Lithium Experiments at the University of Illinois

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Workshop Agenda

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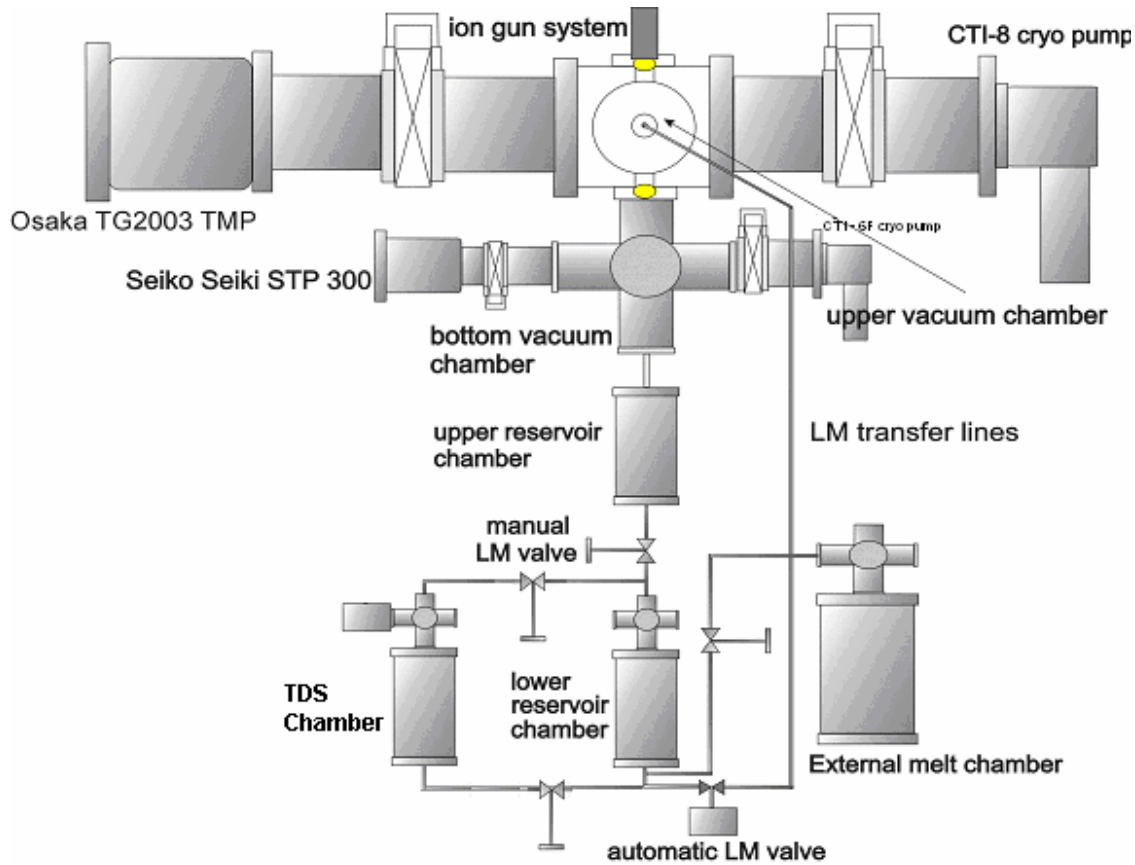
Overview

- Flowing Liquid-metal Retention Experiment (FLIRE)
  - FLIRE experiment design
  - Helium retention and diffusivity merging two-stream lithium flows
  - Helium retention and diffusivity with single-stream lithium flow
  - Improved model for calculating diffusivity
  - Qualitative MHD experiments
- Ion InterAction eXperiment (IIAX)
  - IIAX experiment design
  - Sputtering of yield of solid and liquid lithium
  - Temperature dependence of liquid lithium sputter yield
  - Mechanisms for temperature dependence of sputter yield

FLIRE Experiment Design

- The vacuum system is composed of 2 TMPs and 2 cryo pumps
- SPECS IQE 11/35 Ion gun source provides 10^{14} ions/cm^2/sec
- Upper and lower chamber are connected by 0.3 cm^2 orifice
- Upper and lower reservoirs hold and transport liquid Li
- New magnetic sector mass spec for bottom and TDS chambers
- RGA-QMS for upper chamber
- New magnet/electrode design for MHD exps (details later)
- LM compatible valves



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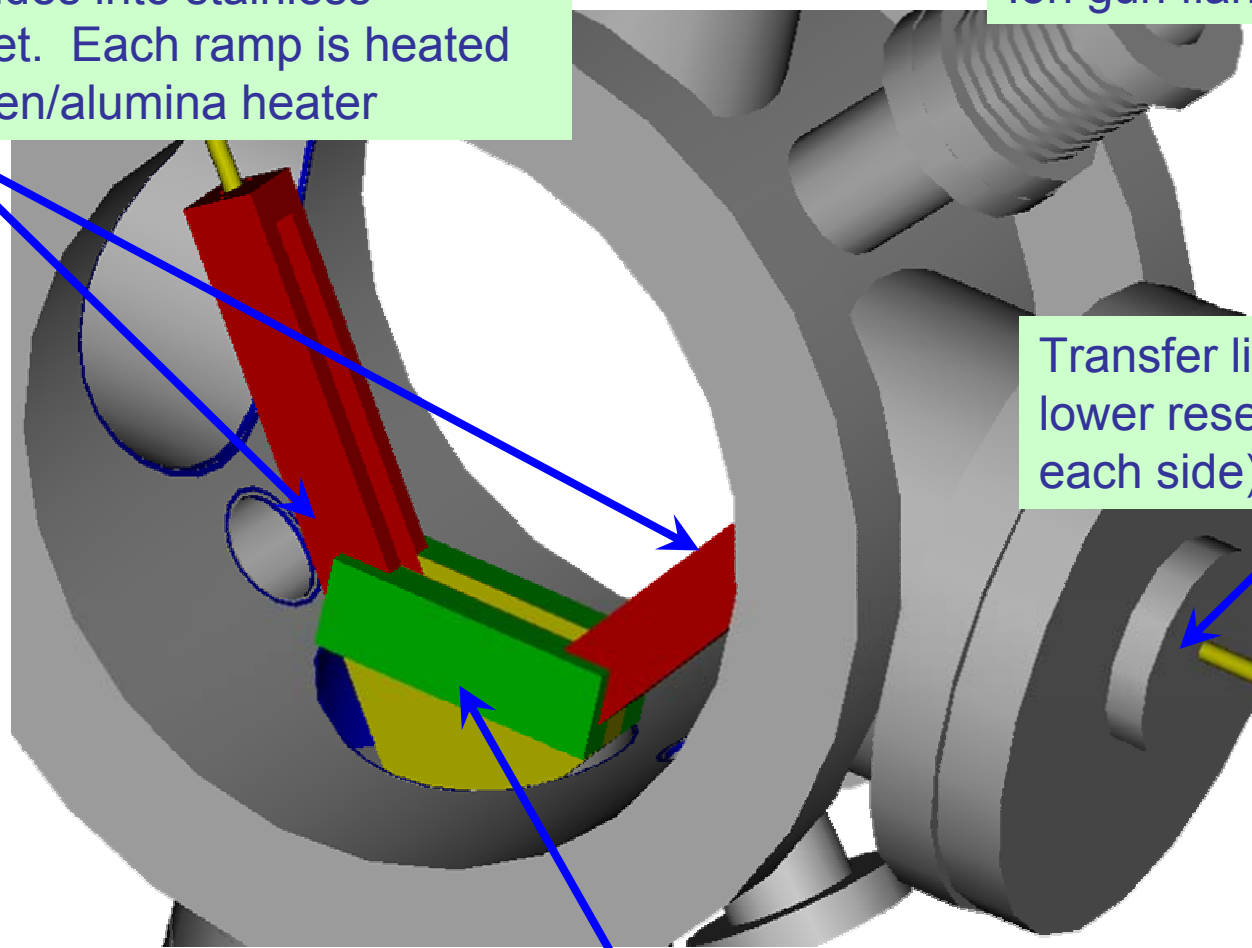
Upper vacuum chamber design with ramps and bracket

SS ramp slides into stainless steel bracket. Each ramp is heated by a tungsten/alumina heater

Ion gun flange location



Transfer line tube from lower reservoir (one on each side)

SS bracket is welded to a 6” flange attached to the upper chamber

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Lithium Flowing Down Ramps

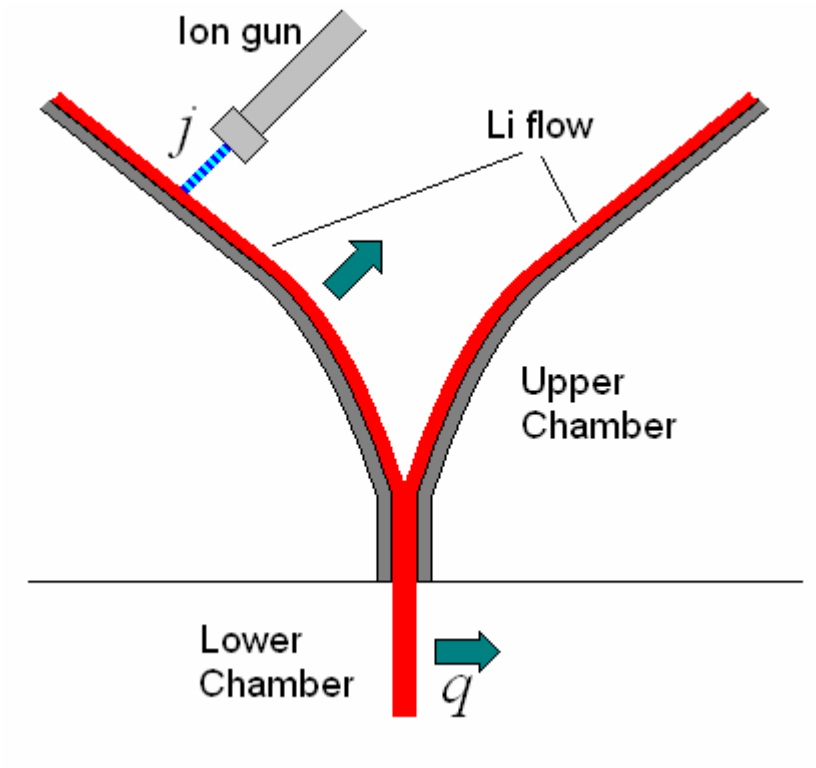
Definition of retention coefficient

- The retention coefficient is given by:

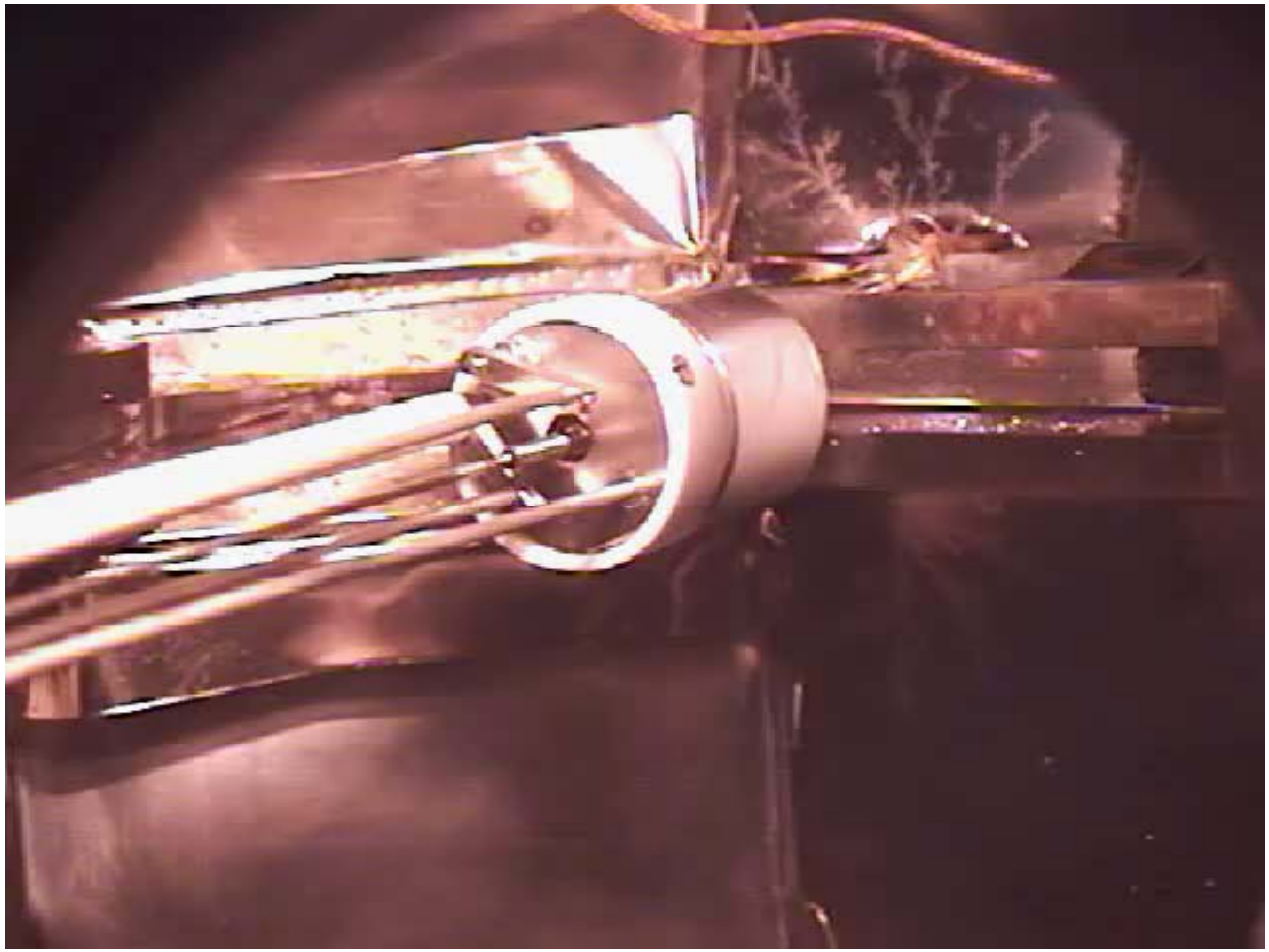
$$R = \frac{q}{j}$$

q: release rate in the lower chamber

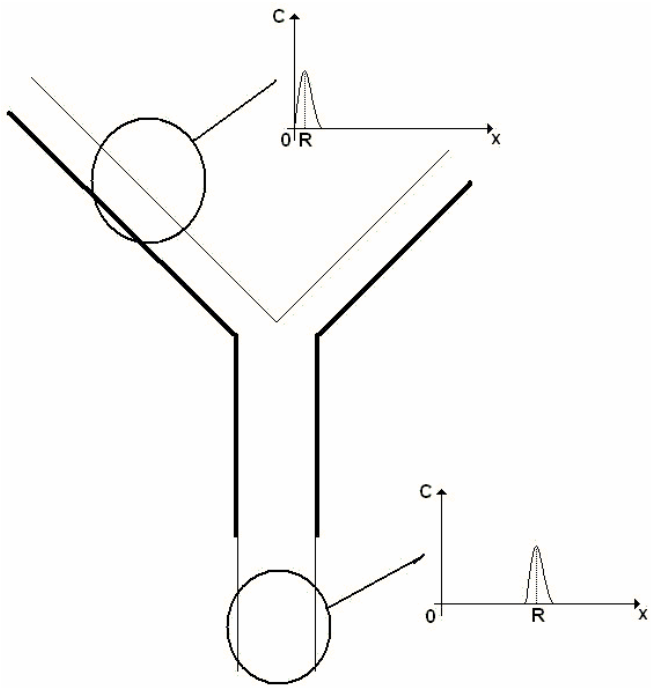
j: injection rate in the upper chamber

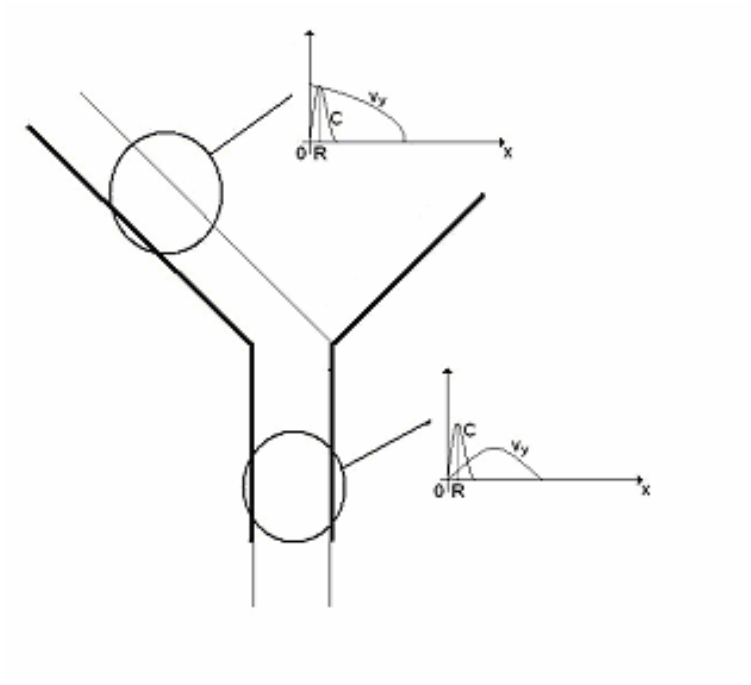


Lithium Flow with Ion Gun



Flow Configurations



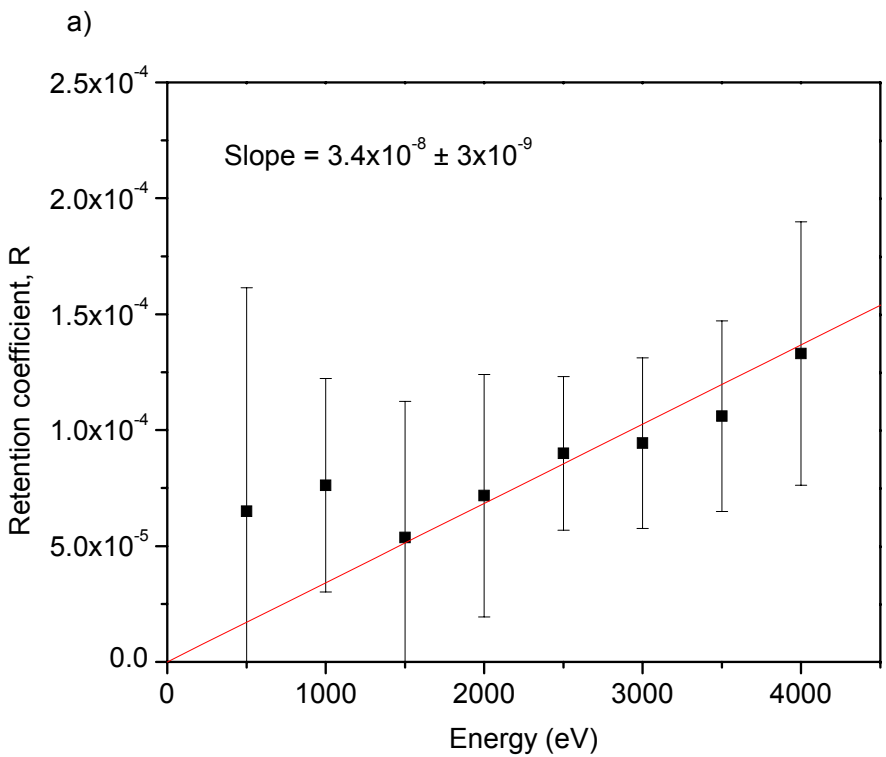


- Double stream run Concentration profiles shown
- Is surface ”folding” an issue in the measurement of *R* and *D*?

- Single flow run Concentration profiles shown
- Is the quality of inter-chamber seal affected by using 1 stream only?

Double Flow Retention (Helium)

- Retention increases with implantation energy
- High retention at low E is unexplained
- Retention decreases with increasing temperature (as expected)



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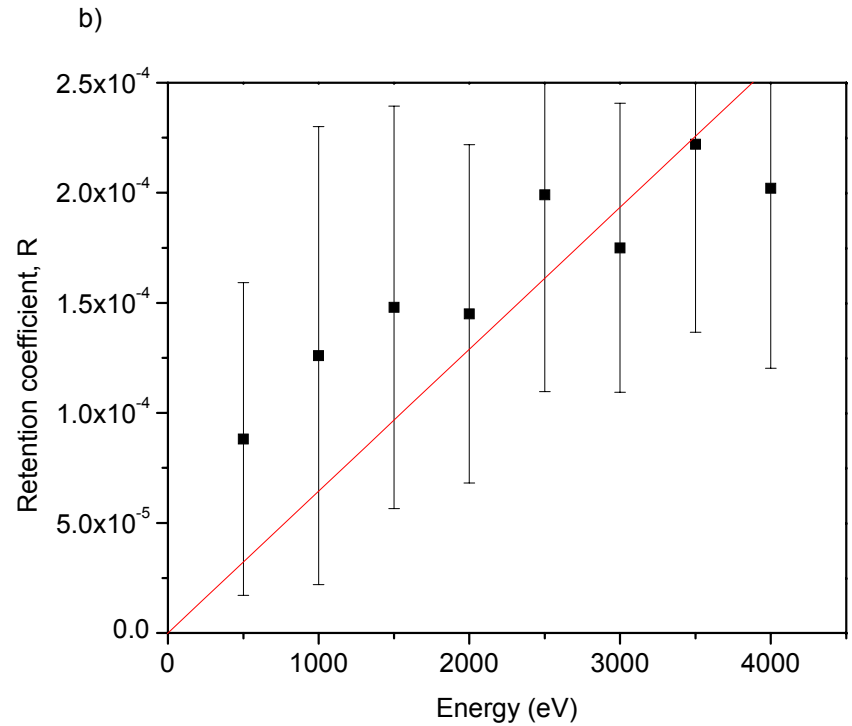
Single Flow Retention (Helium)

- Retention increases more quickly with implantation energy
- Greater slope could be due to higher flow rate for single-flow sealing, but more experiments needed
- Retention still decreases as temperature increases



Simple Calculation of D

- Simplest model assumes
  - Semi-infinite medium
  - Implantation distribution is delta function

$$R = erf\left(\frac{1}{2\sqrt{\theta}}\right)$$

$$\theta = \frac{DL}{vr^2}$$

$$D = \frac{vr^2}{4L\left[erf^{-1}(R)\right]^2}$$

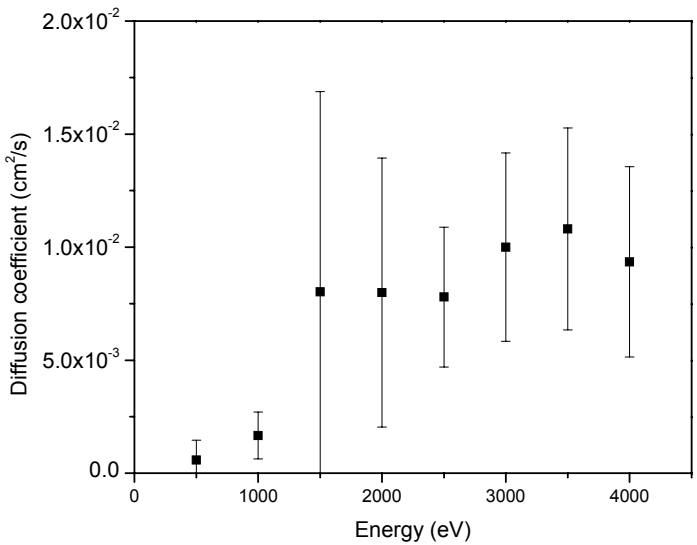
v: flow velocity

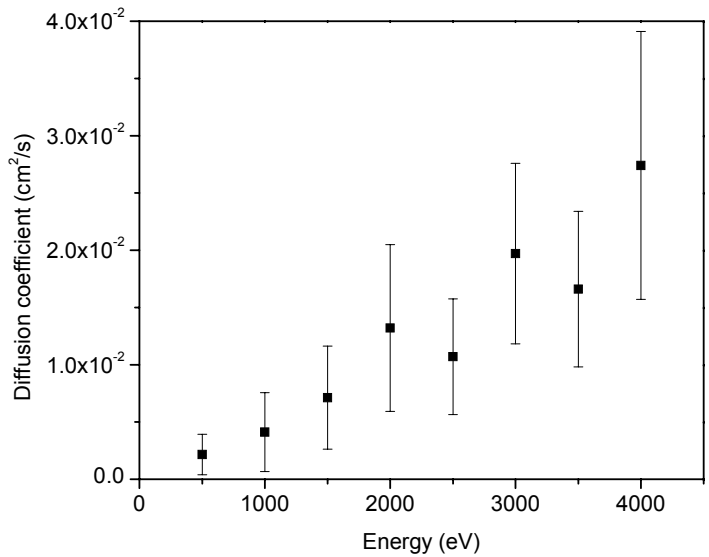
r: mean implantation range

L: path length from striking point to exit

Diffusion Coefficient (Simple Model)

- Diffusion coefficient should be energy independent





- Double flow
  - Calculated diffusion coefficient is constant for high energies
  - Low-energy points unexplained

- Single flow
  - Calculated diffusion coefficient increases with implantation energy
  - Suggests flaw in simple model

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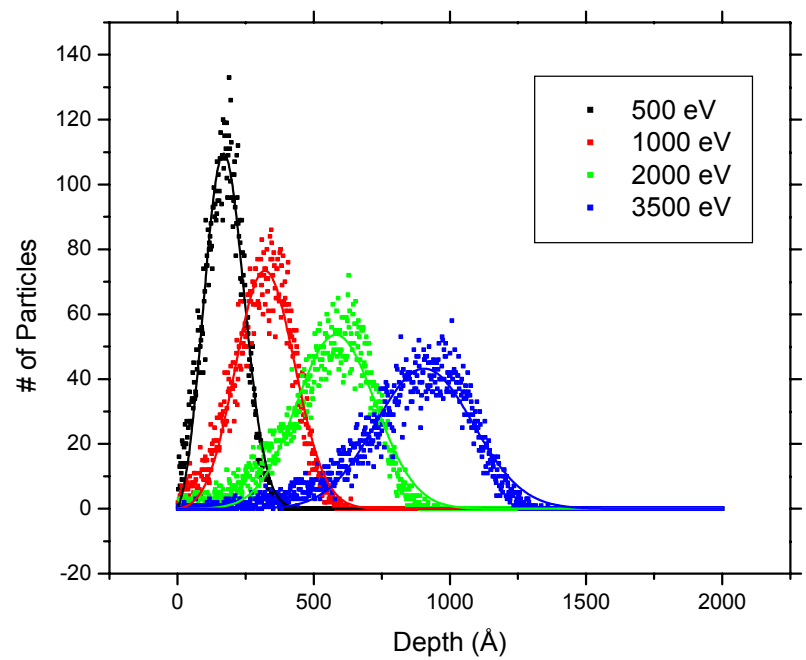
New Model for Calculating D

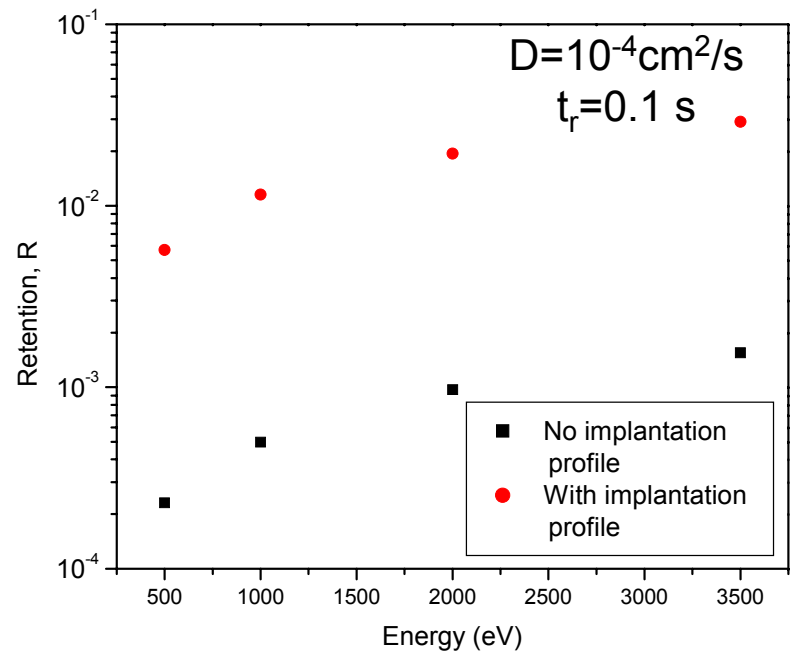
- Improved model assumes Semi-infinite medium
  - Good assumption, based on TRIM results
- Particle depth distributed
  - Linearly skewed Gaussian fit of distribution predicted by TRIM
- Still delta function ion-beam width



$$f(x,t) = \frac{A}{\sigma} x e^{-\left(\frac{x-\mu}{\sigma}\right)^2} \delta(t)$$

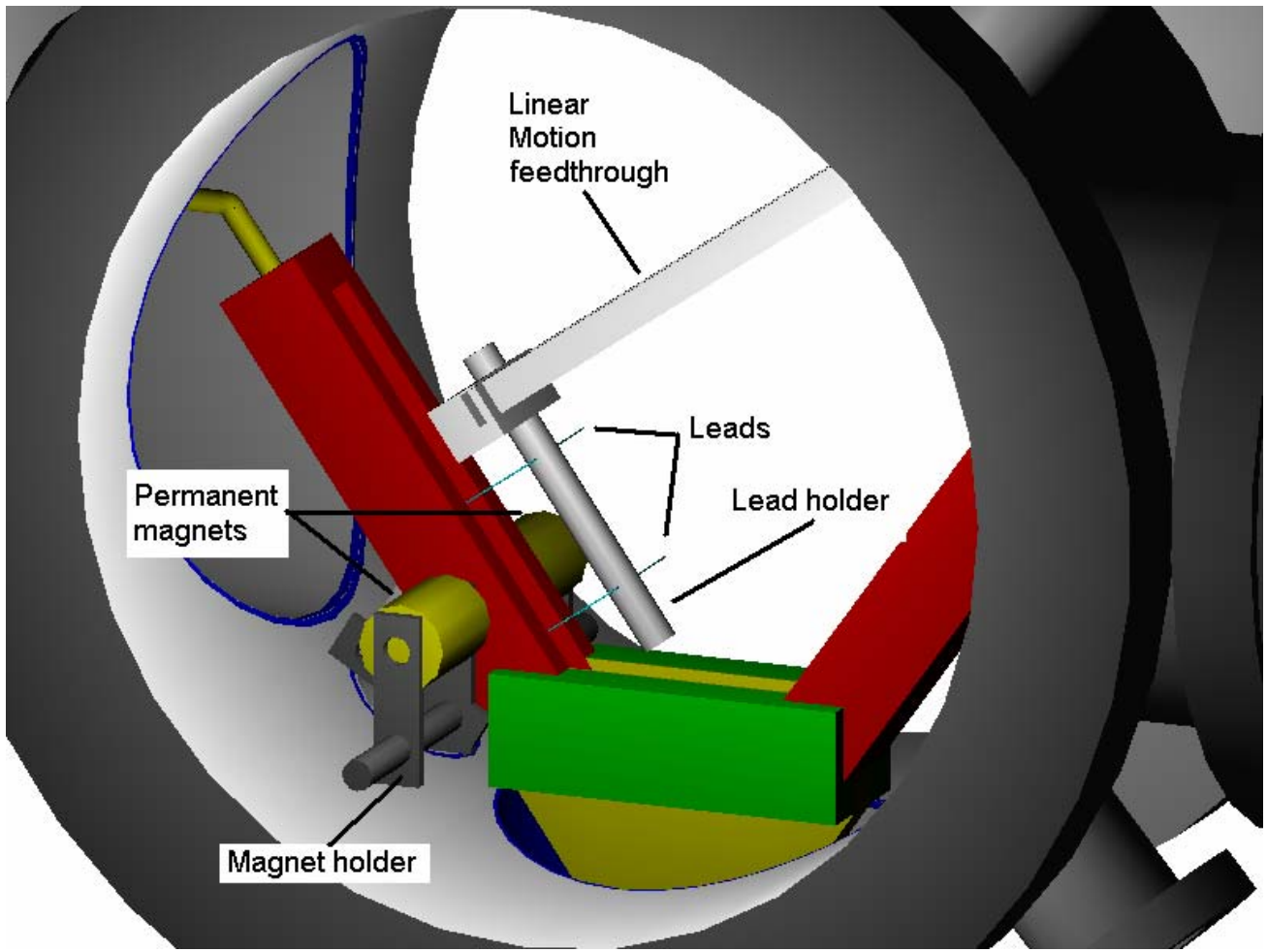
New Model (Cont'd)

- New analytical solution is complicated, but should yield better results (show theoretical increase in R with E)
- Results not yet analyzed with new model
- Additional detail may still be required



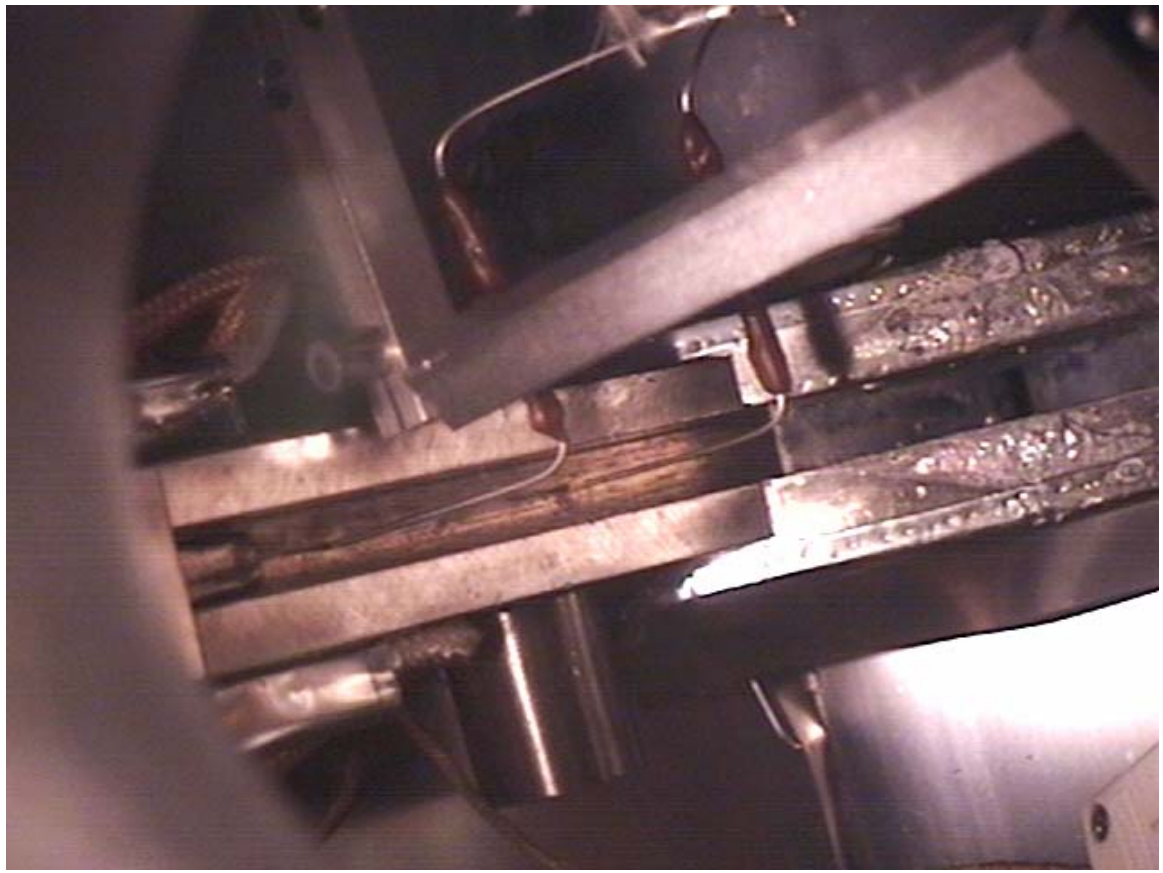
$$R = \frac{\dfrac{A}{\sigma\sqrt{4\pi D t_r}} \int_0^\infty dx \int_0^\infty e^{-\left(\frac{\xi-\mu}{\sigma}\right)^2} \xi \left[e^{-\left(\frac{\xi-x}{4Dt_r}\right)^2} - e^{-\left(\frac{\xi+x}{4Dt_r}\right)^2} \right] d\xi}{\dfrac{A}{2\sigma}\left[\mu\sigma\left(1 - erf\left(\dfrac{\mu}{\sigma}\right)\right) + \sigma^2 e^{-\left(\frac{\mu}{\sigma}\right)^2} \right]}$$

Addition of MHD Experimental Capability in FLIRE



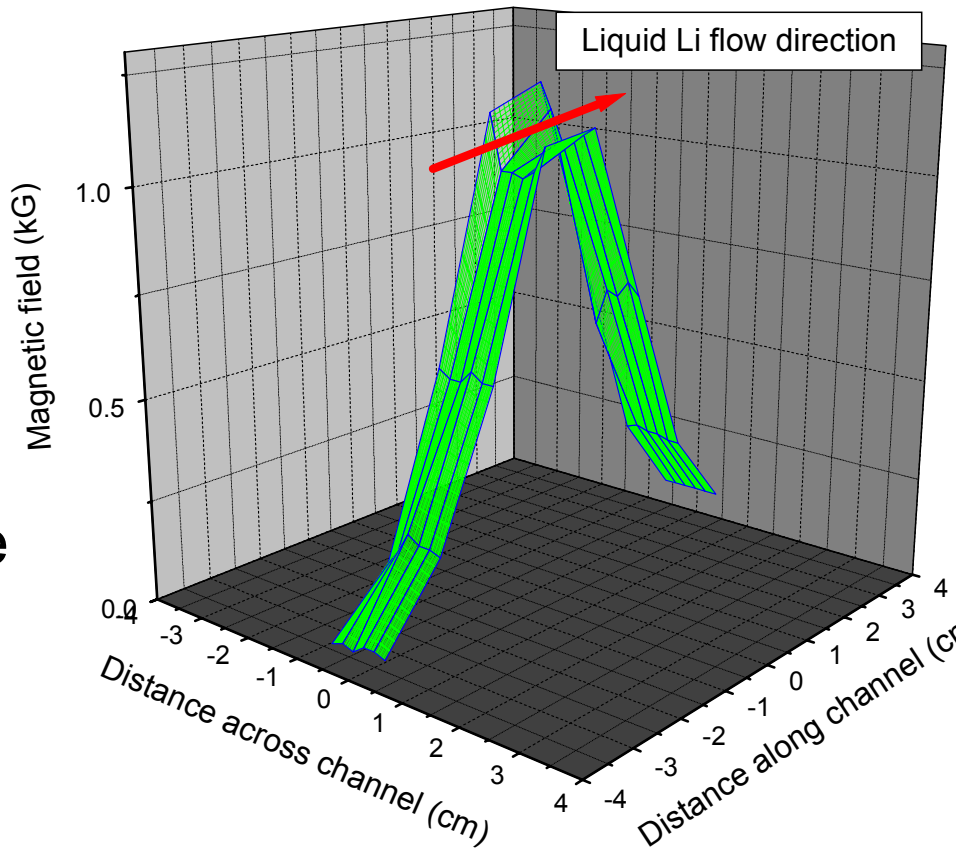
Addition of MHD Experimental Capability in FLIRE (cont'd)

- Permanent magnets provide a 600 G field across flow (after exposure to heat)
- Up to 6 A of current can be passed through the leads in the flow direction

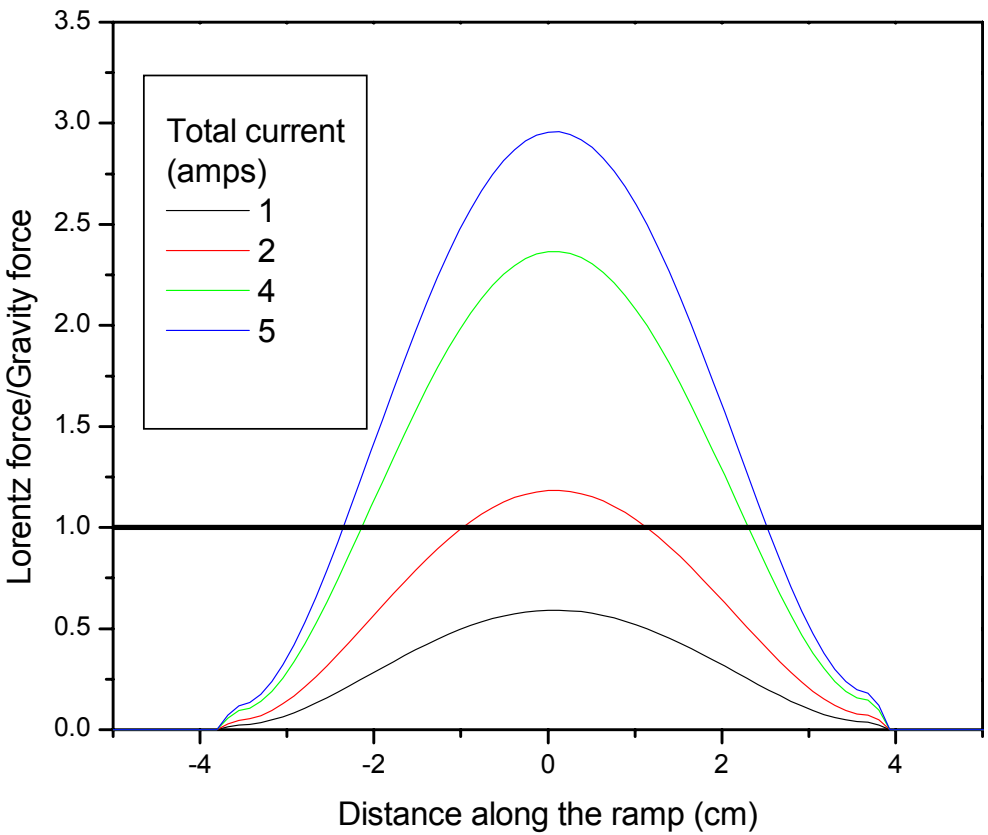


Magnetic Field Strength Along Ramps

- High uniformity across flow, 2 cm region along flow near 1000 G
- After 1 day of operation, field intensity drop of 40% to 600 G at the peak
- Steepest gradient is along the direction of the flow, 1.14 T/m (after demagnetization)

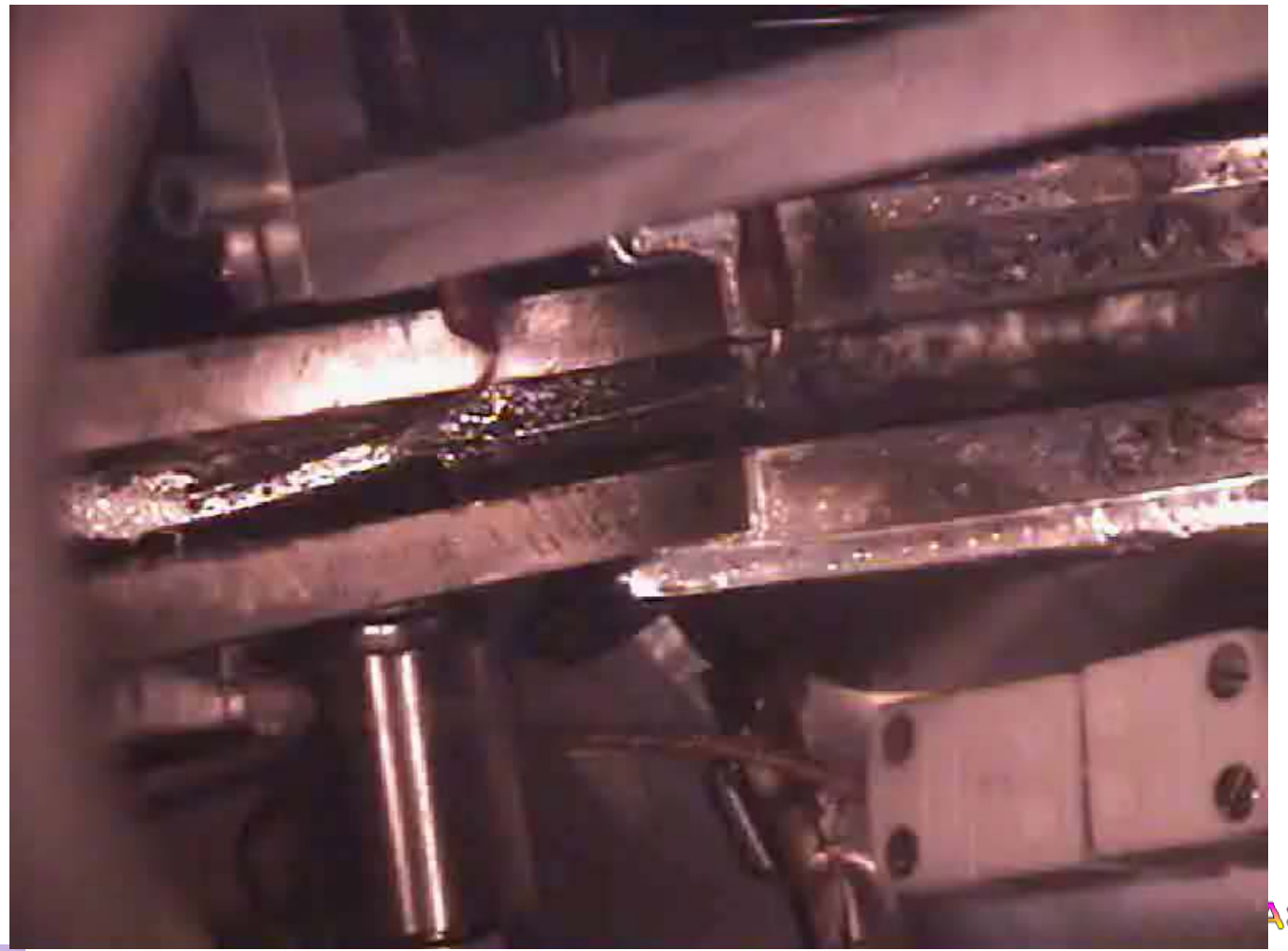


Force Estimates Compared to Experimental Results



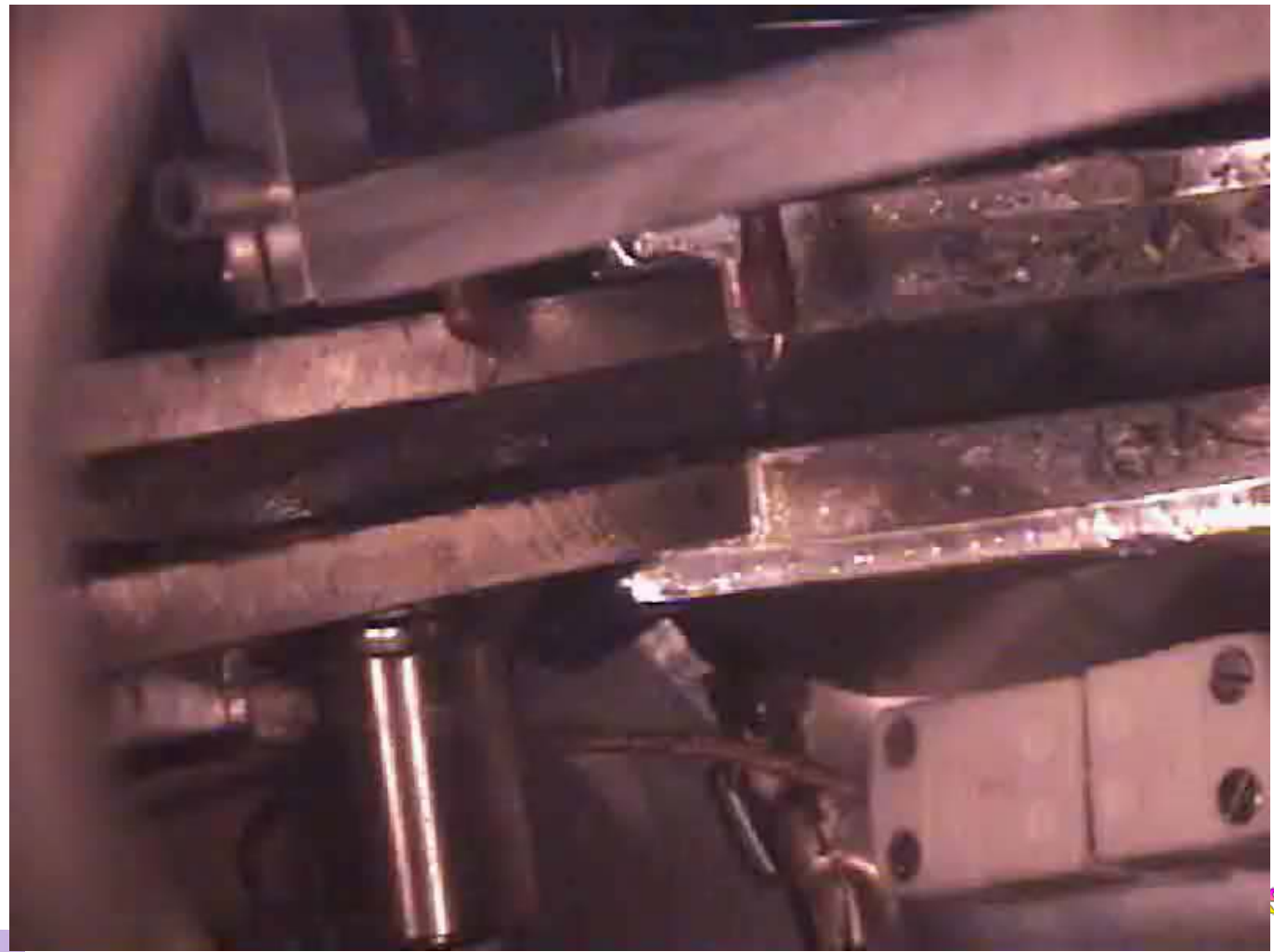
- At 1 A, no lift was observed in the experiments
- At 5 A, the flow lifted from the floor of the ramp but did not detach from the ramp
- Calculations with magnetic field after thermal demagnetization

Lithium Flowing with Magnetic Field, No Current

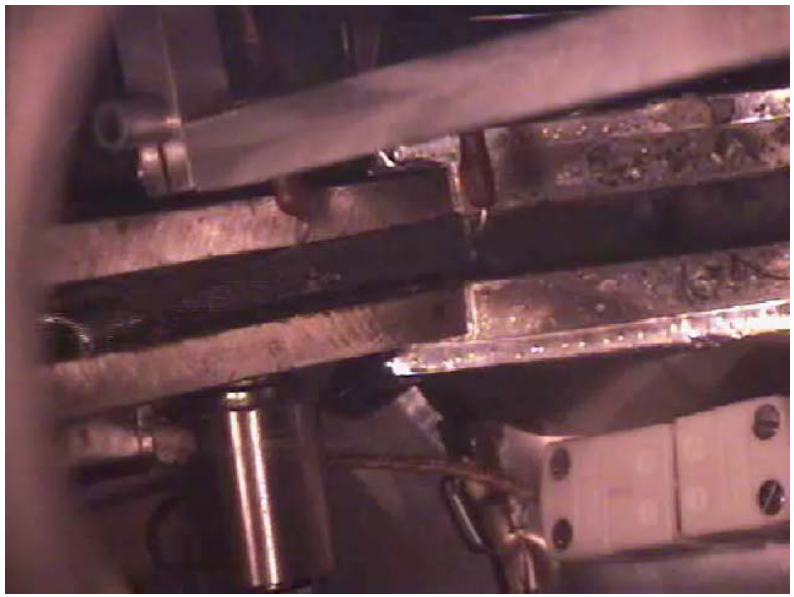


Effect of Lifting Force on the Flow

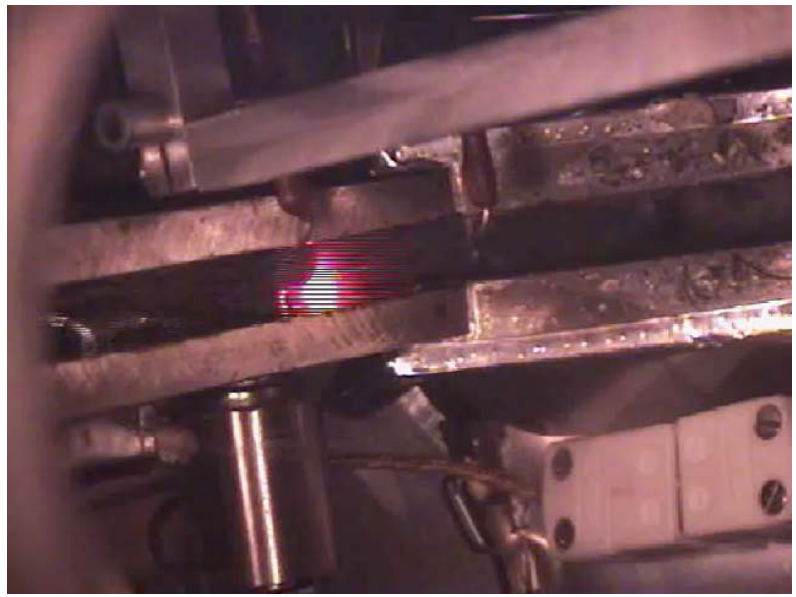
- Magnetic field points from bottom to top of picture
- Current (5 A) going to the right (down the ramp)



Effect of Lifting Force on the Flow (cont'd)

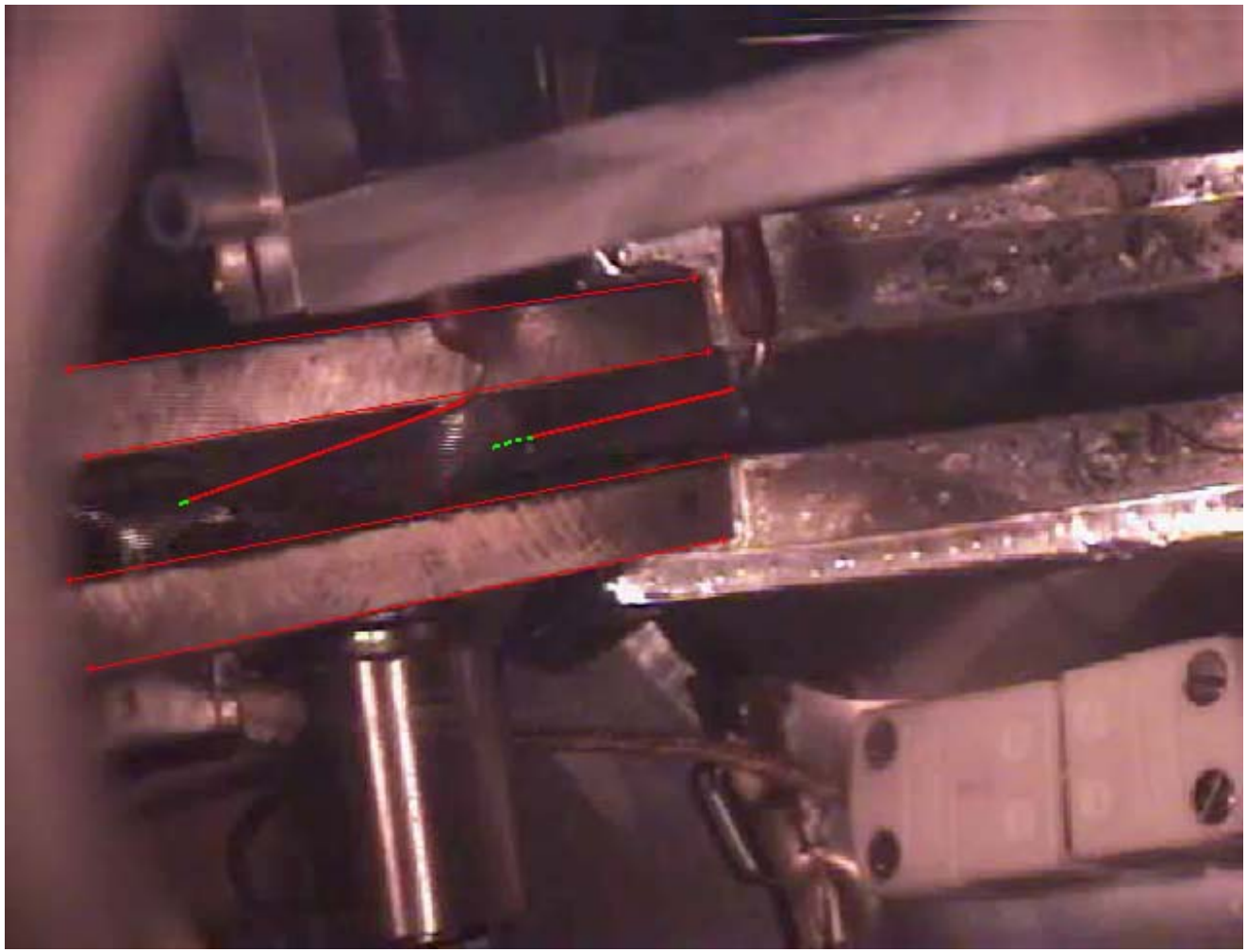


Flow just started, touching top lead only



Two frames later (1/15 sec), the flow makes contact with the bottom lead – note spark

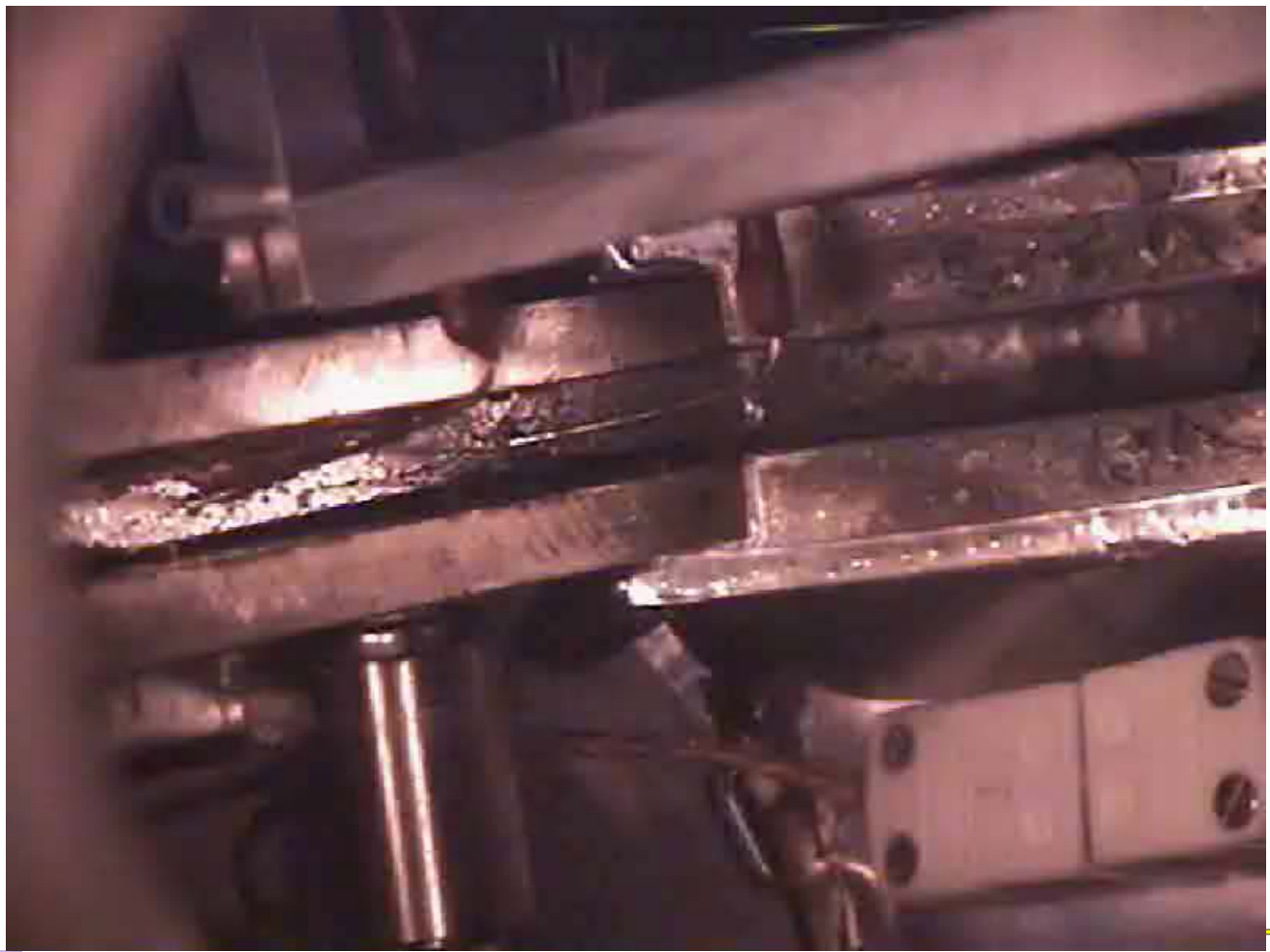
Effect of Lifting Force on the Flow (cont'd)



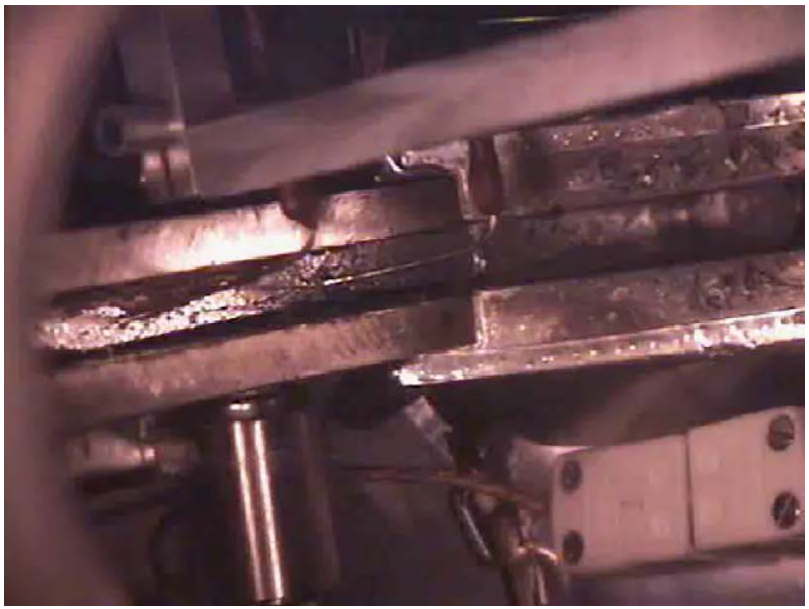
A significant portion of the bottom lead is covered by the lithium, indicating that it has been lifted above the ramp floor although it is still in contact with the bottom of the ramp

Effect of Pushing Force on the Flow

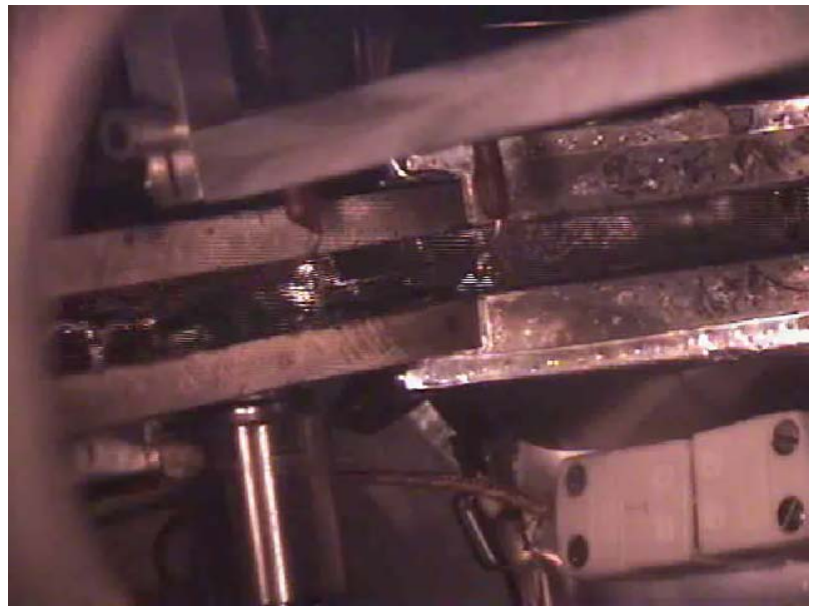
- Magnetic field points from bottom to top of picture
- Current (5 A) going to the left (up the ramp)



Effect of Pushing Force on the Flow (cont'd)

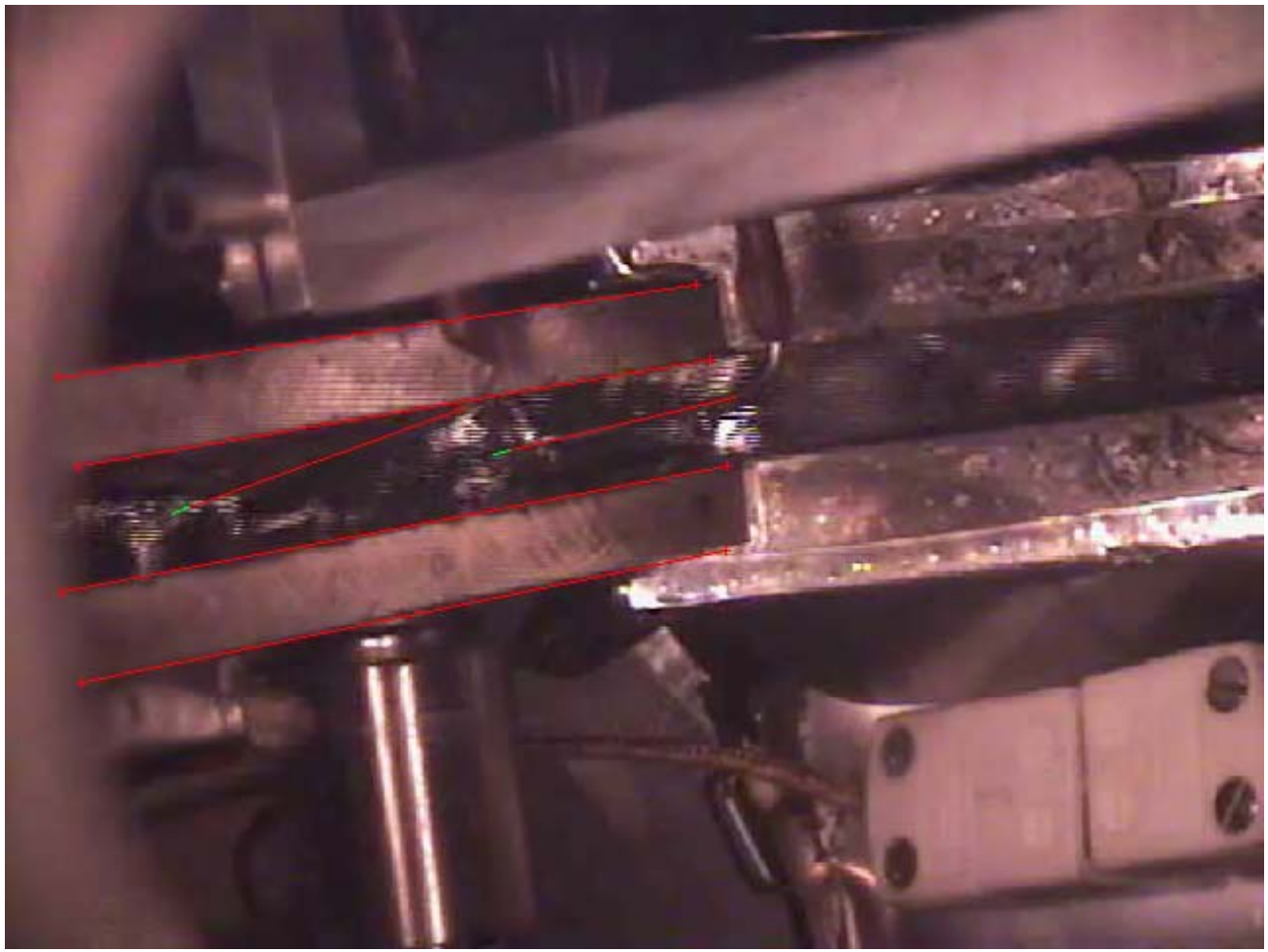


Empty ramp, no flow has started yet



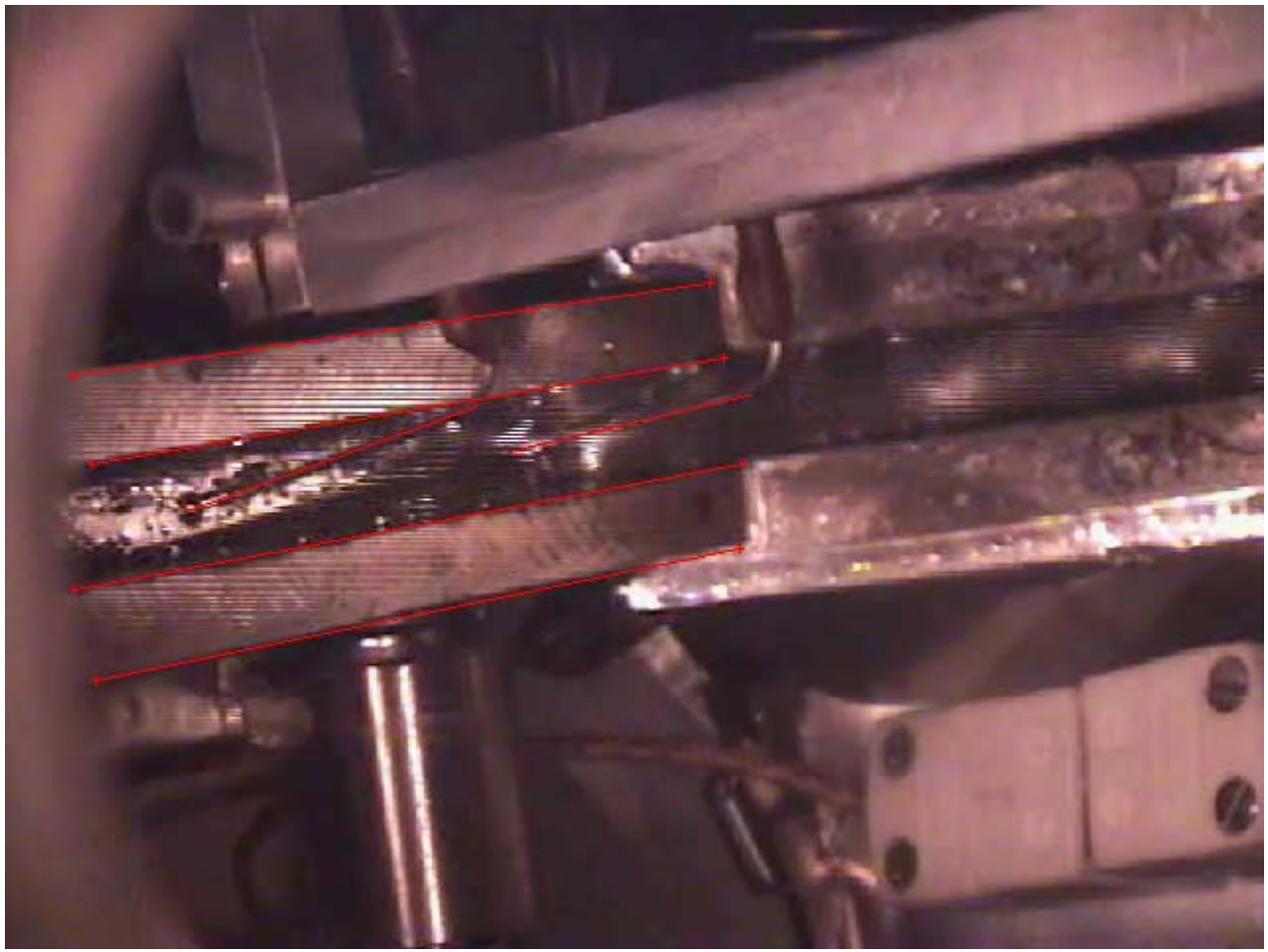
Flow starts and both leads get covered

Effect of Pushing Force on the Flow (cont'd)



During flow, only the lead tips get covered with lithium, indicating thin flow. Also the curvature seems to disappear where the magnets are

Effect of pushing force on the flow (cont'd)



After the flow stops, both leads are exposed again

Summary of FLIRE Results

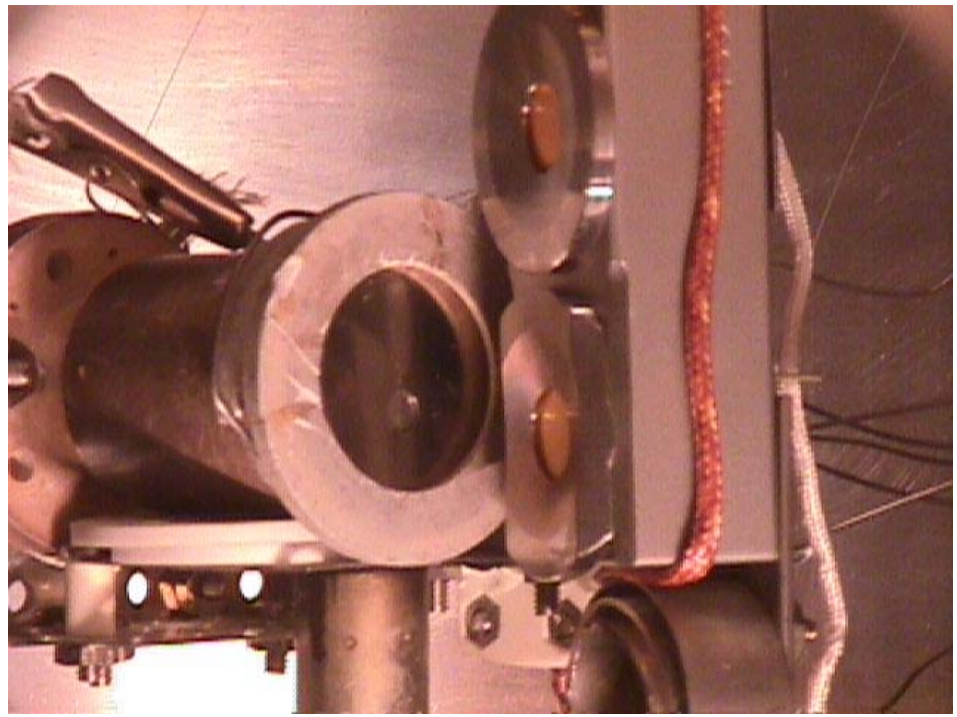
- Double flow
  - Measured retention increases with implantation energy
  - Calculated diffusion coefficient roughly constant
  - High measured retention at low implantation energy needs explaination
- Single flow
  - Measured retention increases more quickly with energy
  - Calculated diffusion coefficient increases with implantation energy
  - Suggests a better model may be needed for diffusion coefficient calculation
- MHD
  - Demonstrates qualitative capability for MHD effects
  - Surface tension can keep Li on ramp, despite lifting force (~3G and still on ramp)

Future Work Plan in FLIRE

- Long-term evolution of implanted He and H particles versus temperature (non-prompt release) using thermal desorption spectroscopy
- How much LiH formed (FLIRE can measure)
- H^+ particle and H-plasma exposures
- He^+ particle and He-plasma exposures
- Gallium retention and diffusivity measurements (Coming this fall, budget permitting)
- Installation of high heat flux source

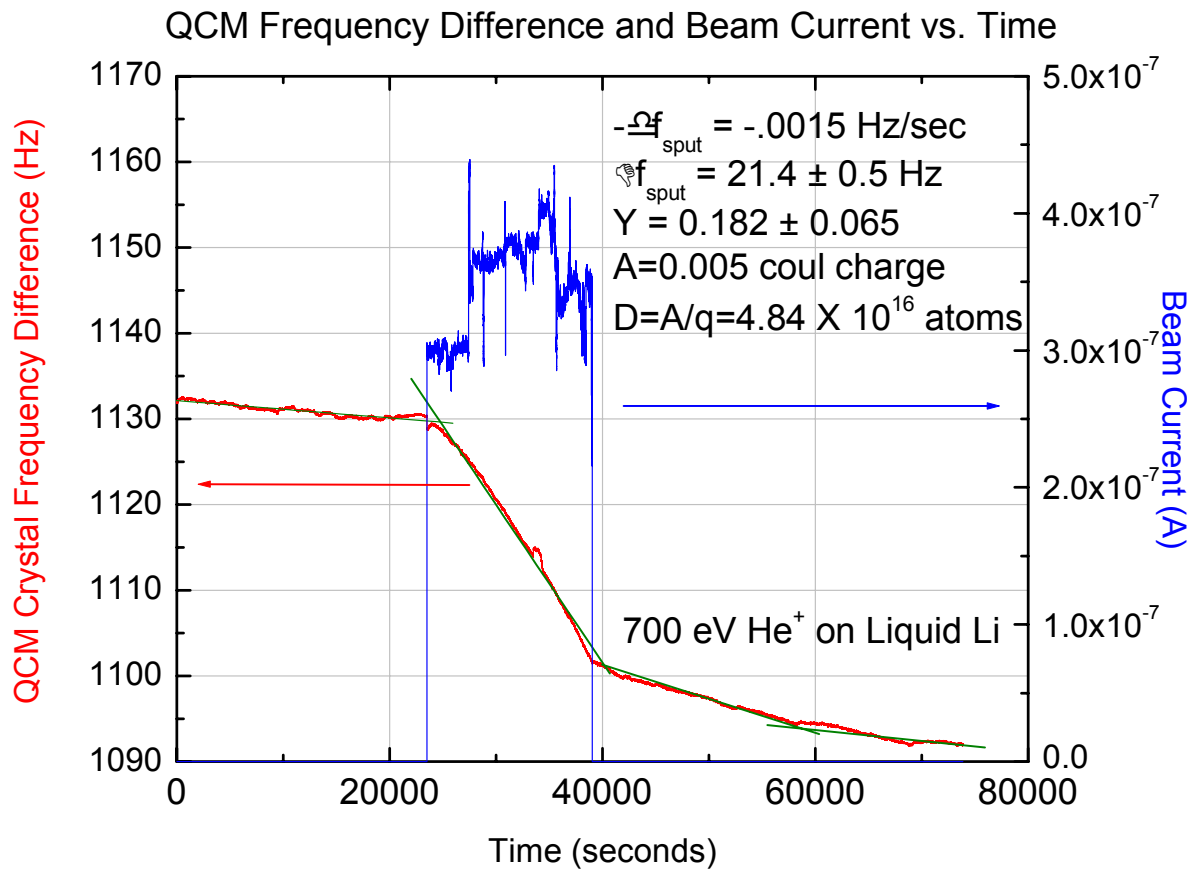
IIAX Experimental Design

- Colutron ion source (>10^{14} ions/cm^2/s) for both Gaseous and metal species: H+, D+, He+, and Li+
- A cleaving arm removes thin oxide layer on liquid-metal sample
- Both evaporation and sputtering measured with quartz crystal microbalance (QCM)
- The DCU-QCM is used to address background temperature variation
- Erosion measurements on static liquid metals



QCM Frequency Difference and IIAX Beam Current Time Plots

- Before liquid target is irradiated with ion beam, an evaporation flux measurement is completed
- QCM frequency difference slope increases when beam hits target measuring evaporation + sputtering fluxes
- When beam is off, some oxidation follows until original evap flux is obtained



$$-\delta f_{sput} = \left|\delta f_{sput+evap} - \delta f_{evap}\right|$$

$$Y = \frac{1}{Df_i S\Omega m_{Li2O}} \frac{\Delta f}{f_{final}} M_{crystal}\left(1 + R_j Y_j \Omega_j\right)$$

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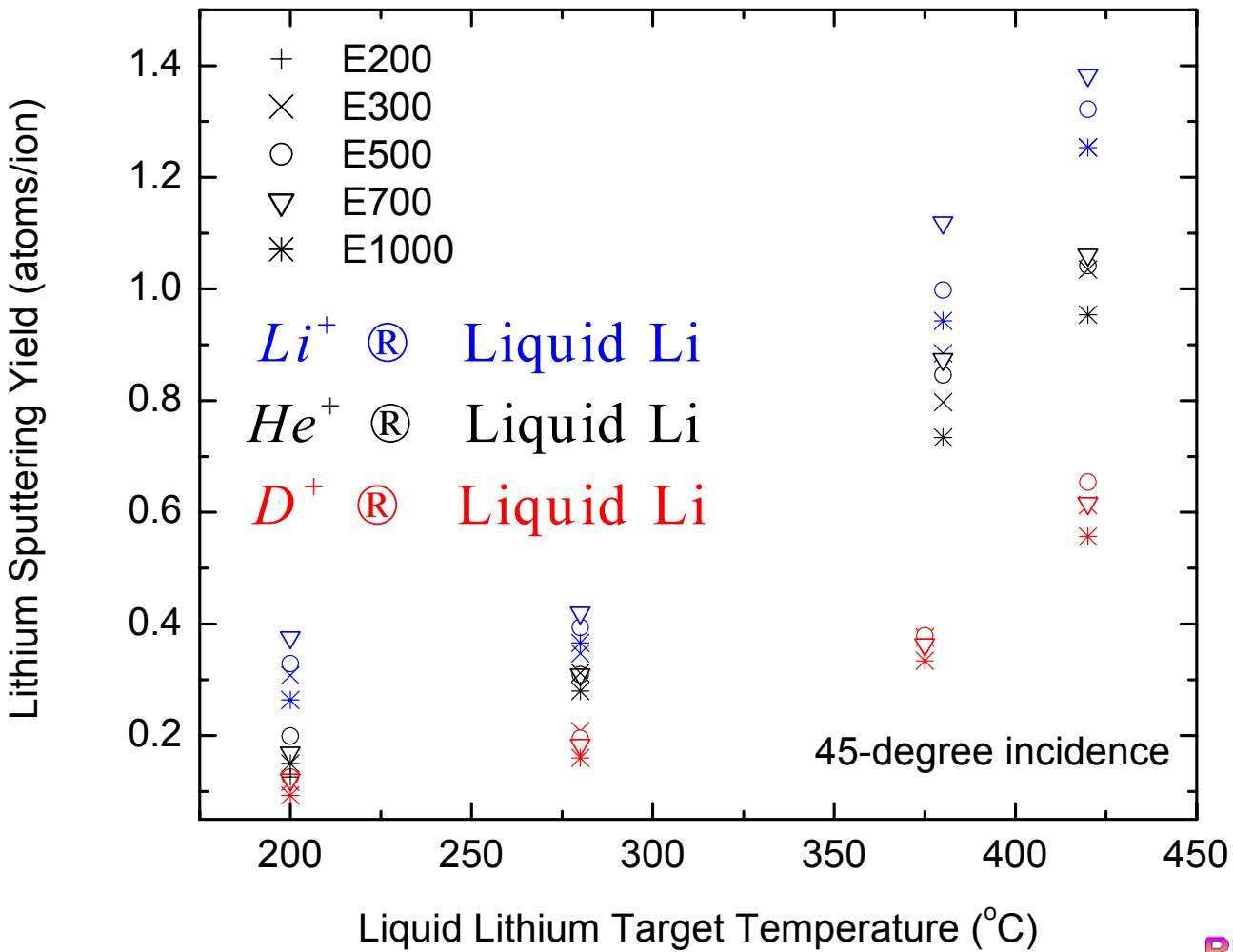
IIAX Temperature-Dependent Yields for Various Incident Particle Energies



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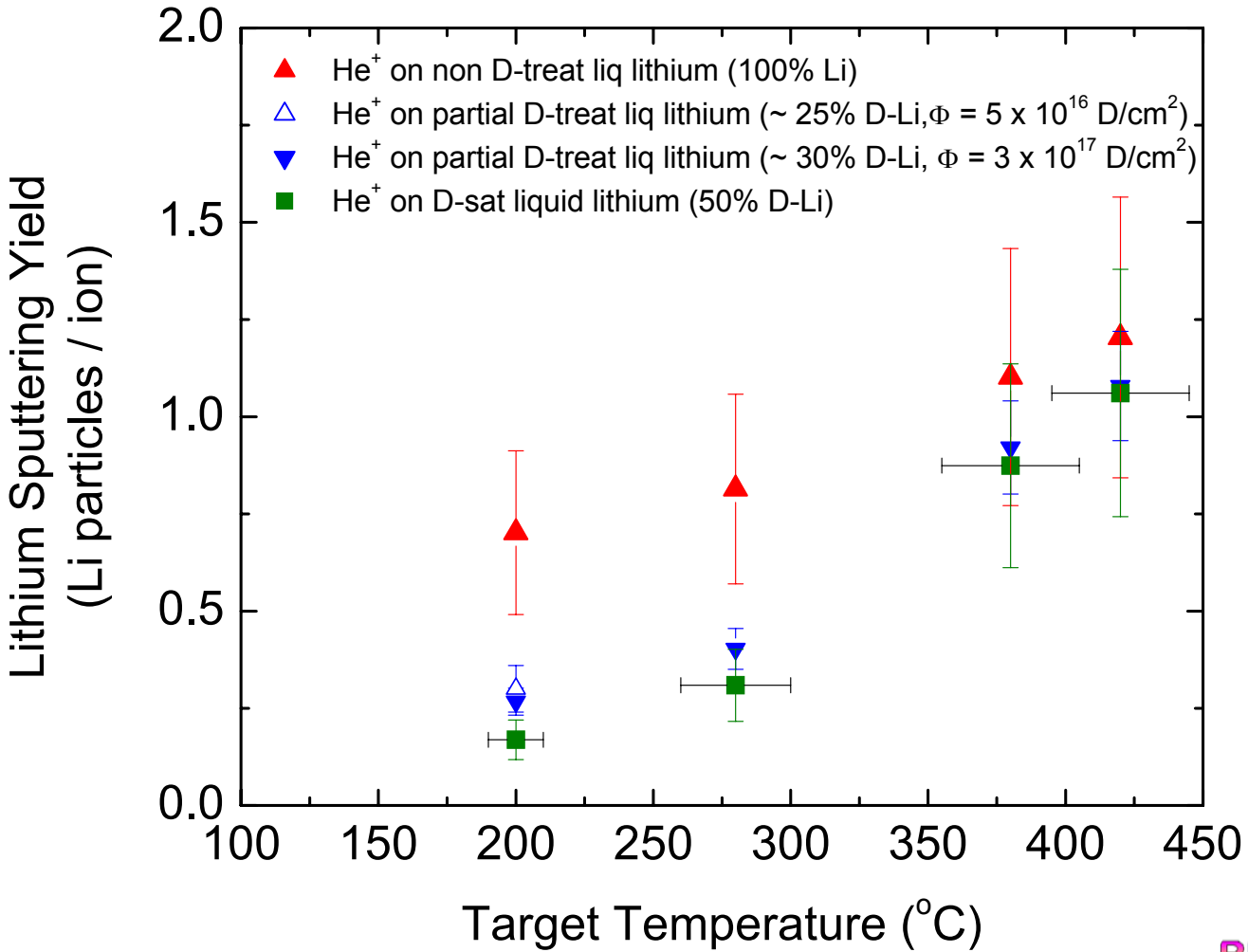
D-Treatment of Liquid Li Surfaces Versus Target Temperature (He^+)



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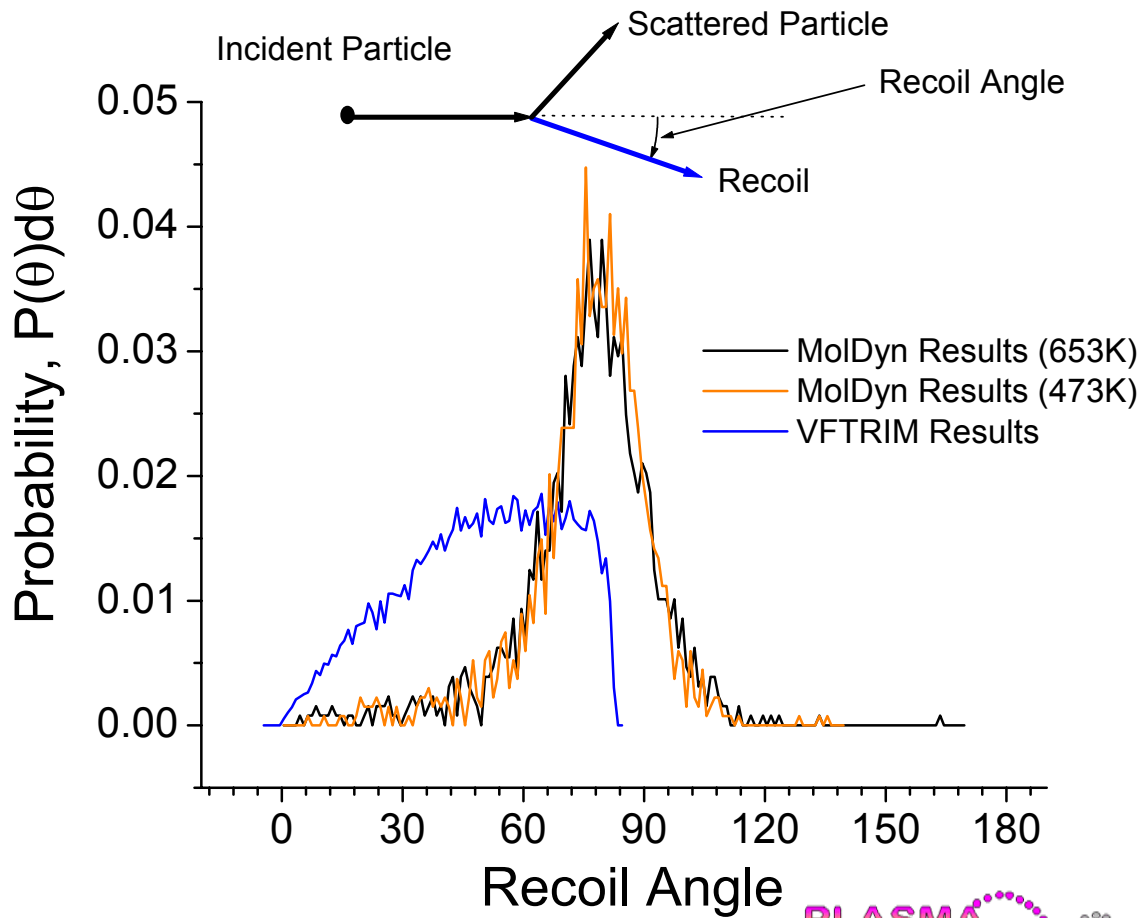
Recoil Angular Distribution from MD Simulations

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



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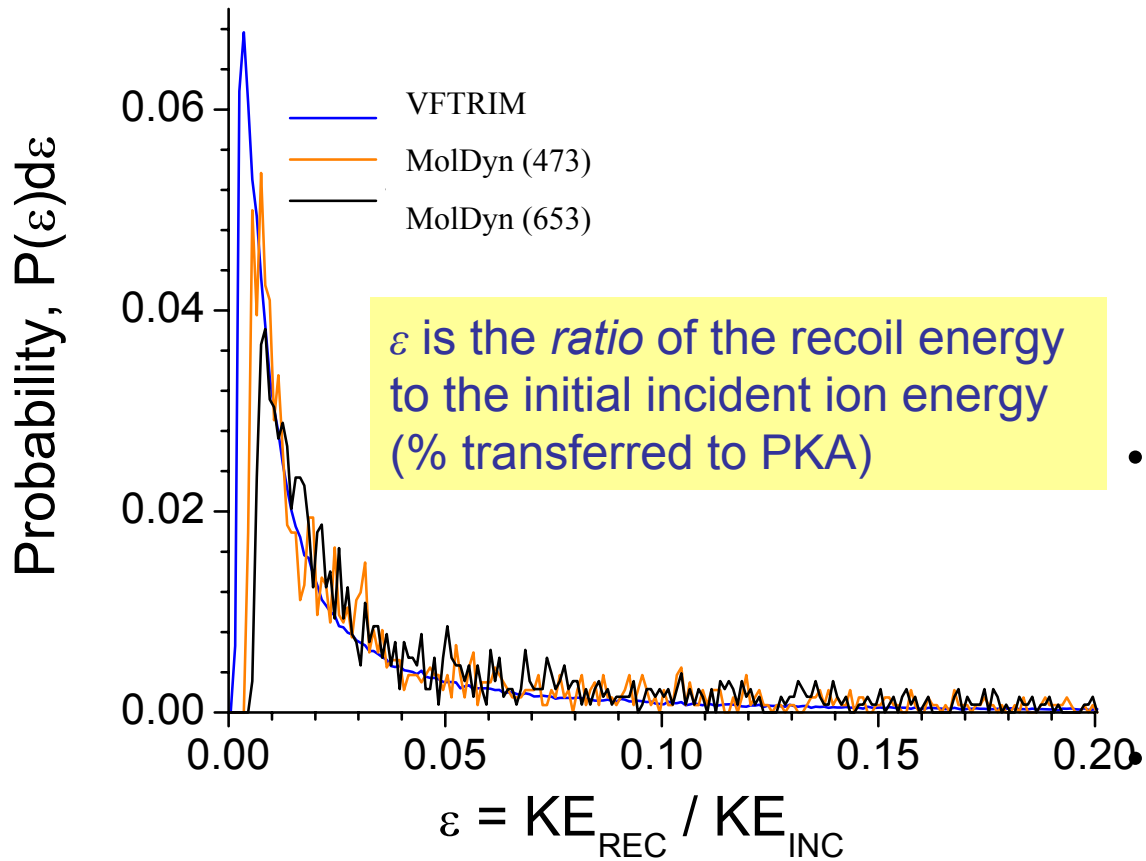
Recoil Energy Distribution from MD Simulations



- 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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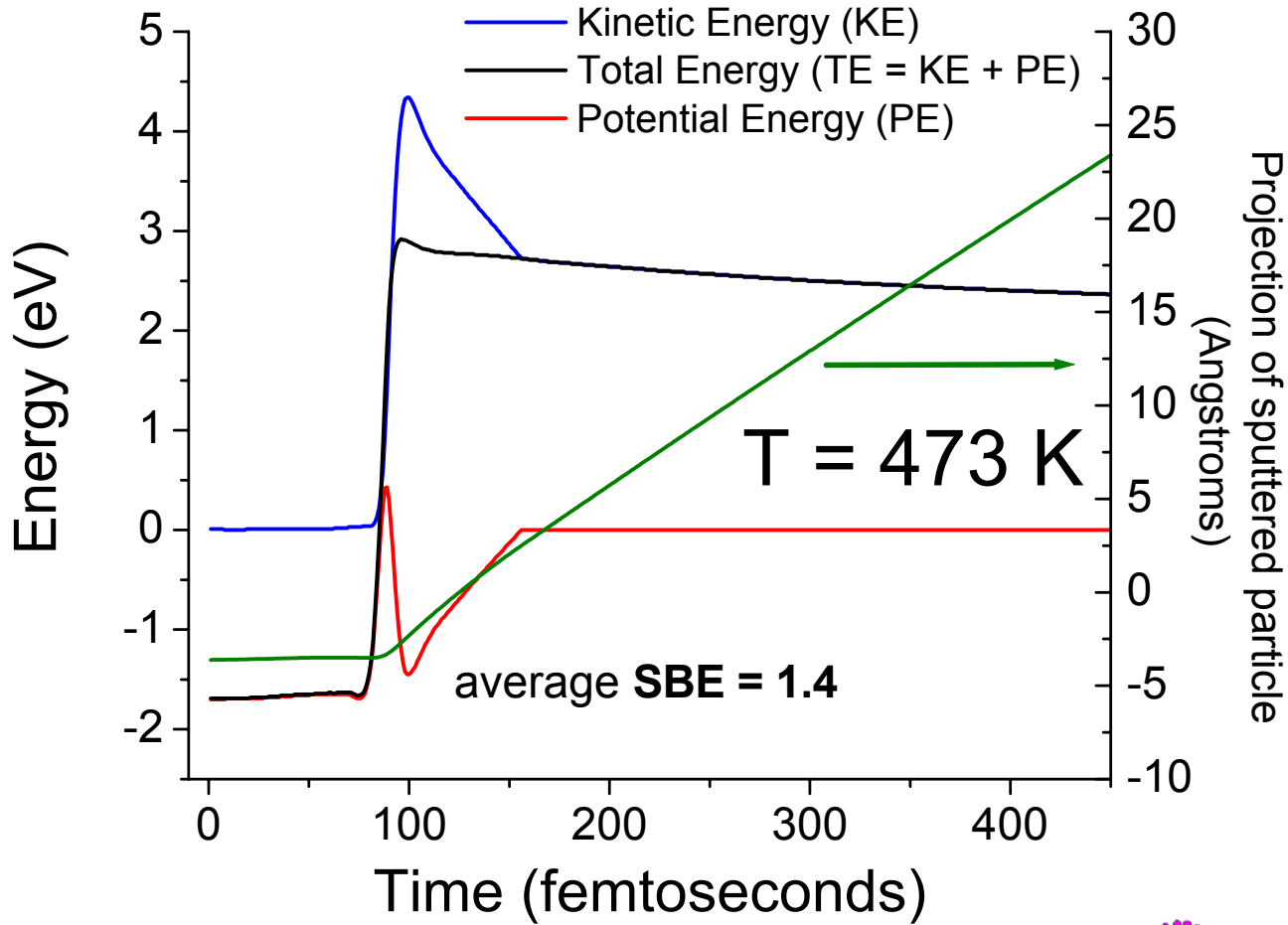
How Surface Binding Energy is Obtained from MD Simulations (473 K)

- 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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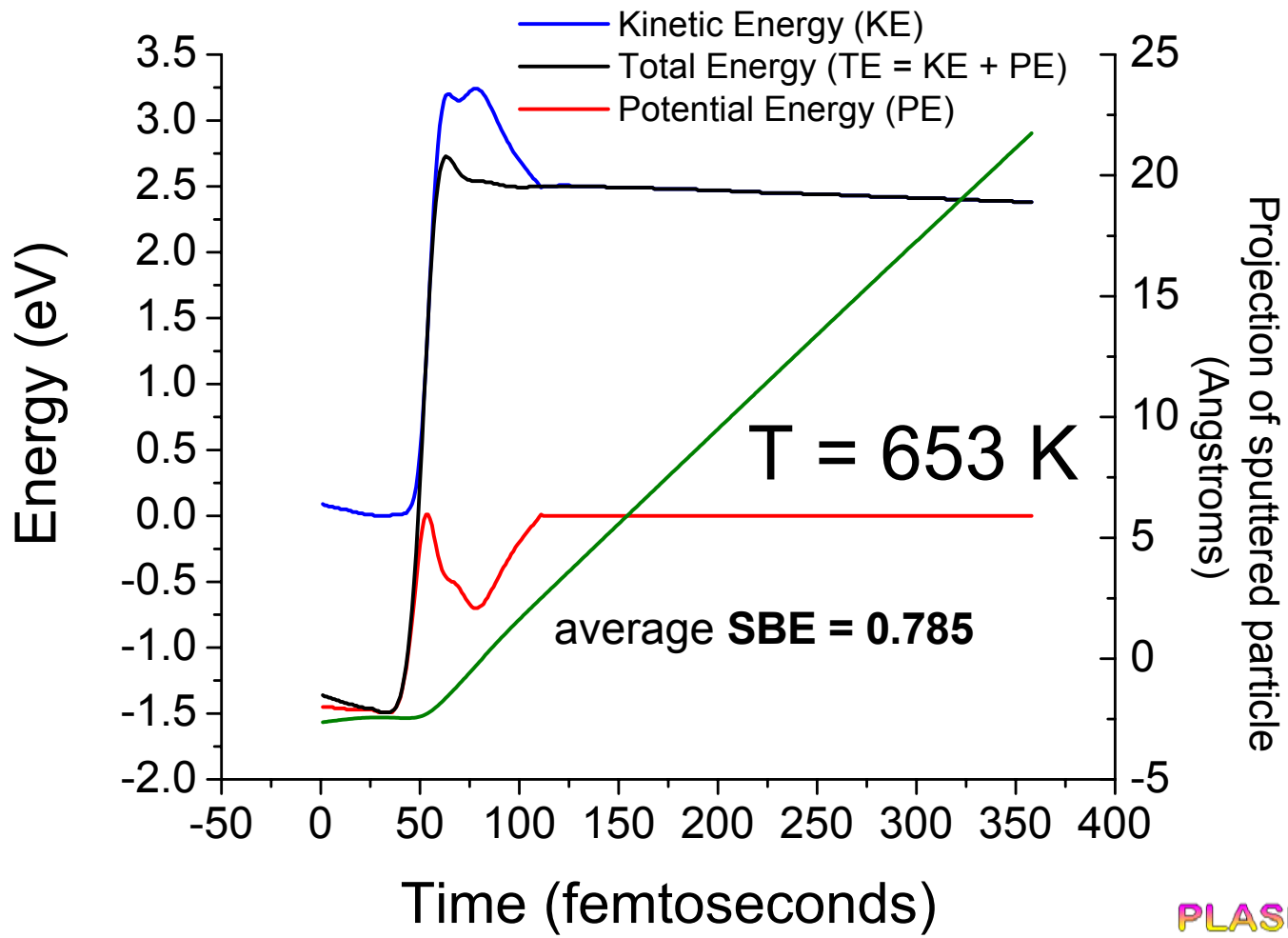
Surface Binding Energy from MD Simulations at 653 K is lower !



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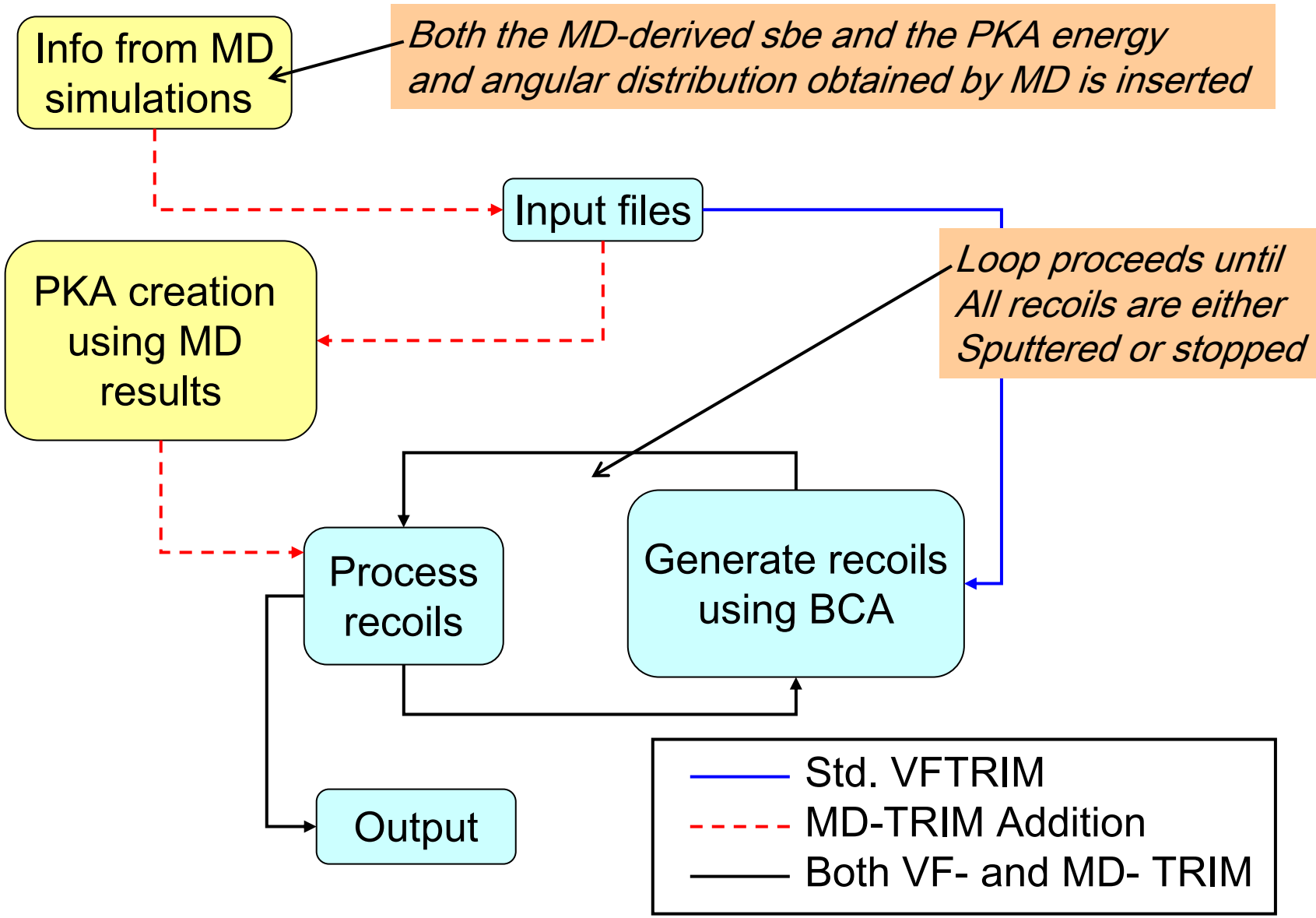

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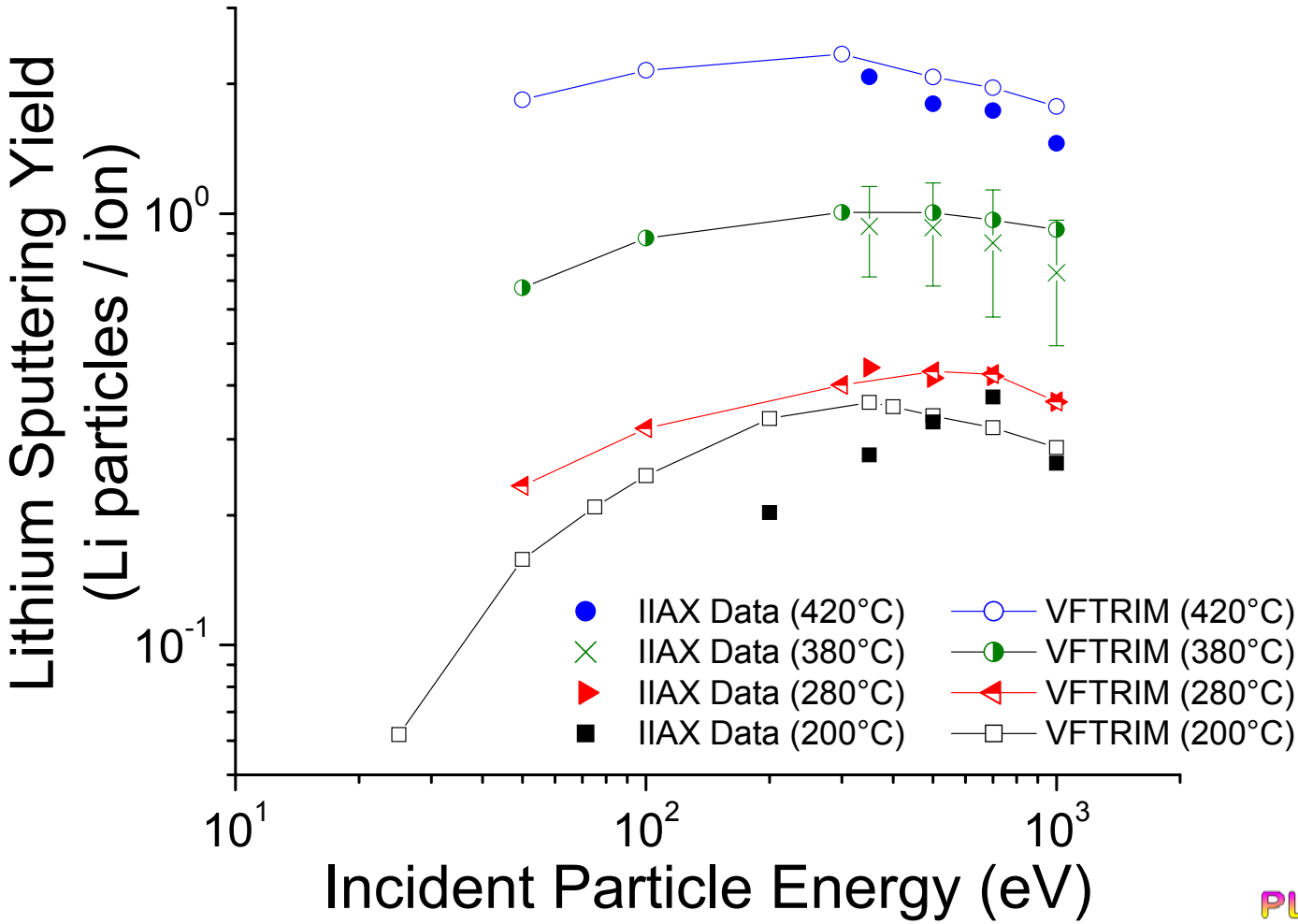
Li^+ on Liquid Li (D-treated) IIAX Data with ad-hoc VFTRIM-3D Model



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MD-TRIM Results

Estimated Experimental Results : 0.8 1.2

PKA Dist. Type / sbe	VFTRIM (Std. Ver.)	MD-TRIM Results		
		VFTRIM (BCA Dist.)	473°K (MD Dist.)	653°K (MD Dist.)
0.79 eV	0.8415	1.1130	1.1827	1.2938
1.40 eV	0.4915	0.6430	0.7549	0.8084
1.68 eV	0.4152	0.5180	0.6378	0.7048

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Mechanisms that Explain Enhancement (Allain-Ruzic Model)

- Near-surface energy deposition to “weakly-bonded”, mobile lithium atoms leads to non-linear erosion even for low-incident particle energies (true for materials with low cohesiveness and sublimation heat such as: alkali metals or the alkaline earths, others: Ga, In, Sn, Sn-Li)… This occurs even for solid-phase materials but becoming more conspicuous in the liquid state
- In addition, the nature of the binding of the sputtered atom relative to its nearest neighbors and how this changes with system temperature
- Surface stratification (characteristic of liquid-metals) could in fact play a role in the enhancement of erosion

Summary of IIAX Results

- Liquid-metals do not erode much differently than in their solid state just above the melting point
- IIAX data of Li erosion from D-treated and non D-treated samples suggest that the chemical state of the surface (with D-treatment) decreases the sputtering yield of lithium
- Lithium erosion is enhanced as temperature increases for a variety of incident particle energies (50 eV – 1 keV) and incident species: D+,He+, Li+
- Other liquid-metals where erosion enhancement has been observed: Ga, Sn and Sn-Li at low incident particle energies
- The Allain-Ruzic model (verified with MD results) fits and explains observed liquid-metal sputtering temperature dependence
  - Near-surface energy deposition to “weakly bonded” mobile lithium atoms leads to nonlinear erosion, even for low incident energies
  - Nature of binding of sputtered atoms to nearest neighbors changes with temperature (decreases)

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- ALPS/DOE funding
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