking ratios in the initial stage
- Saturation is not obtained due to the insufficient time scale (2 *ps*)



- The actual concentration can't stay at such a high level according to the phase diagram
- Compare how sputtering yield and reflection coefficient depend on the lithium hydride concentration



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Conclusion

- Sputtering yield increases with temperature. Hydrogen atoms are more likely to be sticking at low incident energies (<50eV)
- Reflection coefficient significantly decreases due to the liquid properties of lithium lattice
- Reflection coefficient, sputtered energy and angle, and reflected energy are not likely affected by temperature
- LiH system needs longer time scale in order to get saturation at proper concentration
- The simulation results should be improved if employing a better spline potential by properly splitting the universal potential and H-Li potential

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Future Work

- Develop a better H-Li spline potential, along with larger lattice size and longer time scale
- Verify the agreement of our MD sputtering yield and VF-TRIM result
- Investigate the sputtering yields and reflection coefficients with a wider incident energy range
- Look at the effects of incident angle on the sputtering and reflection
- Predict sputtering yield as a function of surface temperature
- Respond to the needs of community

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