Experiments and modeling of charged particle/ free-surface flowing liquids

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ALPS Meeting, Grand Canyon, Arizona
April 9-11, 2003

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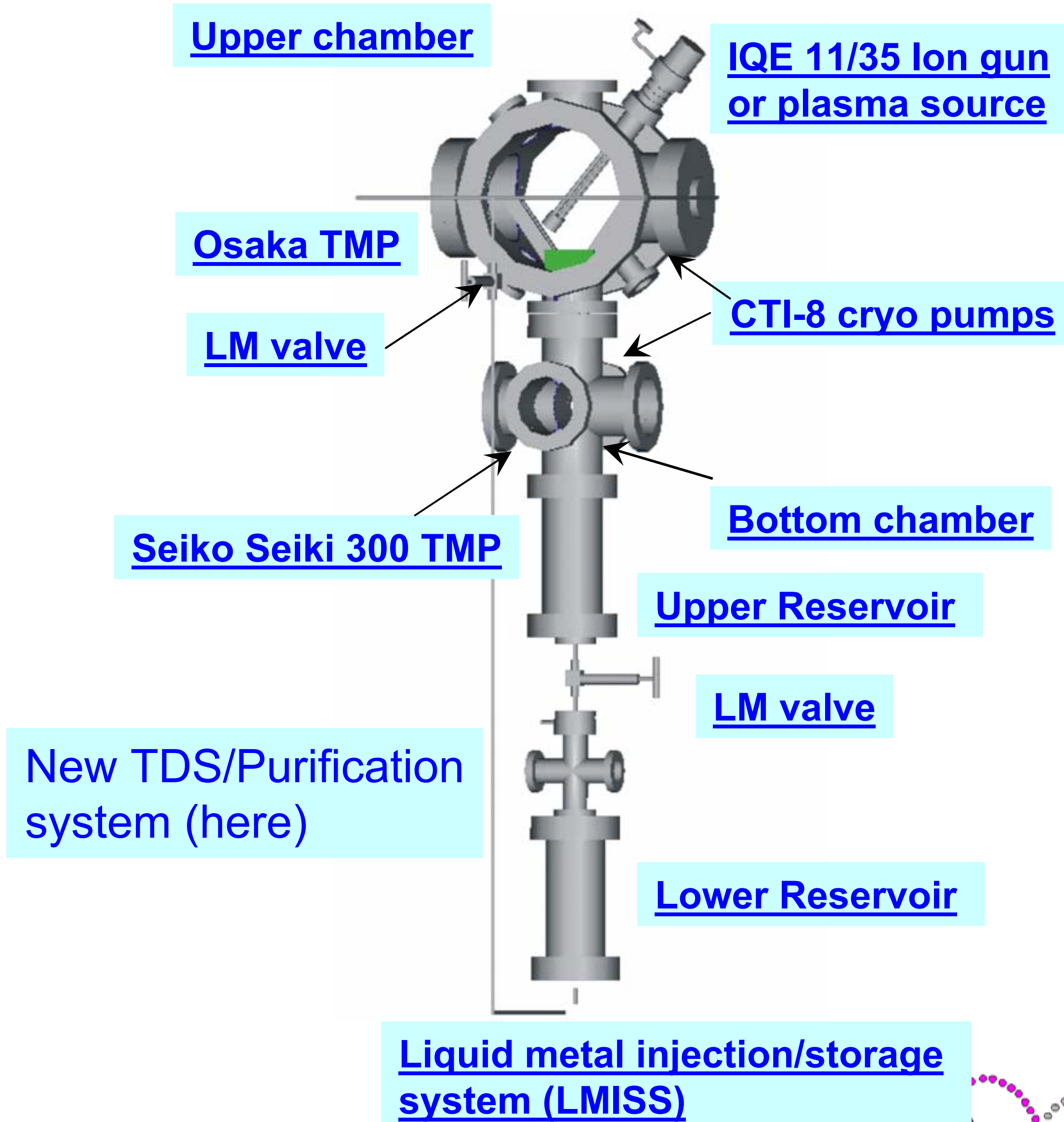
Outline

- Overview of the Flowing Liquid Retention Experiment (FLIRE) at Illinois
- Recent modifications to FLIRE
- MHD experiments on FLIRE
- Future work plan for FLIRE
- Molecular Dynamic Modeling of liquid Li
- Explanation of temperature enhanced sputtering --- a new code: MDTRIM
- Summary and acknowledgements

General FLIRE Experimental 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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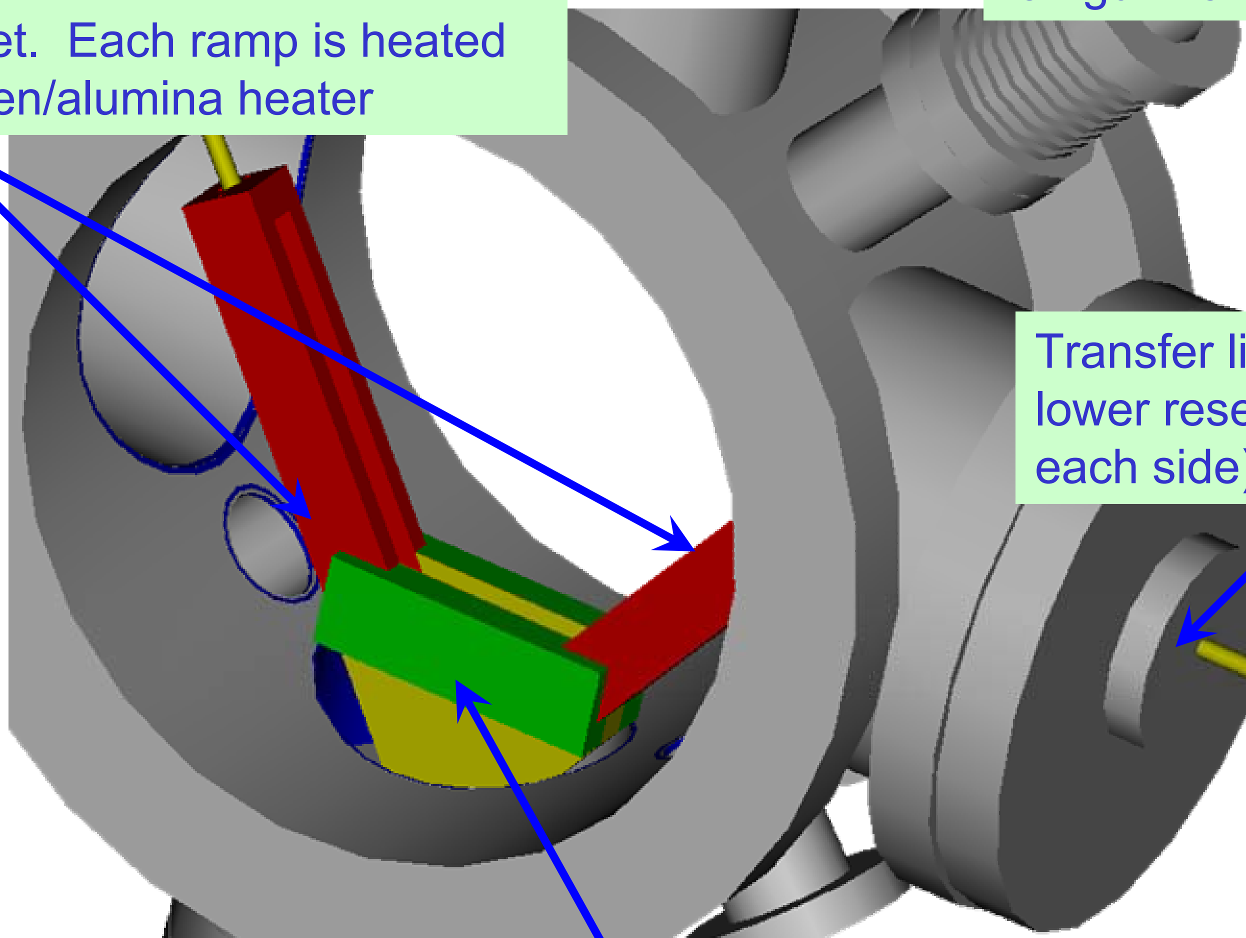
Upper vacuum chamber design with ramps and bracket



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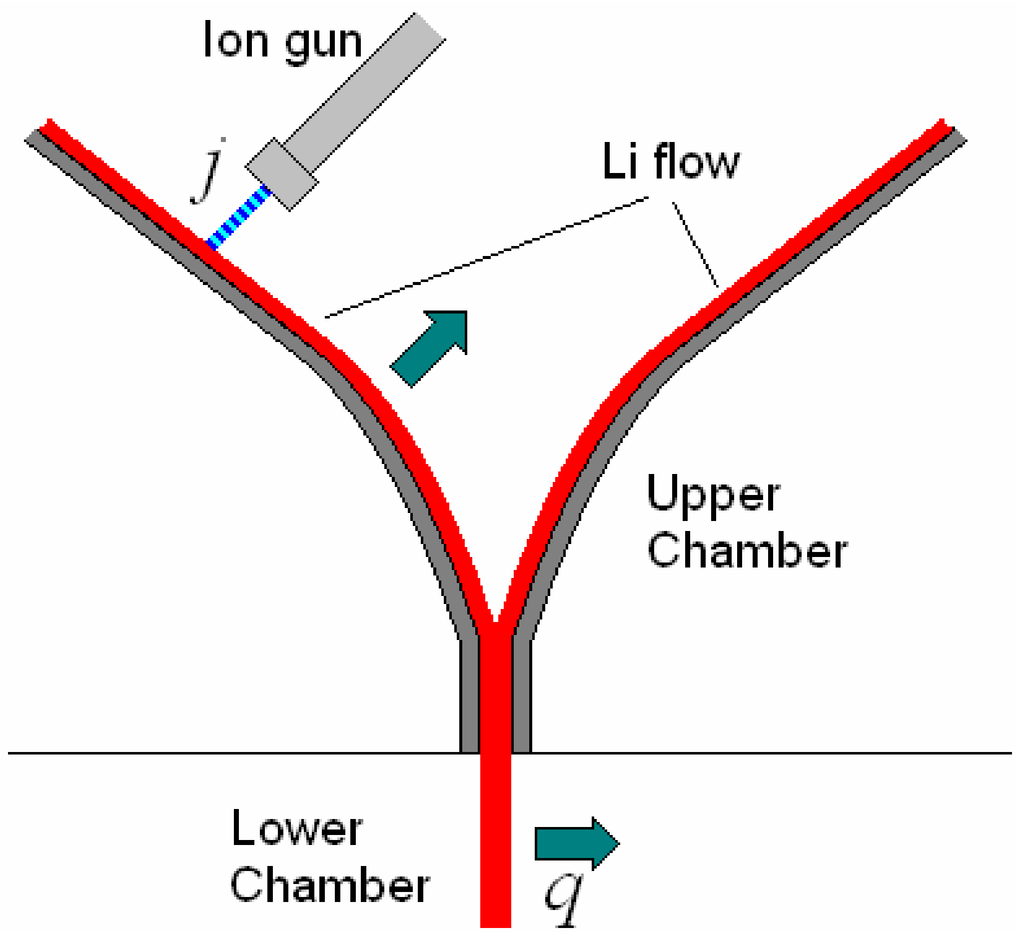
Definition of retention coefficient

- The retention coefficient is given by:

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

q: release rate in the lower chamber

j: injection rate in the upper chamber



Calculation of D from He retention data

- From analytical model, the retention coefficient is given by:

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

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

v: flow velocity

r: mean implantation range

L: path length from striking point to exit

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

M. Nieto, et al., J. Nucl. Mater. 313-316 (2003) 646

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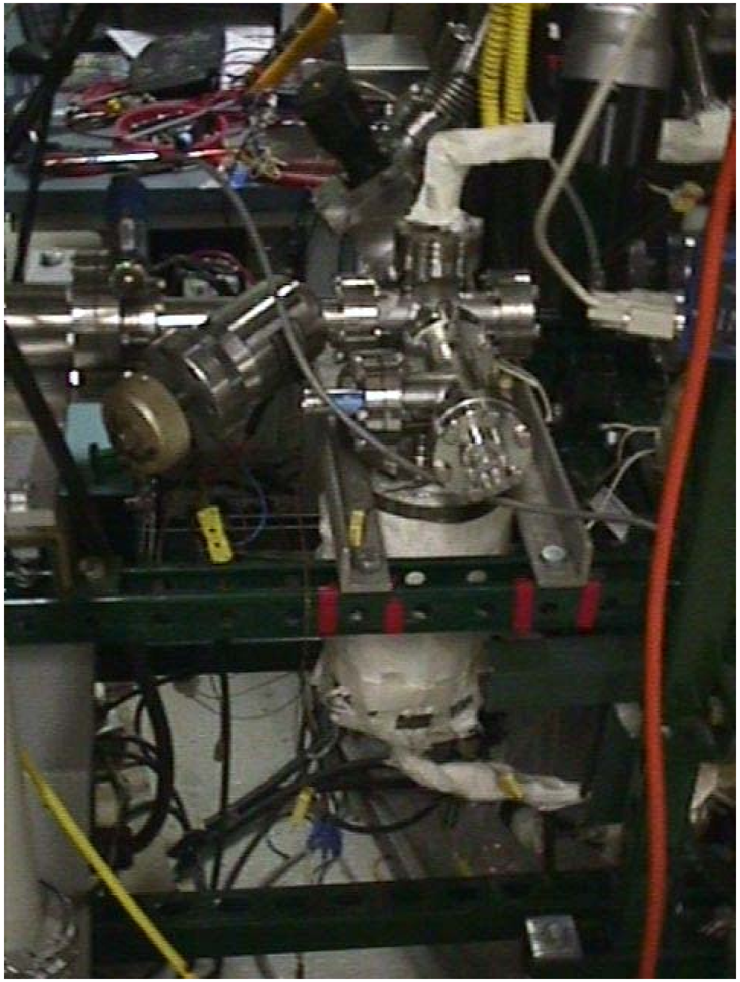
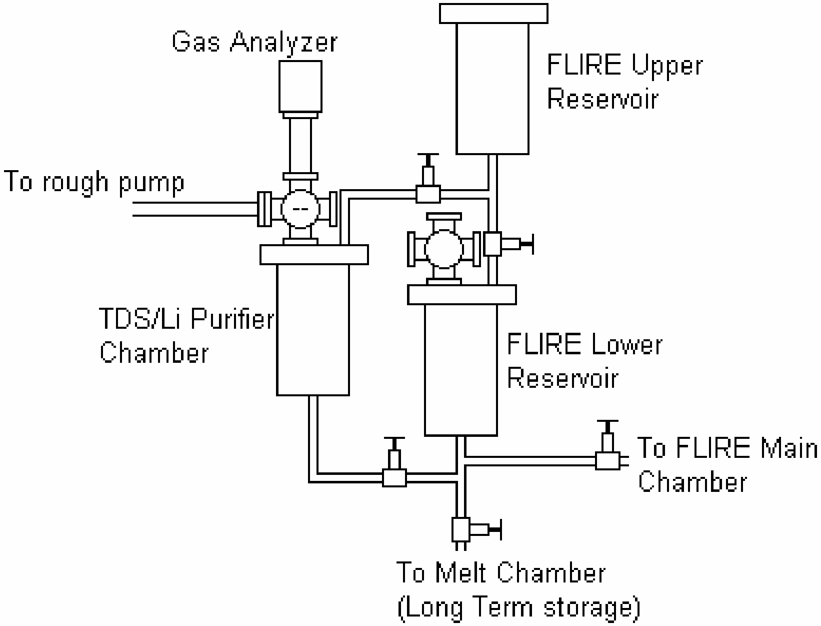
New TDS/Purification System major components





- New layout of TDS (thermal desorption spectroscopy)/ Purification chamber installed in FLIRE to measure long-term retention/diffusivity of implanted helium and chemically-bound hydrogen
- The new design also works to remove implanted species from liquid-metal to be recycled for additional runs in FLIRE

TDS/Purification System

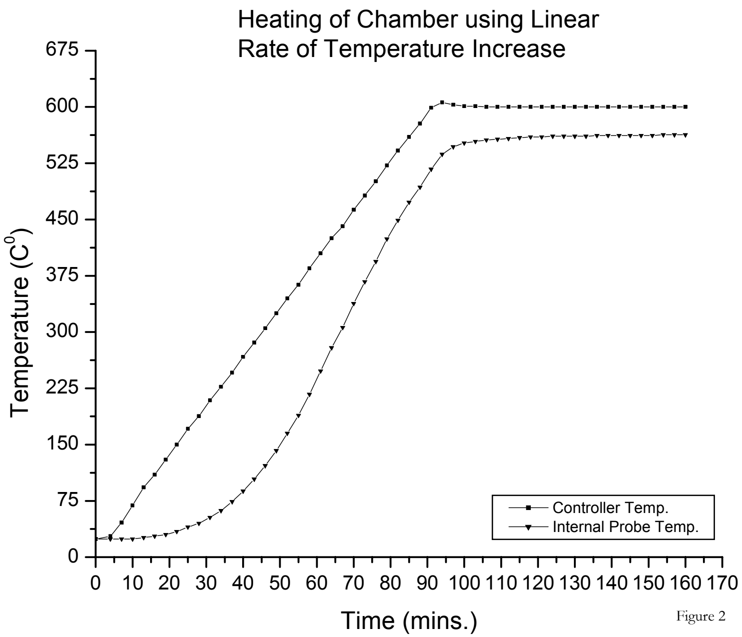


Figure 2

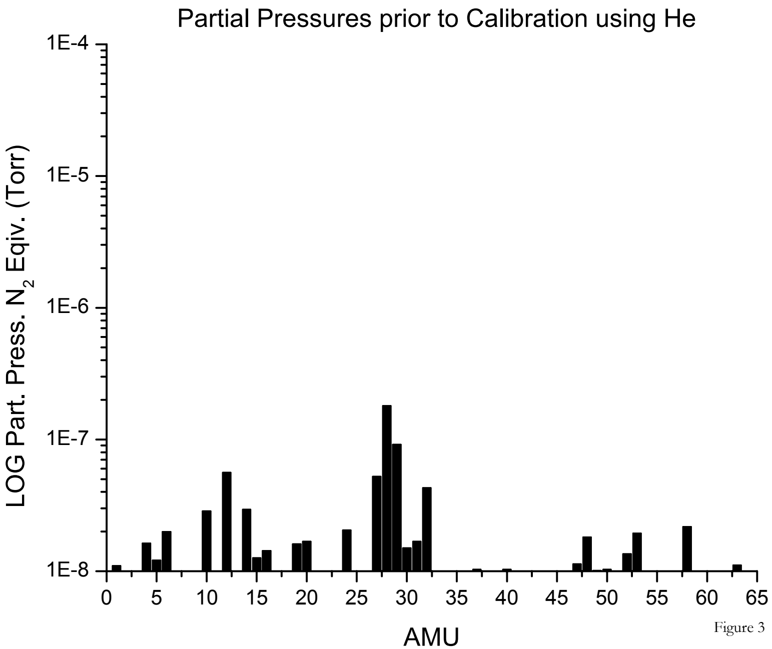
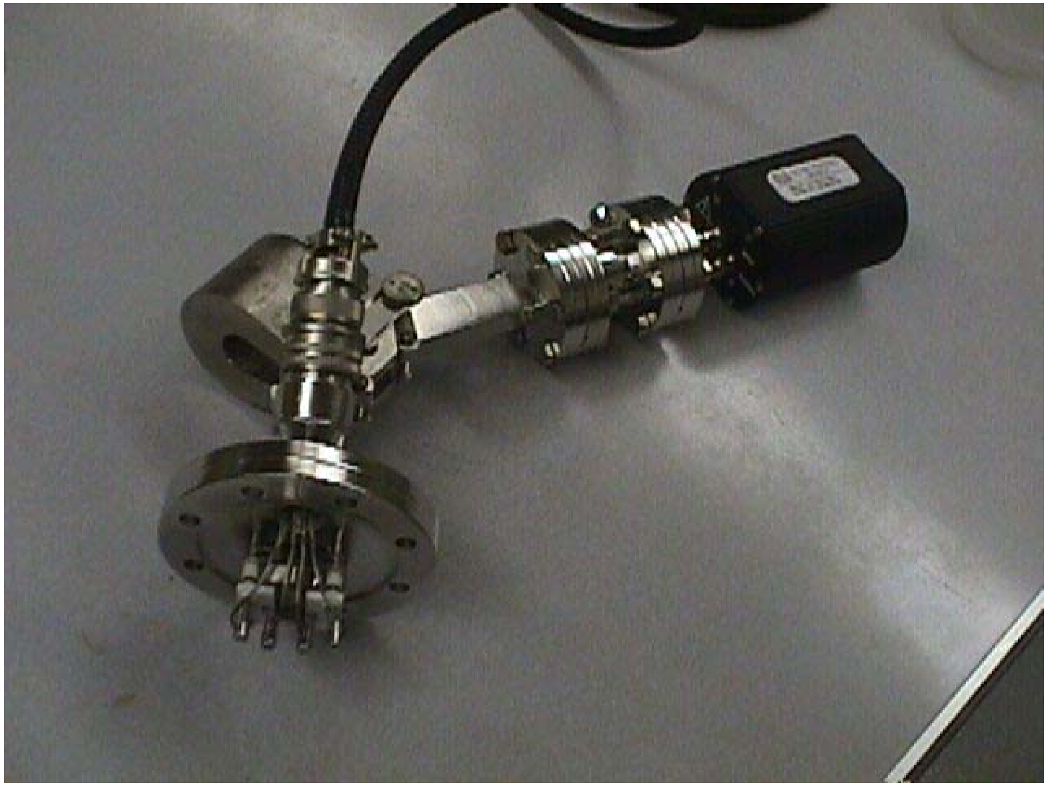


Figure 3

- Can get to temperatures above the decomposition temperature of LiH (660° C)
- Main impurity is air, not water or hydrogen
- Temperature ramp-up and control system tested

Magnetic Sector Mass Spectrometer for residual gas analysis

- VTI Odyssey system
- Low-mass capability
- no “zero blast” issues as in QMS systems
- Mass range: 1-100 amu
- 5 X 10^{-14} Torr min. detectable pressure with electron multiplier
- Spectrometer is shared between the new TDS system and FLIRE bottom chamber



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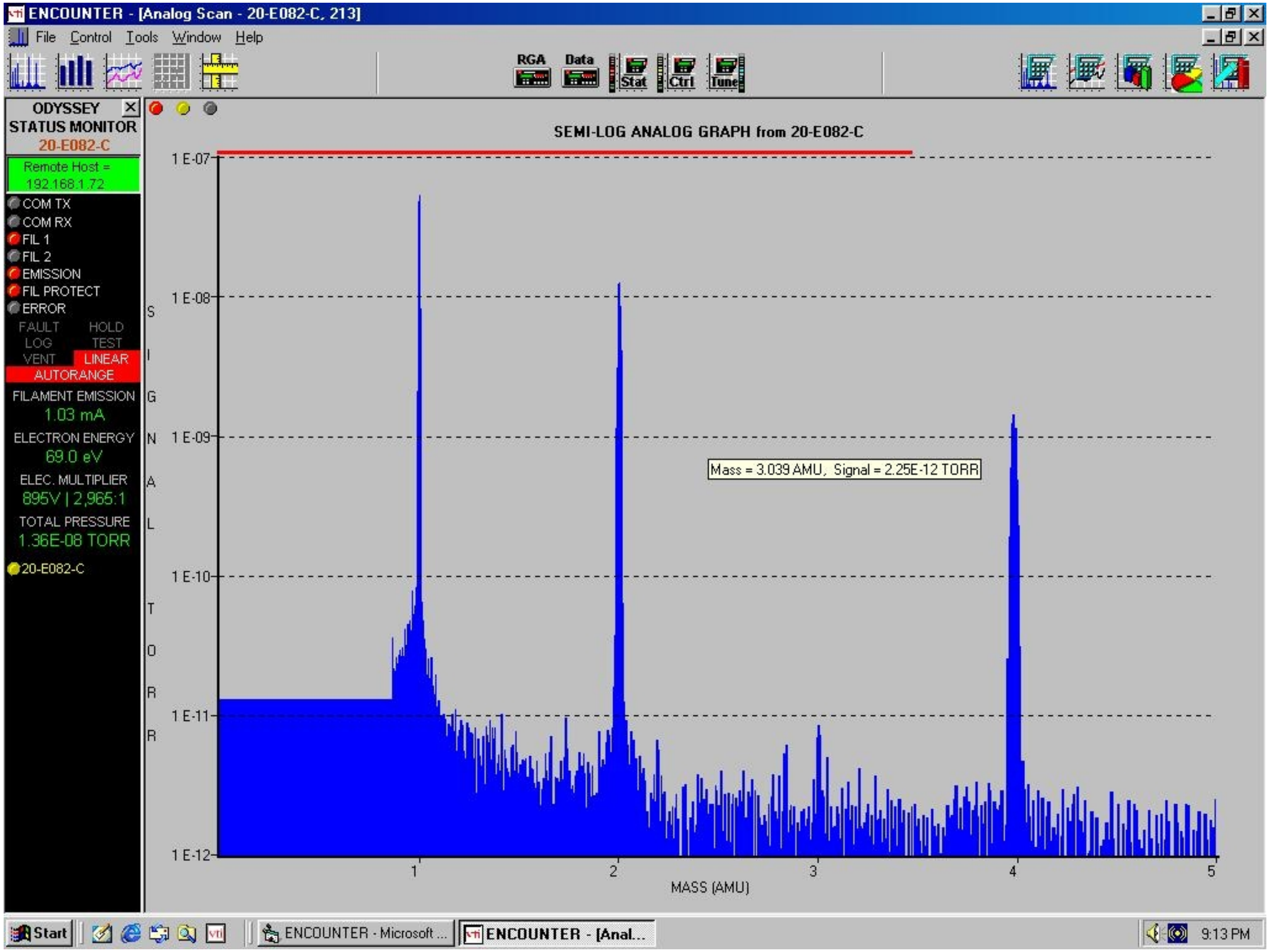
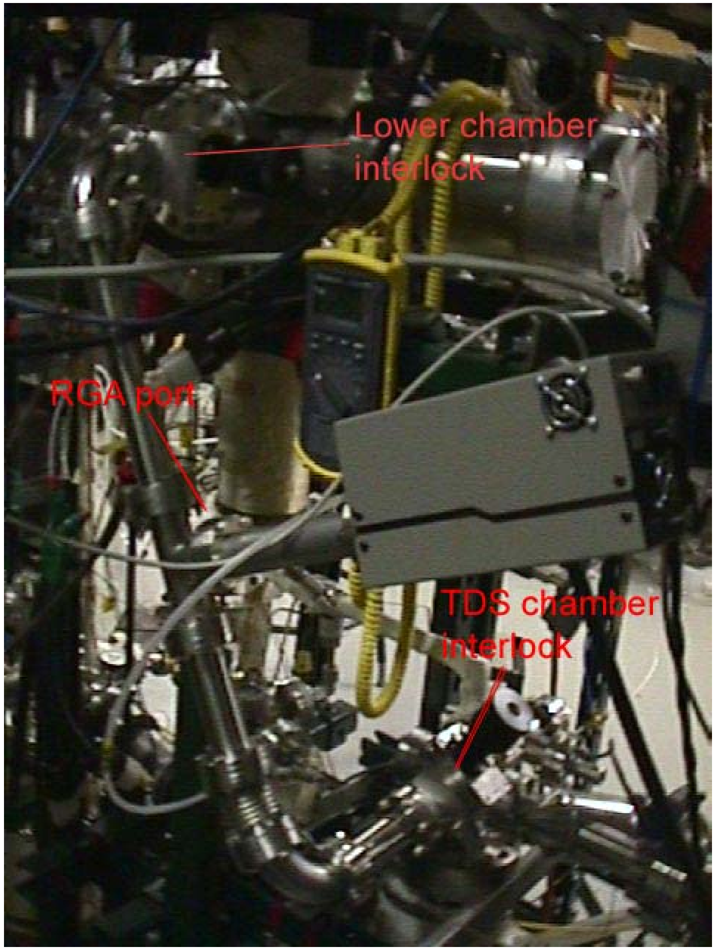
Sample magnetic sector RGA scan

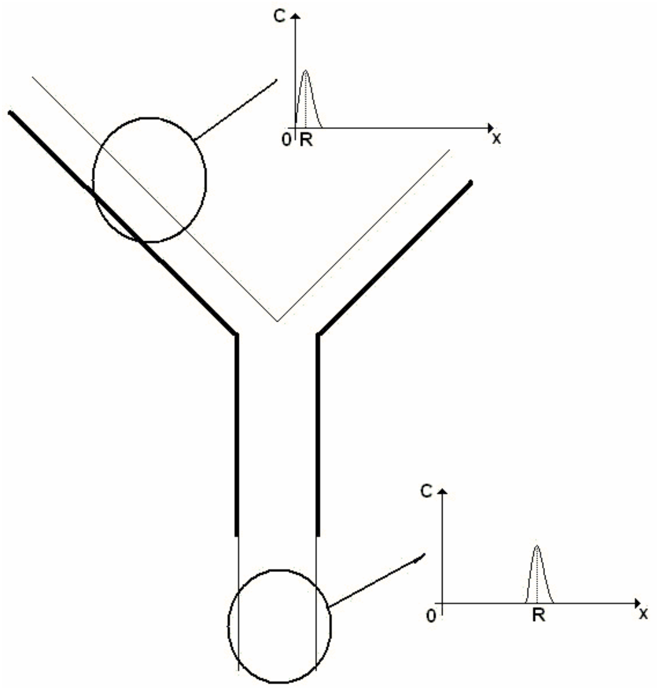


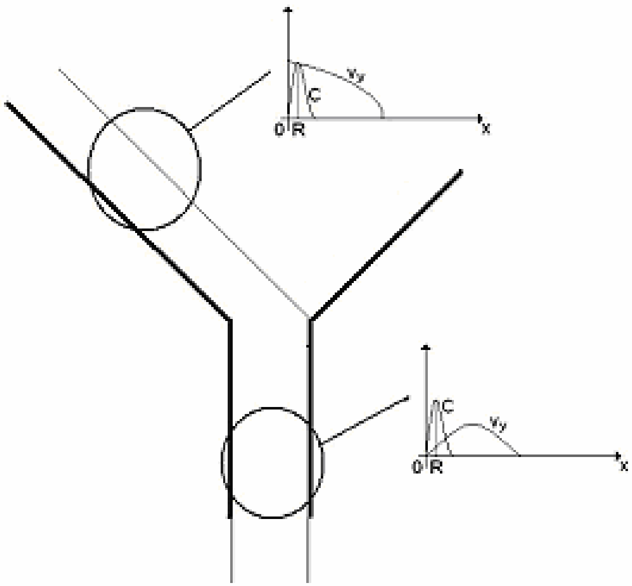
Mass Spectrometer sharing

- Both lower and TDS chambers require gas analysis capabilities
- Cost constrains do not allow two units with the desired sensitivity
- System of interlocks to "share" the RGA system was designed and installed



New ability to study flow characteristic effects on retention measurements





- On the right, double stream run (normal operation); on the left, single flow run (proposed experiment). Concentration profiles shown
- Is surface ”folding” an issue in the measurement of *R* and *D*?
- Is the quality of inter-chamber seal affected by using 1 stream only?
- Experiments underway to explore this issues

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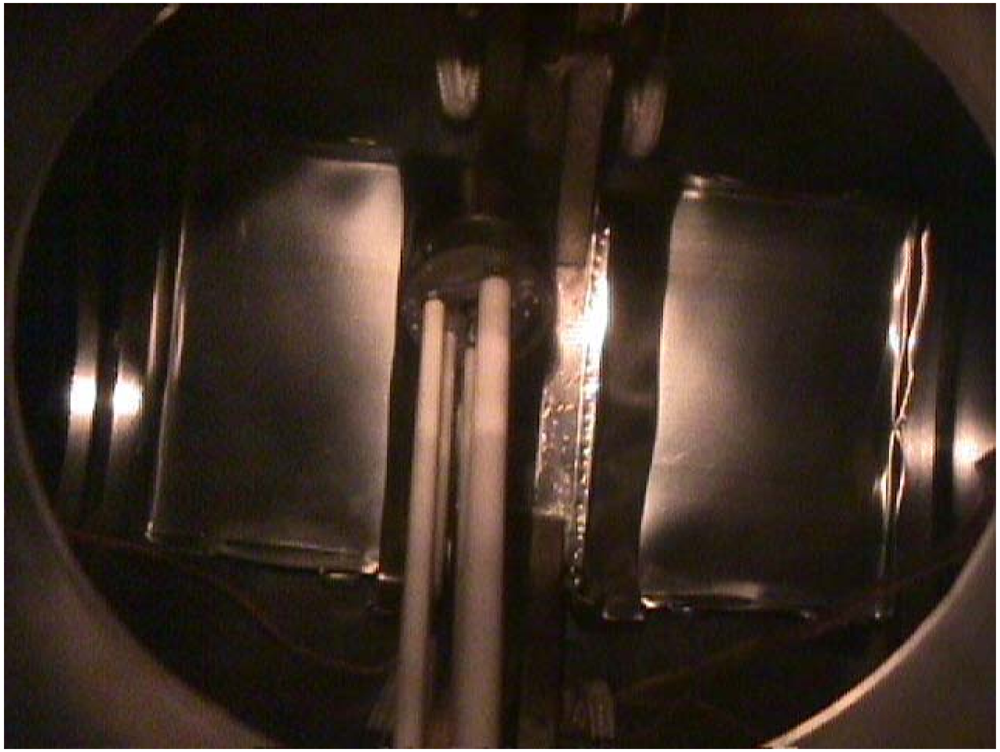
Li contamination mitigation strategies and internal heater upgrades

- Repaired ion gun source
- Improved pressure control in LMISS with new diaphragm gauge
- Internal tray protecting main chamber gaskets
- Custom-made heaters will significantly aid in plasma source experiments
- New heaters also help reduce down-time due to heater failure
- The 4-in. long HV heaters are made of Mo will deliver 100 W able to operate up to temps near 1000 °C



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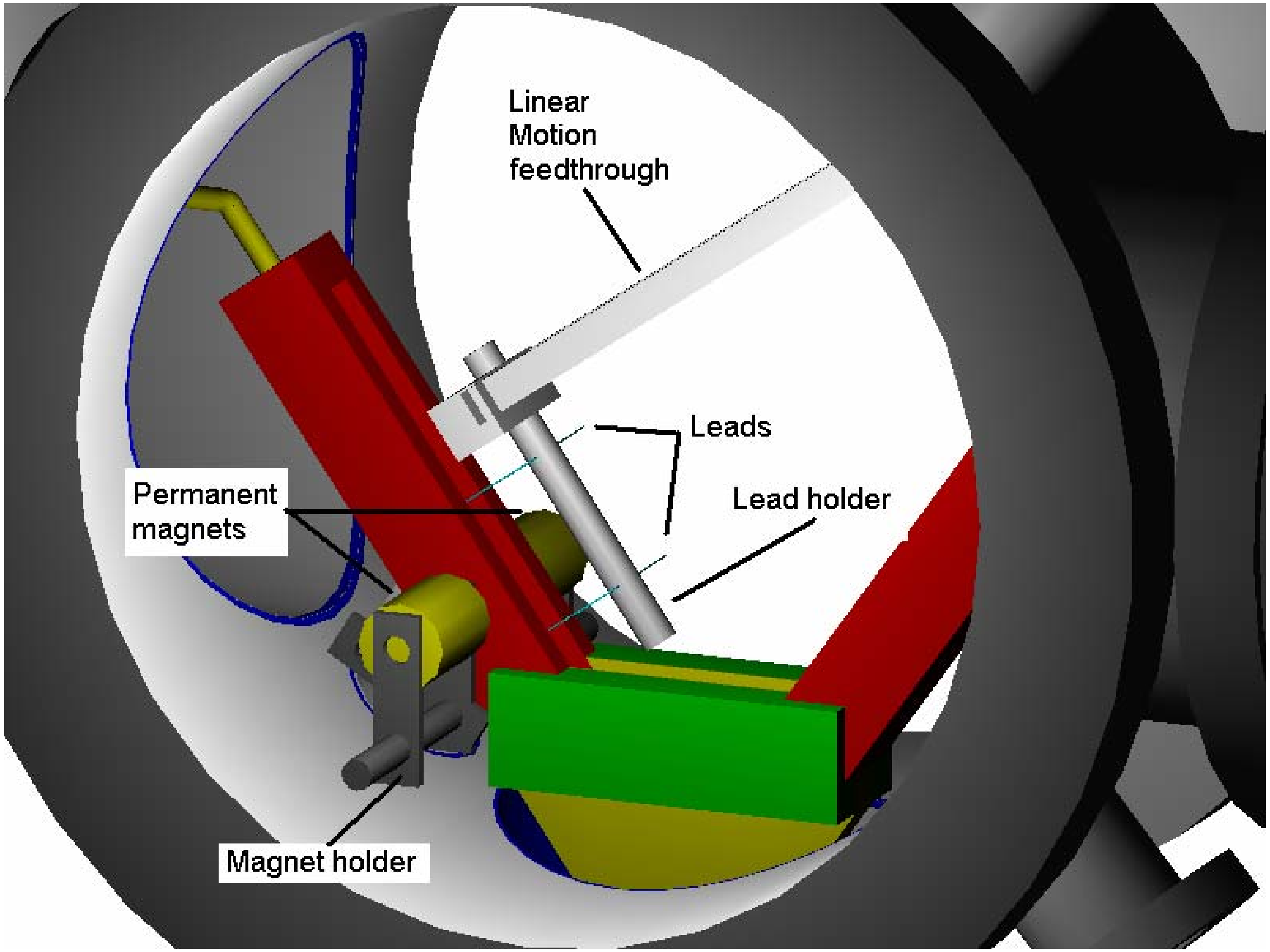
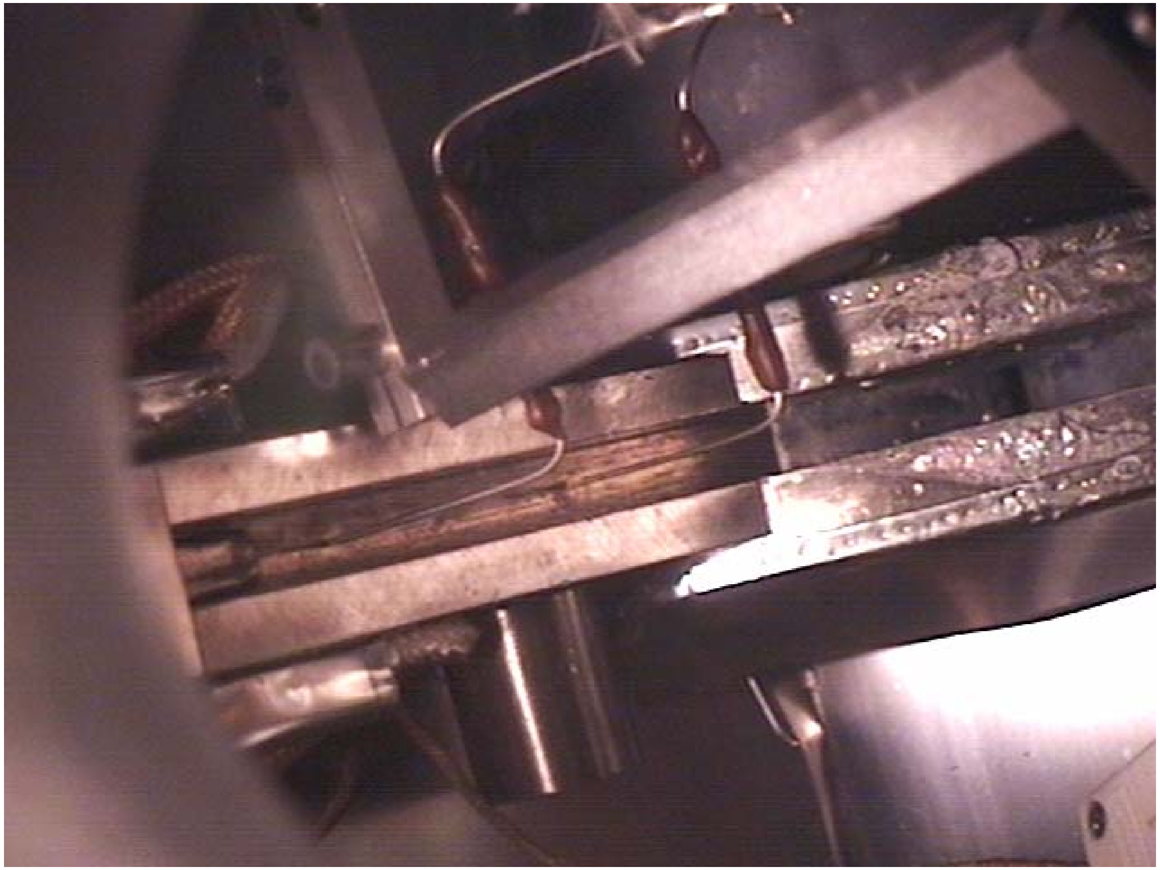
Addition of MHD experimental capability in FLIRE



Addition of MHD experiments capability in FLIRE (cont.)

- 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



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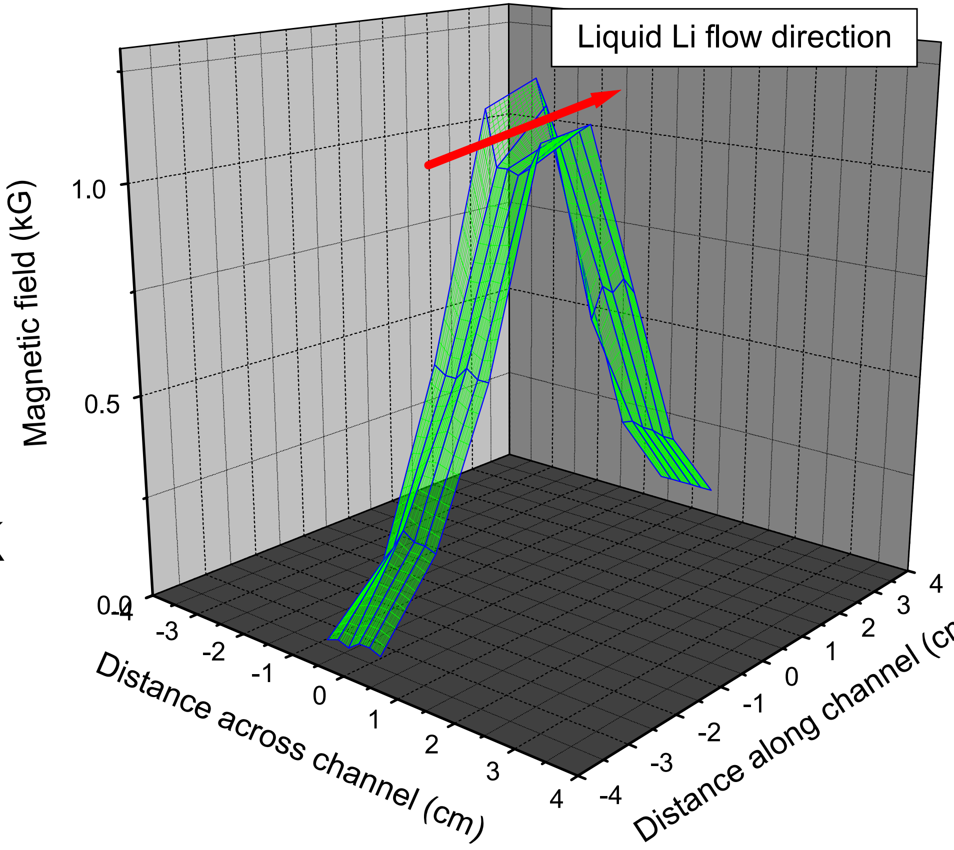
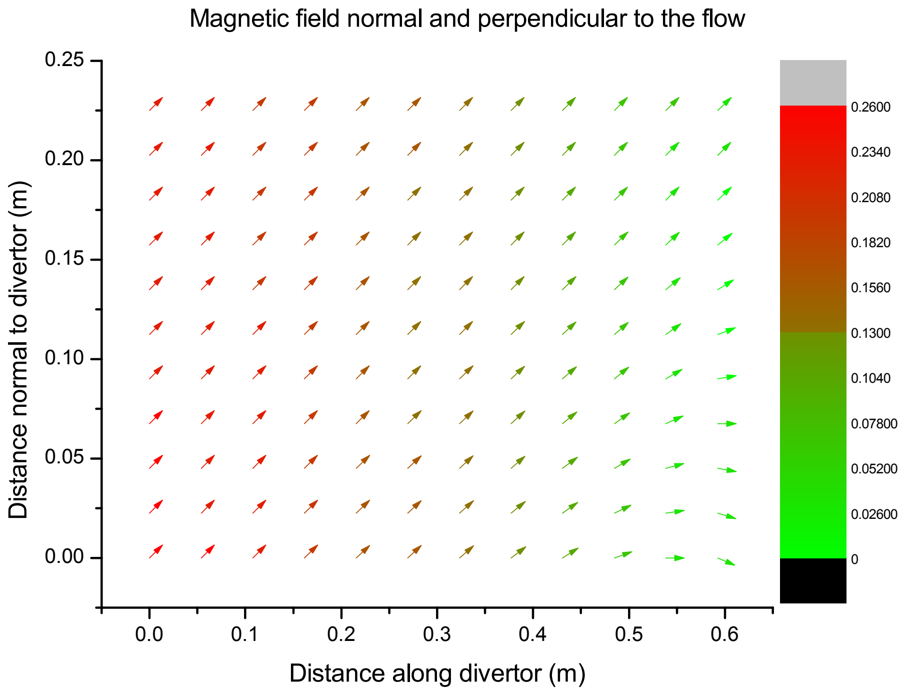
Magnetic field strength along internal ramps

- 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)



NSTX conditions



- Field perpendicular to flow in NSTX varies between 0 and 0.25 T
- Change occurs over a distance of 0.6 m
- Gradient is 0.42 T/m

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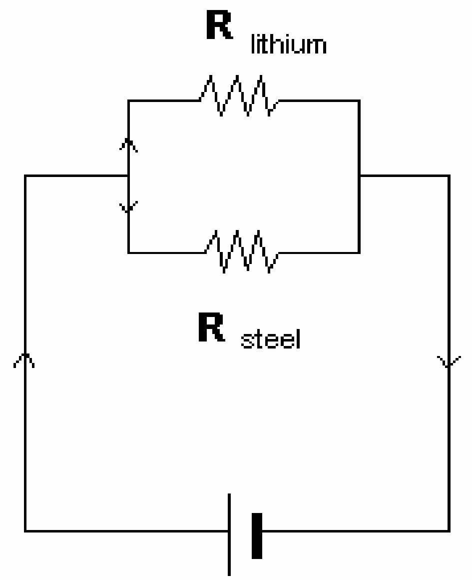
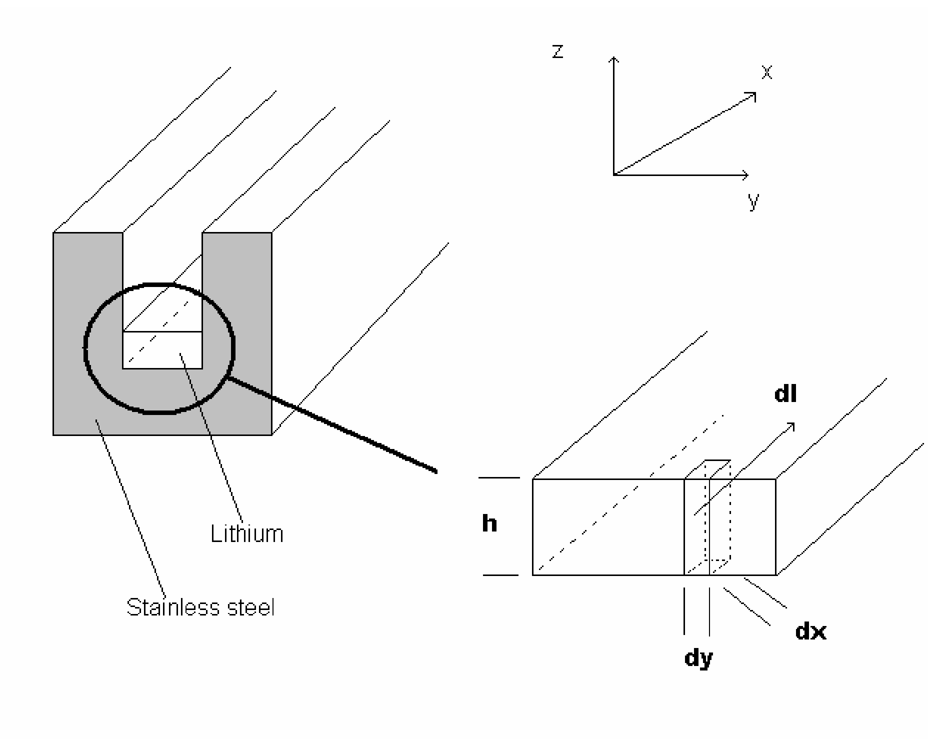
MHD experiments on FLIRE

- Up to 6 A of current passes through the leads
- Model the system as two resistors in parallel
- Estimates of resistivity and cross sectional area of Li flow and SS ramp give a lower limit of 14%, and an upper of 30% passing through Li
- Experimental measurement yielded a value of **23%** of the current passing through the lithium



Force estimates for the FLIRE MHD experiments



- EM force per unit volume on the flow is given by:

$$f_{EM}(x) = \frac{F_{EM}}{V} = j_{Li} B(x)$$

- Gravitational force per unit volume is:

$$f_g(x) = \rho g \cos\theta$$

- For constant volume elements, the ratio of forces is:

$$\frac{F_{EM}}{F_g} = \frac{I_{Li} B(x)}{A_{Li} \rho g \cos\theta}$$

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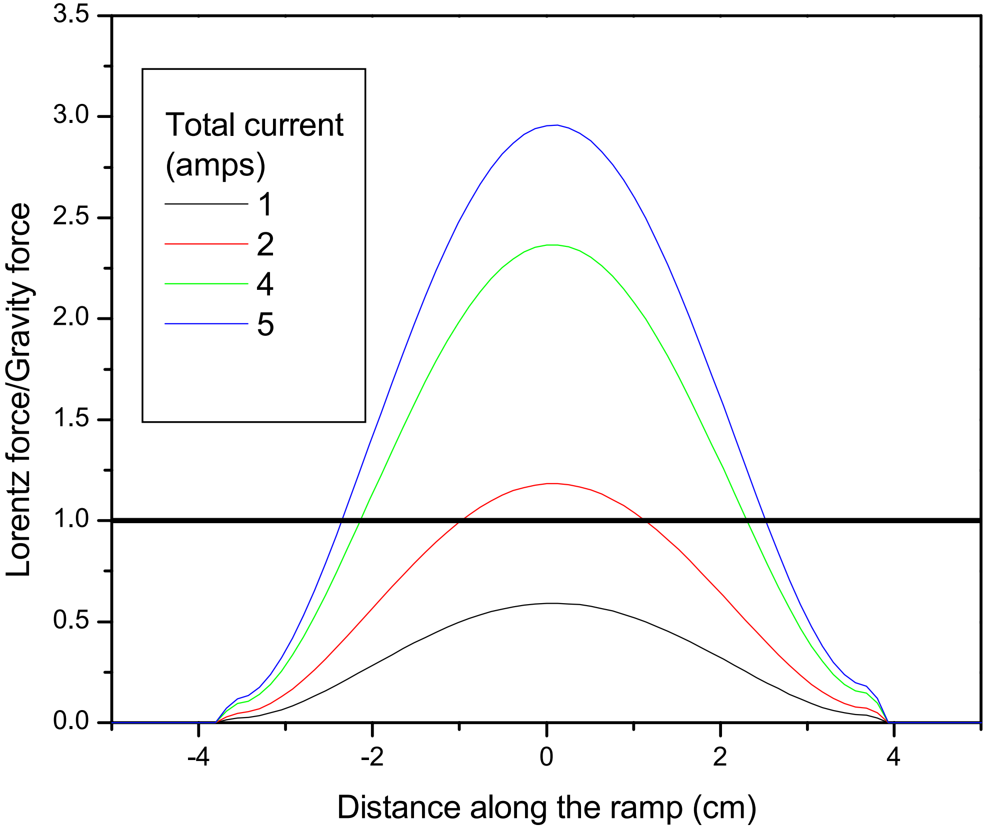
Force estimates compared to experimental results from FLIRE



- At 1 A, no lift was observed on 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

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Lithium flowing down the ramps with no magnetic field

seal, no gun.avi

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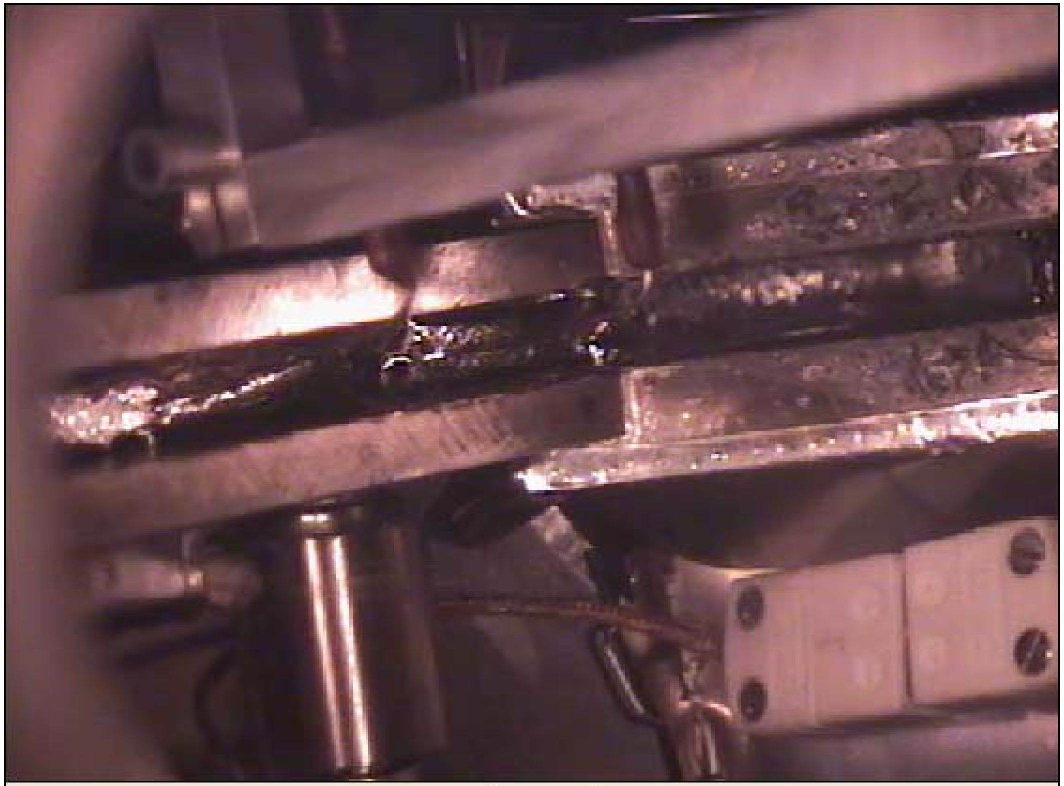
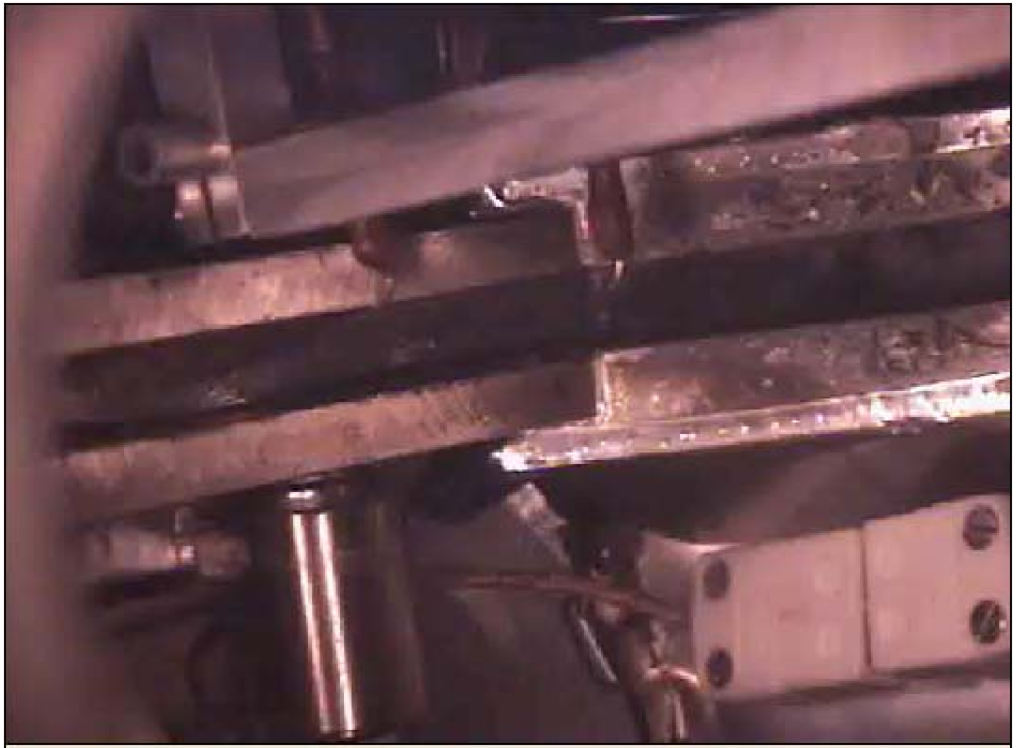
Lithium flowing down the ramps with magnetic field, no current



Run5 (compressed).avi

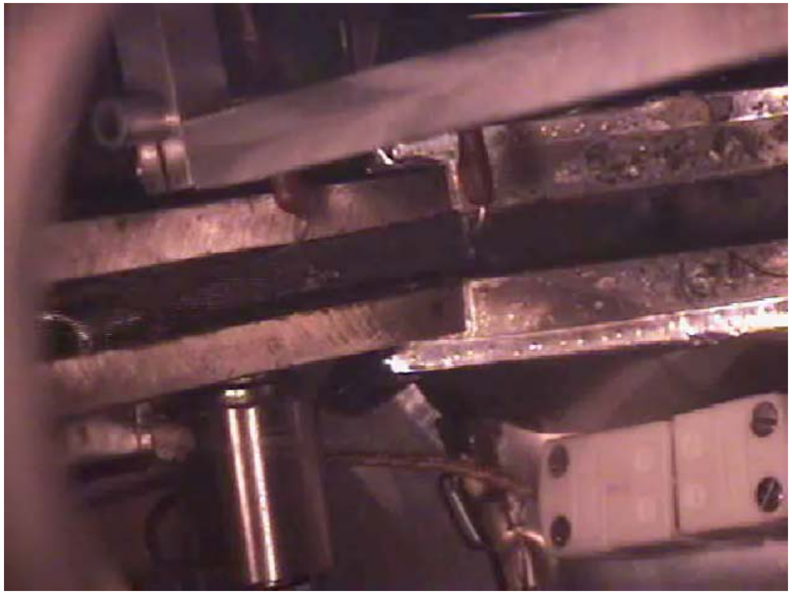
Effect of lifting force on the flow



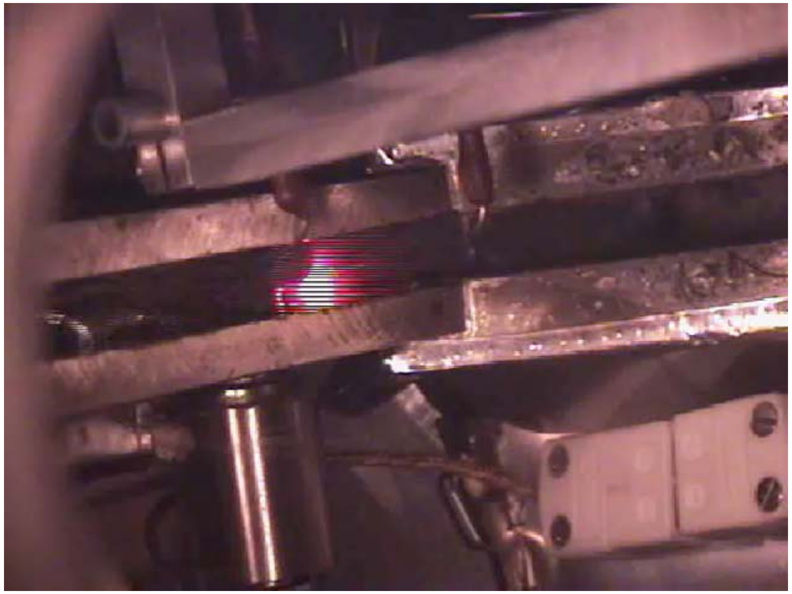
Run1 (compressed).avi

- 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)

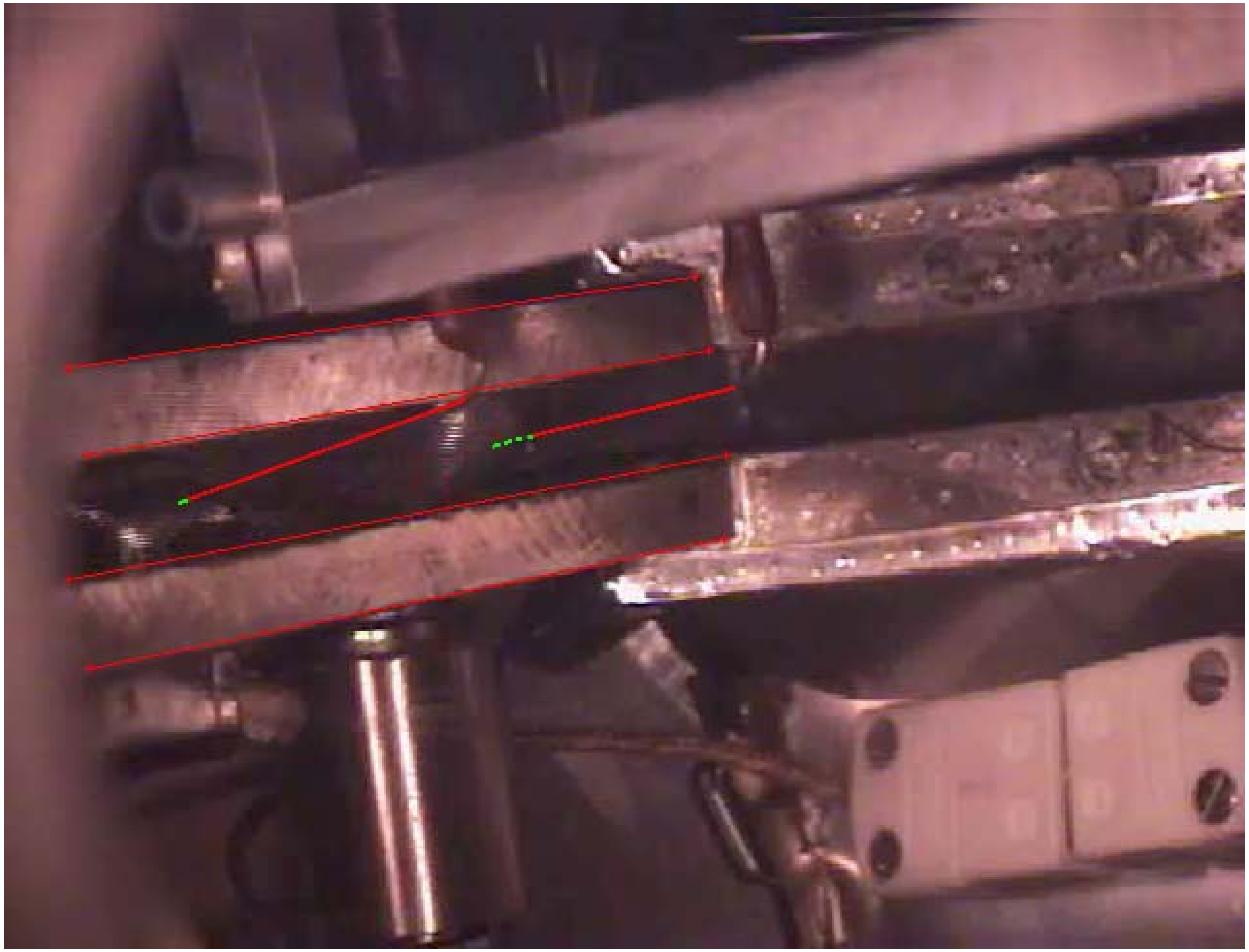


Flow just started, touching top lead only



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

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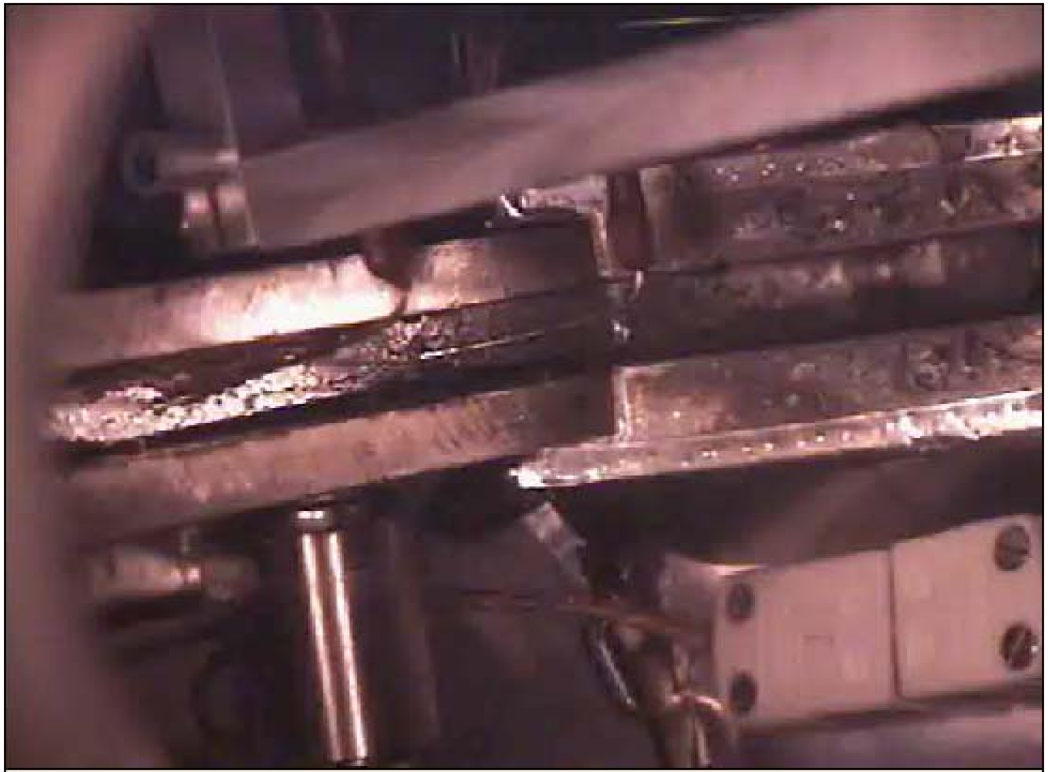
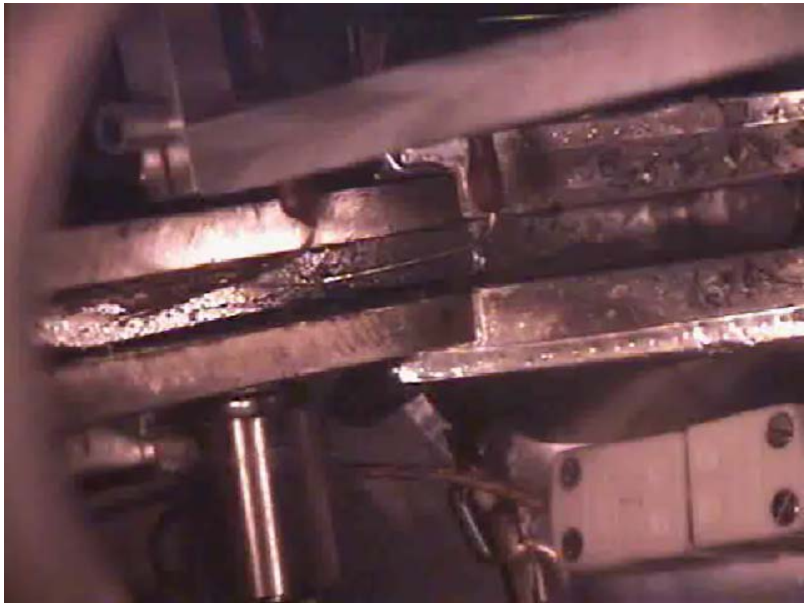
Effect of **pushing** force on the flow



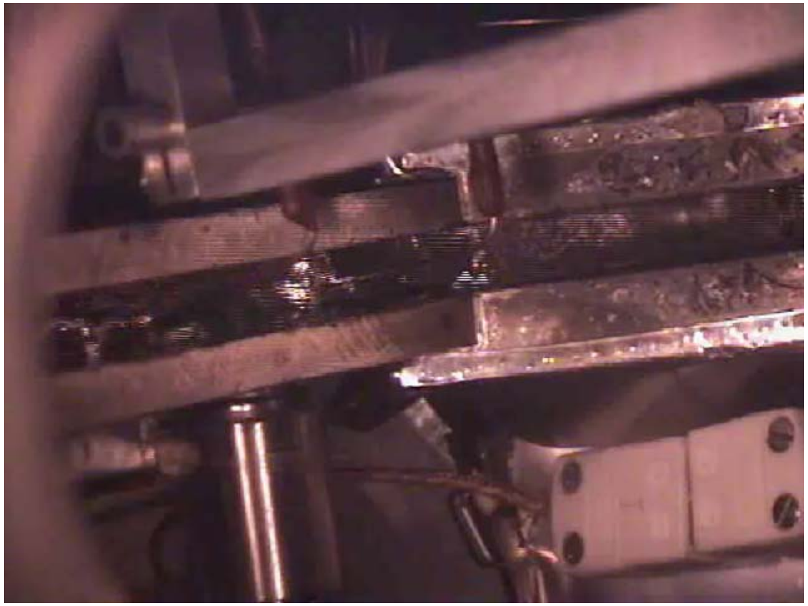
Run6 (compressed).avi

- 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

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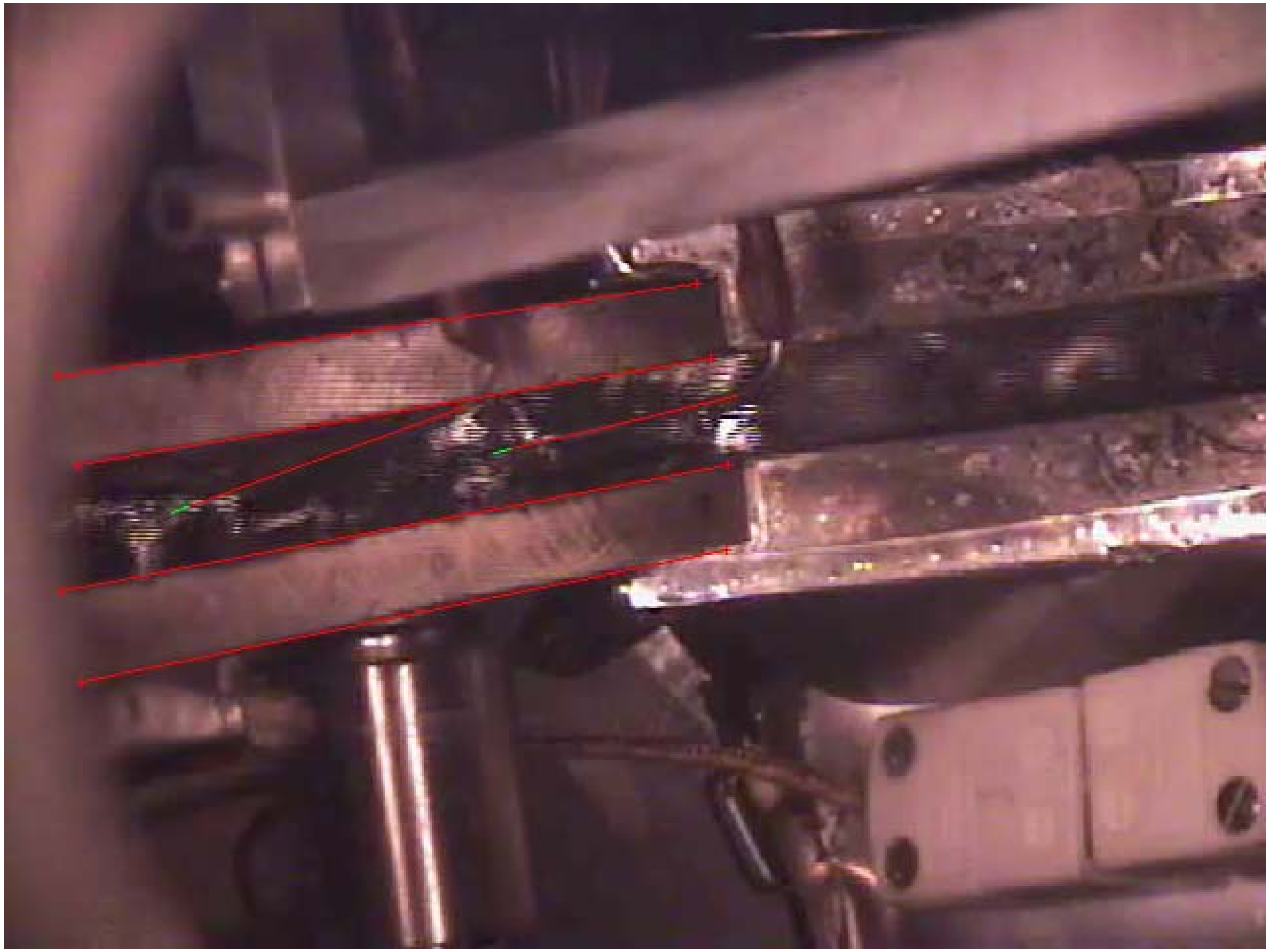
Effect of pushing force on the flow (cont'd)



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

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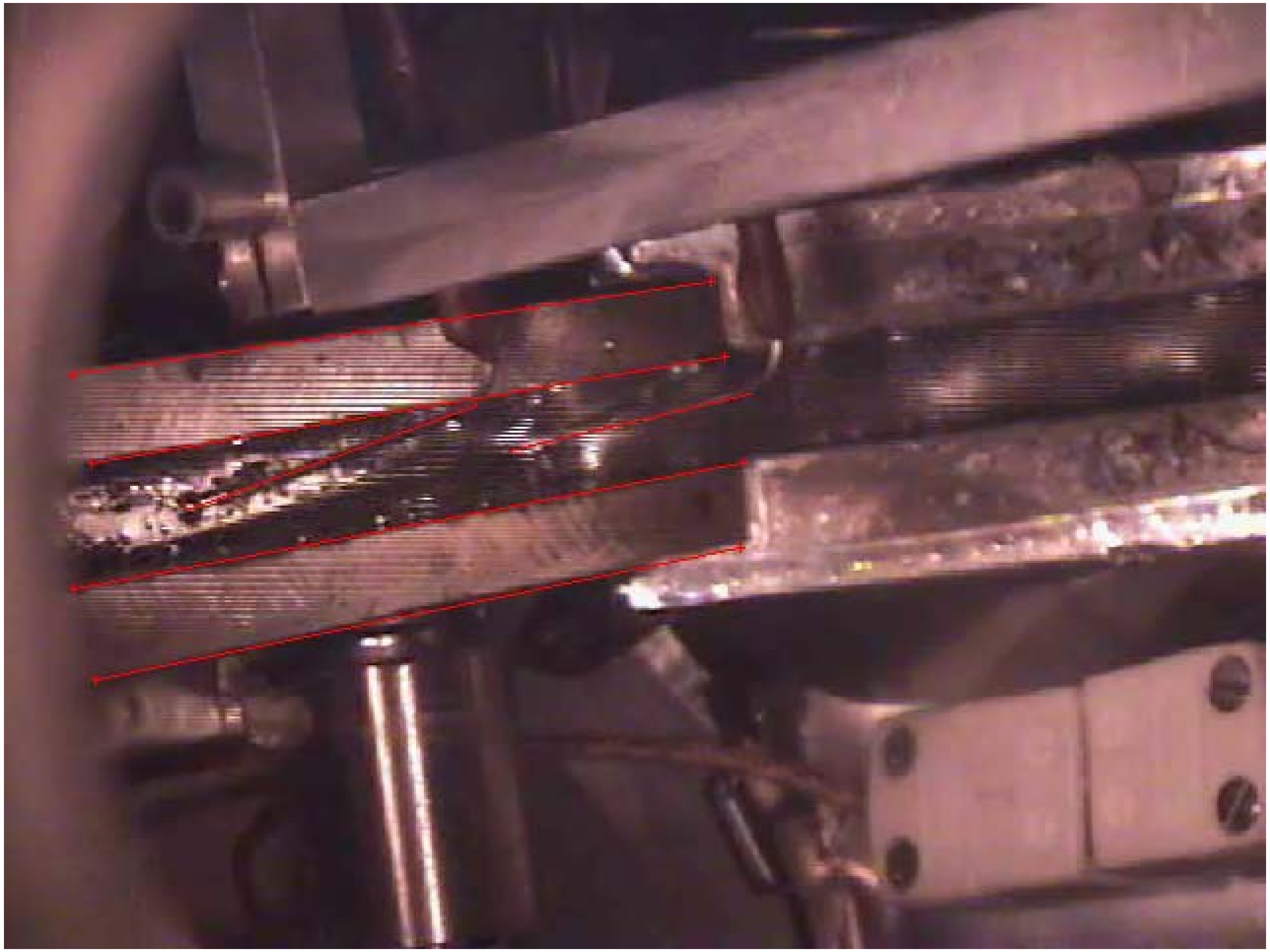
Effect of pushing force on the flow (cont'd)



After the flow is over, both leads are exposed again

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Dimensionless groups relevant to MHD flows

- Reynolds number $$Re = \frac{vh}{\nu}$$
- Hartmann number $$Ha = Bh\sqrt{\frac{\sigma}{\rho\nu}}$$
- Froude number $$Fr = \frac{v^2}{gh}$$
- Capillary number $$Ca = \frac{\rho\nu \cdot \mathrm{v}}{\gamma}$$
- Bond number $$Bo = \frac{\rho g h^2}{\gamma}$$

NOMENCLATURE

v: flow velocity

ν: dynamic viscosity

h: film thickness

g: gravity acceleration

γ: surface tension

σ: electrical conductivity

B: magnetic field

ρ: density

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Dimensionless numbers calculations

Dimensionless parameter	Fusion reactor	FLIRE
Reynolds (inertial vs viscous)	5500	890 – 4400
Hartman (EM vs viscous)	4300	172
Froude (inertial vs gravity)	20	65 – 200
Capillary (viscous vs surf. tension)	0.001	0.001 – 0.002
Bond (gravitational vs surf. tension)	0.3	0.01 – 0.05

- Froude and Hartmann numbers calculated for typical FLIRE conditions:
  - v = 0.8-2.0 m/sec
  - B = 0.1 Tesla
  - h = 1-2 mm
- Proposed conditions in a fusion reactor (S. Molokov, I. Cox, C.B. Reed, Fusion Technology **39** (2001) 880)
  - V = 1 m/sec
  - B = 10 Tesla
  - h = 0.5 cm

T = 300 °C for surface tension, density and viscosity values

Future Work Plan in FLIRE

- Single liquid Li flow tests in FLIRE
  - determine "folding" effect on retention/diffusivity measurements
- Long-term evolution of implanted He and H particles versus temperature (non-prompt release)
- H^+ particle and H-plasma exposures
- He^+ particle and He-plasma exposures

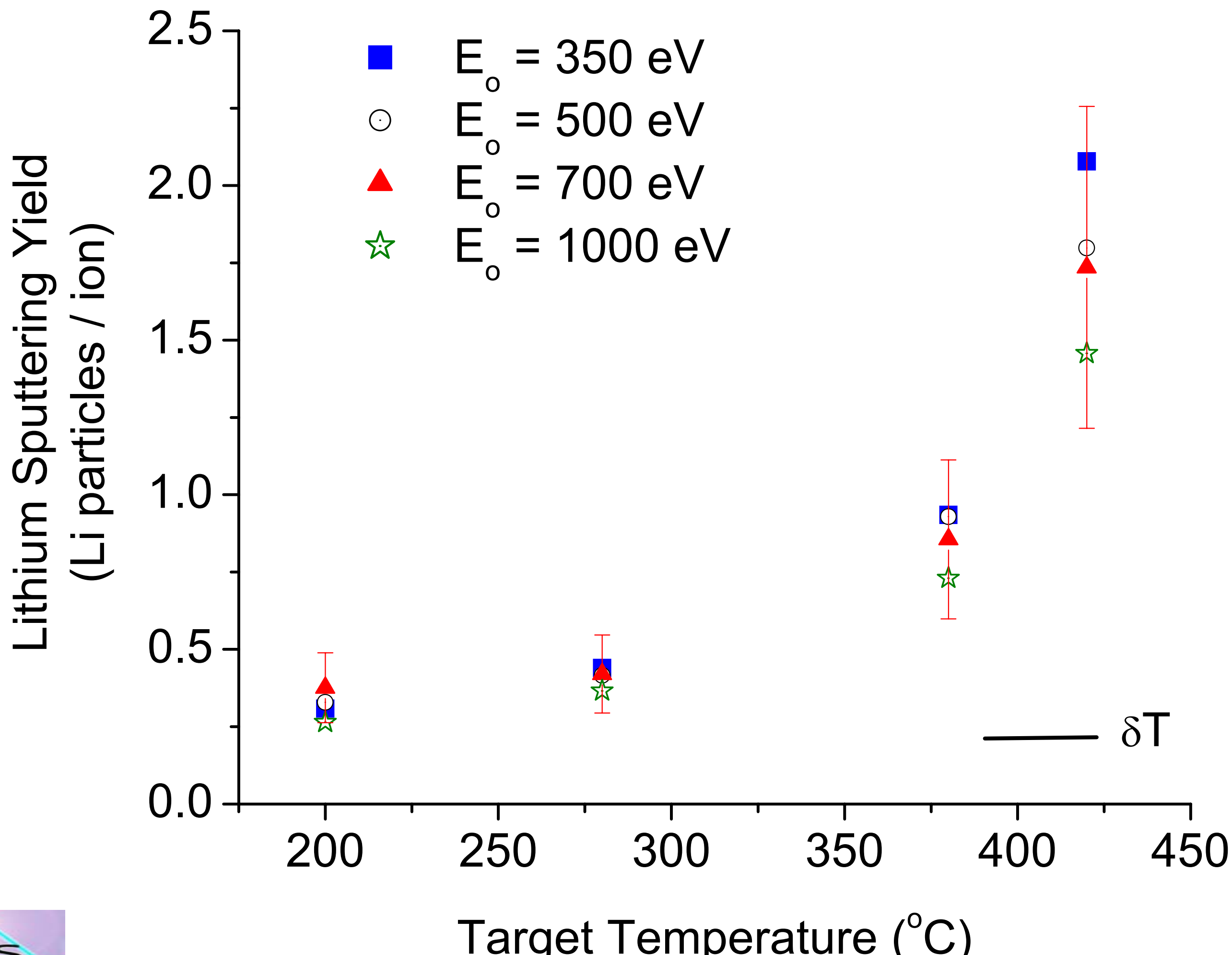
Future Work Plan in FLIRE (cont.)

- Ga experiments (summer 2003)
- More MHD effects on retention/diffusivity in flowing liquid metals (e.g. lithium, gallium)
- Addition of new diagnostics: QCMs for erosion, ultrasonic transducers for film thickness, IR thermography
- Installation of HHF source

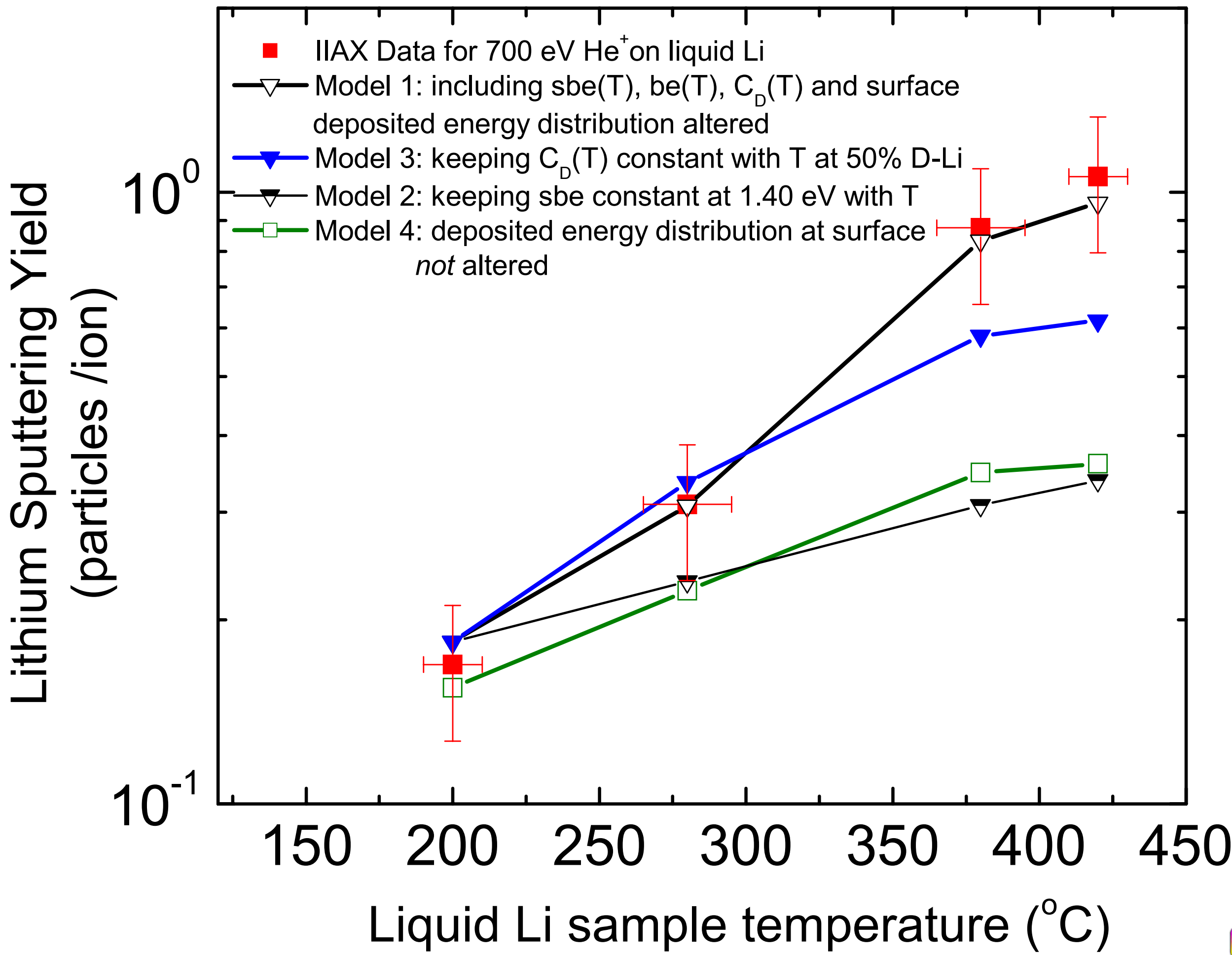
Modeling temperature enhanced liquid-Li sputtering

- Experimental Li erosion data in IIAX and PISCES-B demonstrate enhanced erosion characteristic for temperatures between 200-400 °C and incident particle energies between 50-1000 eV
- A number of conjectures have been made regarding the enhancement, yet no clear model

IIAX data: Li^+ on D-treated Liquid Li vs T for various incident energies

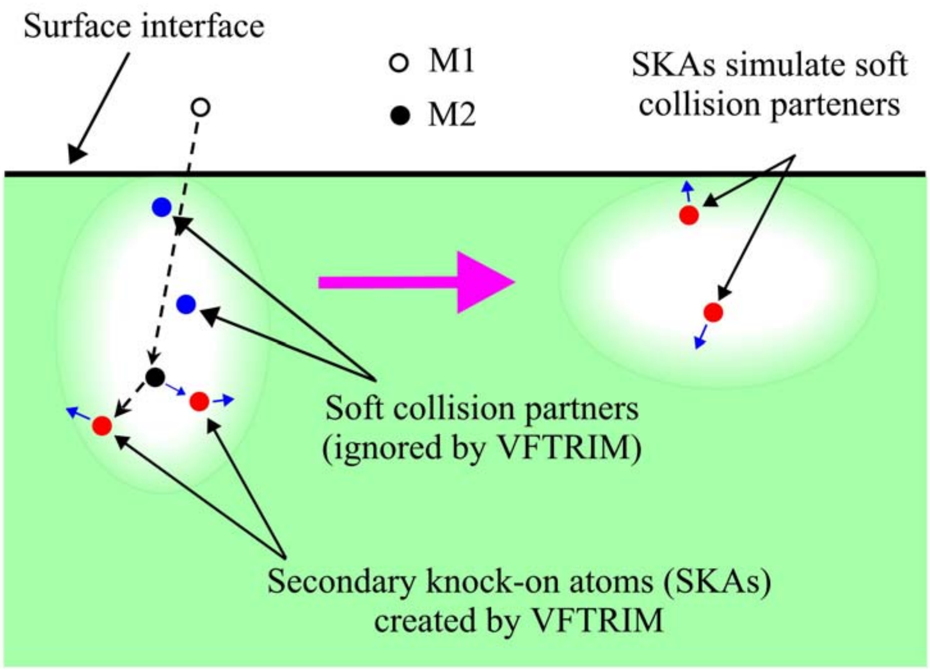


He^+ on liquid Li with ad-hoc model in VFTRIM-3D



VFTRIM-3D used ad-hoc models to determine key mechanisms responsible for enhancement

- Surface binding energy was calibrated to mean ejected energy of sputtered lithium atoms measured in PISCES-B as a function of system temperature
- The SKA portion of collision cascade was juxtaposed along surface to simulate near-surface non-binary collisions absent in the BCA-based code, VFTRIM
- Deuterium surface concentration varied as T/T_m increases (this effect was found to be minor in the enhancement of Li sputtering)



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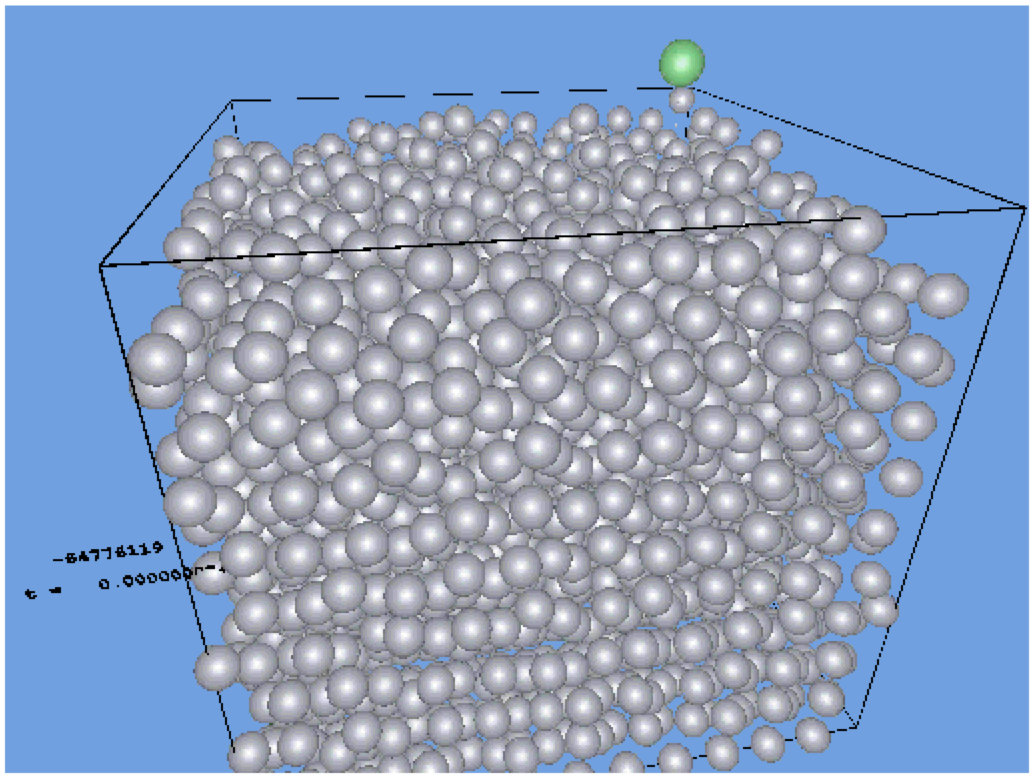
Molecular Dynamics simulations allow detailed knowledge of liquid Li cascade dynamics

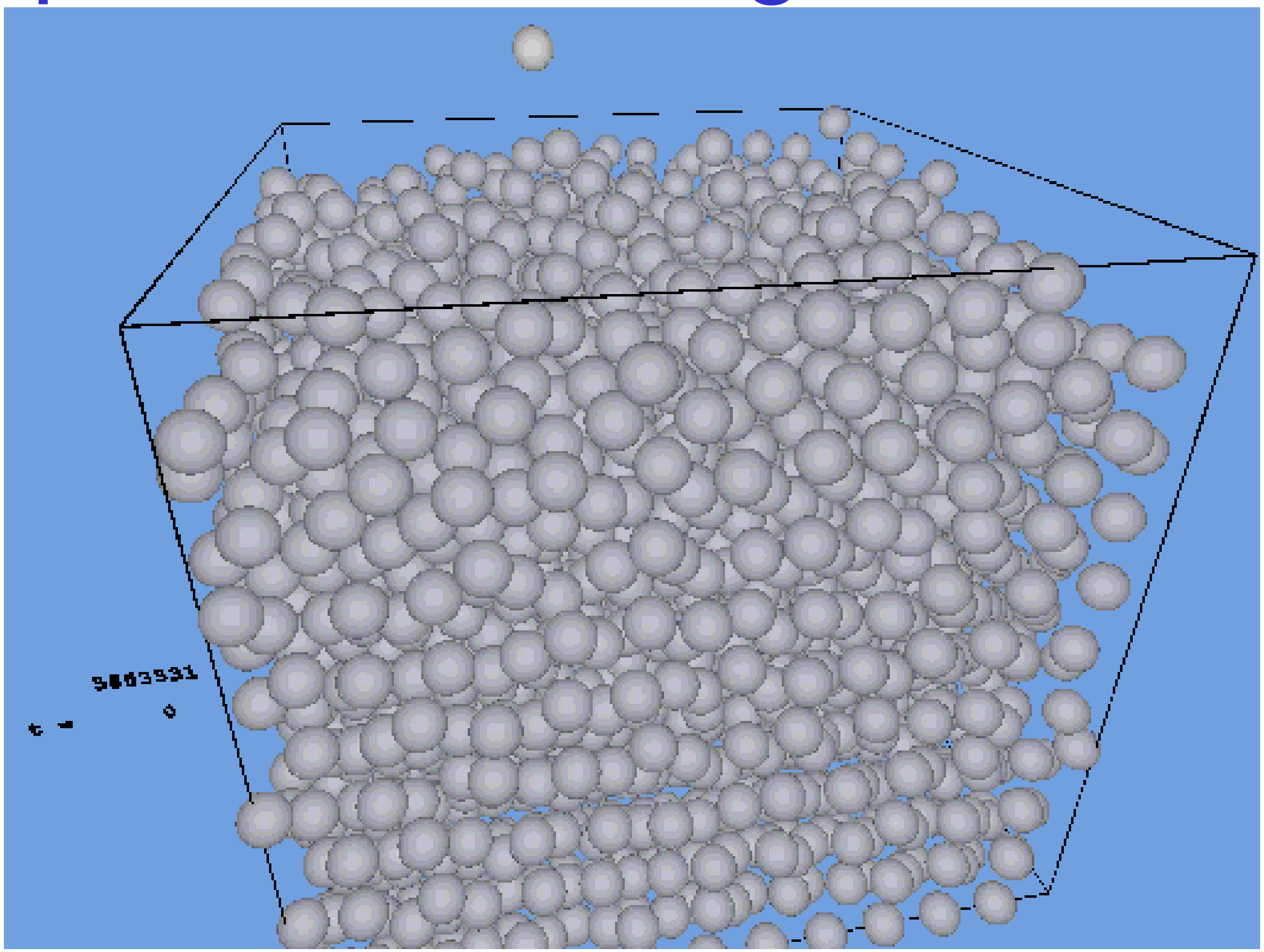
- studied 100 eV Li^+ at 45-degree incidence with 473 and 653 K system temperature (1000+ flights in each MD simulation)
- near-surface energy cascade (~12-15 recoils created per flight in a 40 Å depth)
  - Energy recoil distribution
  - Angular recoil distribution for PKA and incident particle
- surface binding energy obtained from potential energy temporal history of sputtered atom in MD simulations

Collision Cascade is along Surface!

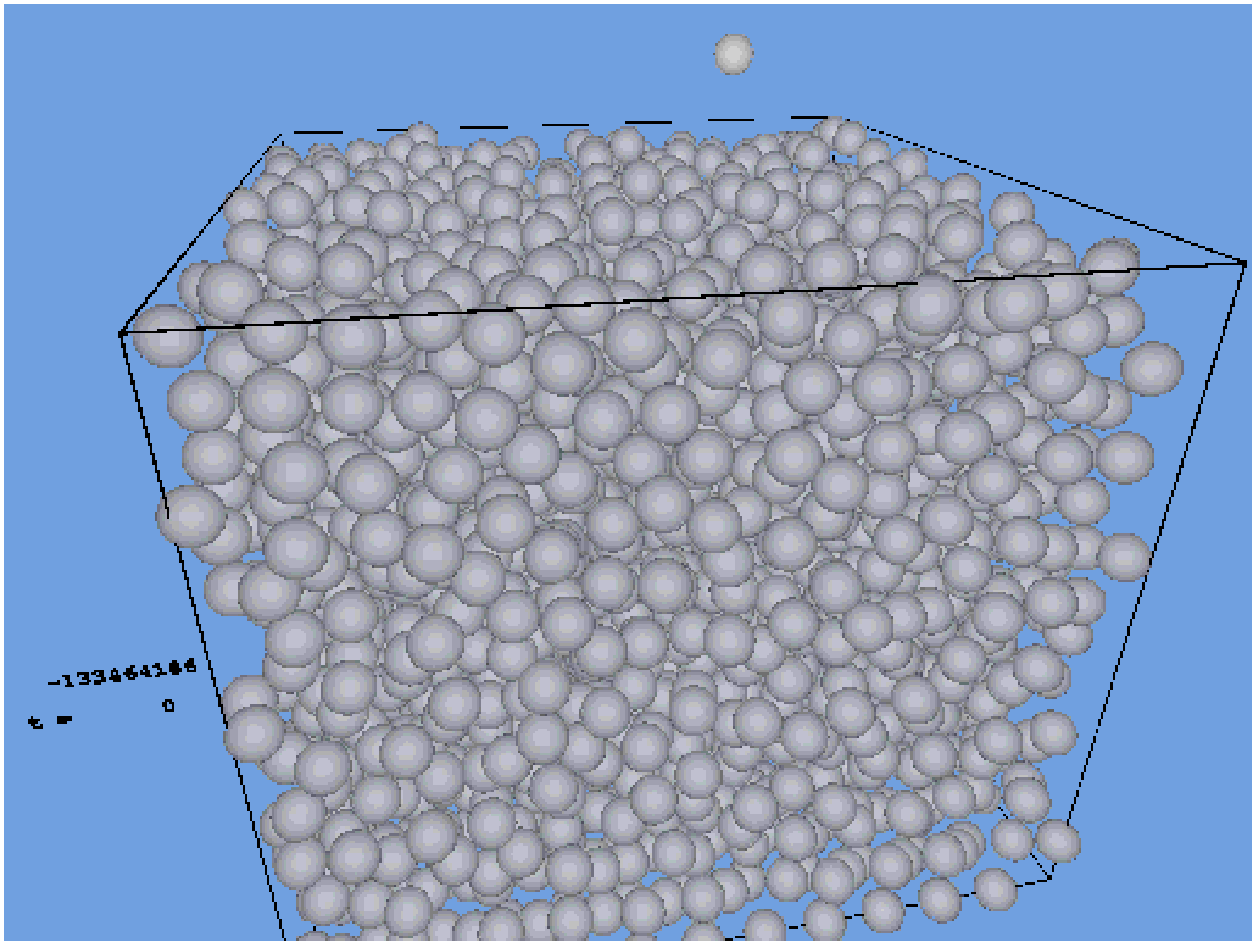
100 eV, 20-degrees, at 473 K



Thermal motion contributes to perpendicular energies --- 473 K



Even greater thermal motion at 653 K



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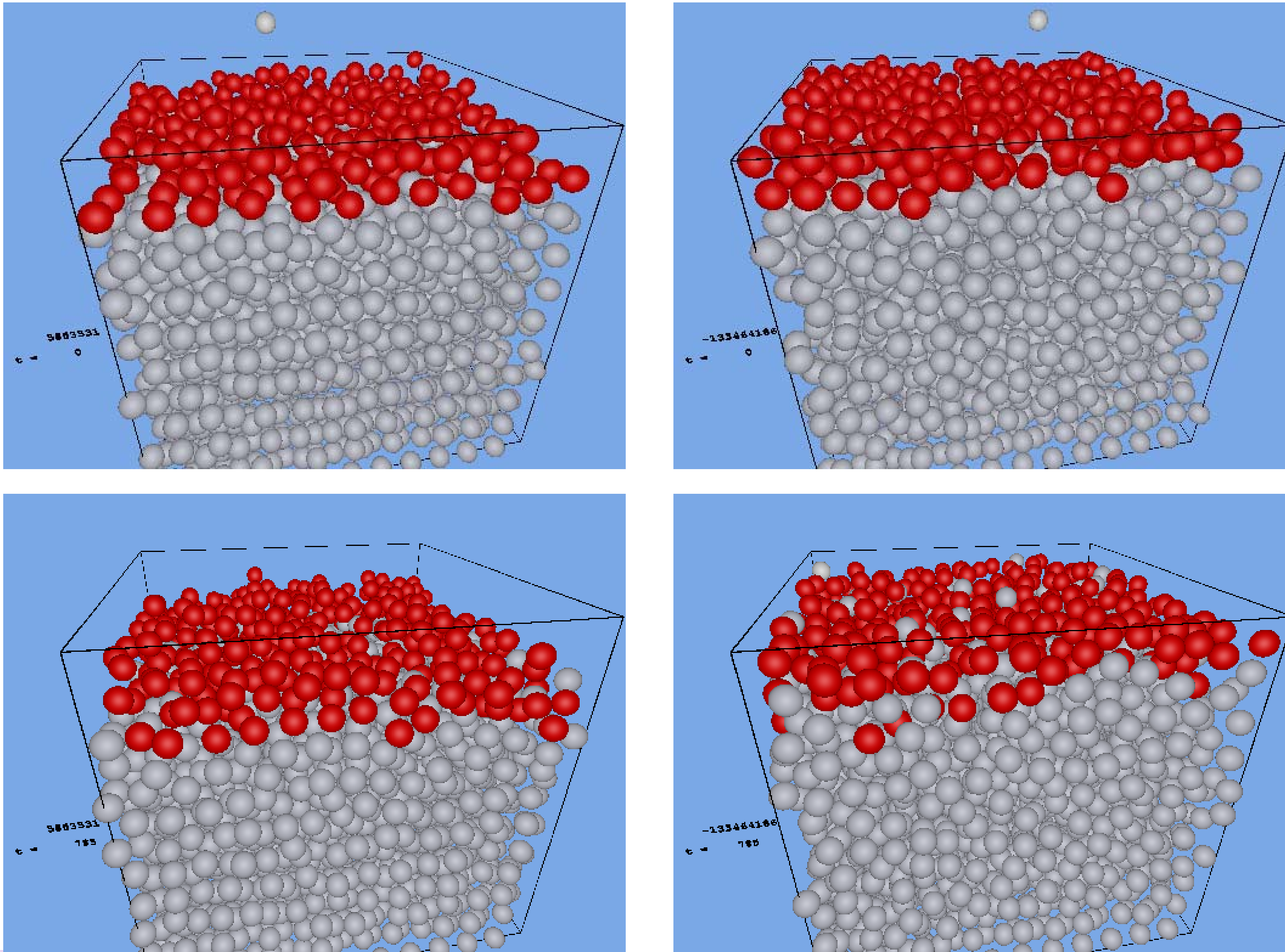
473 K

653 K

Initial

After 50 ps



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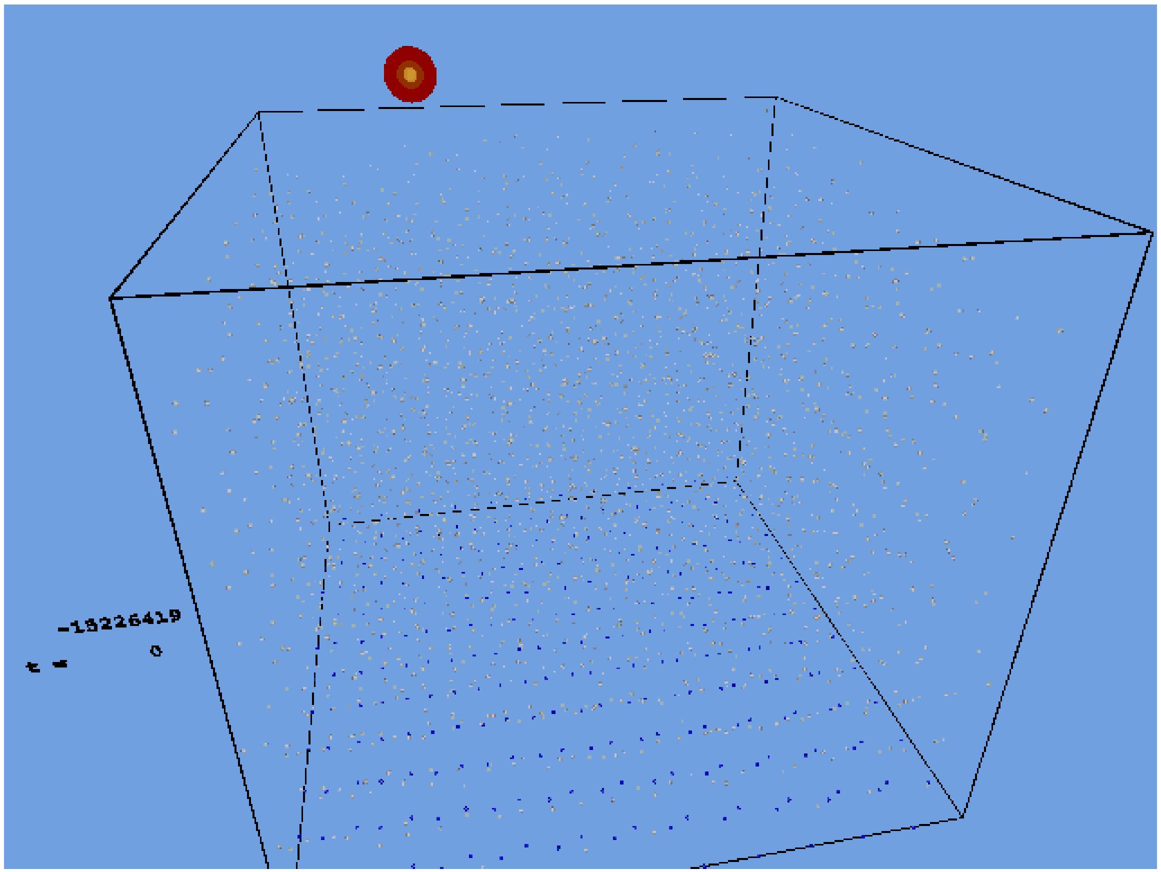
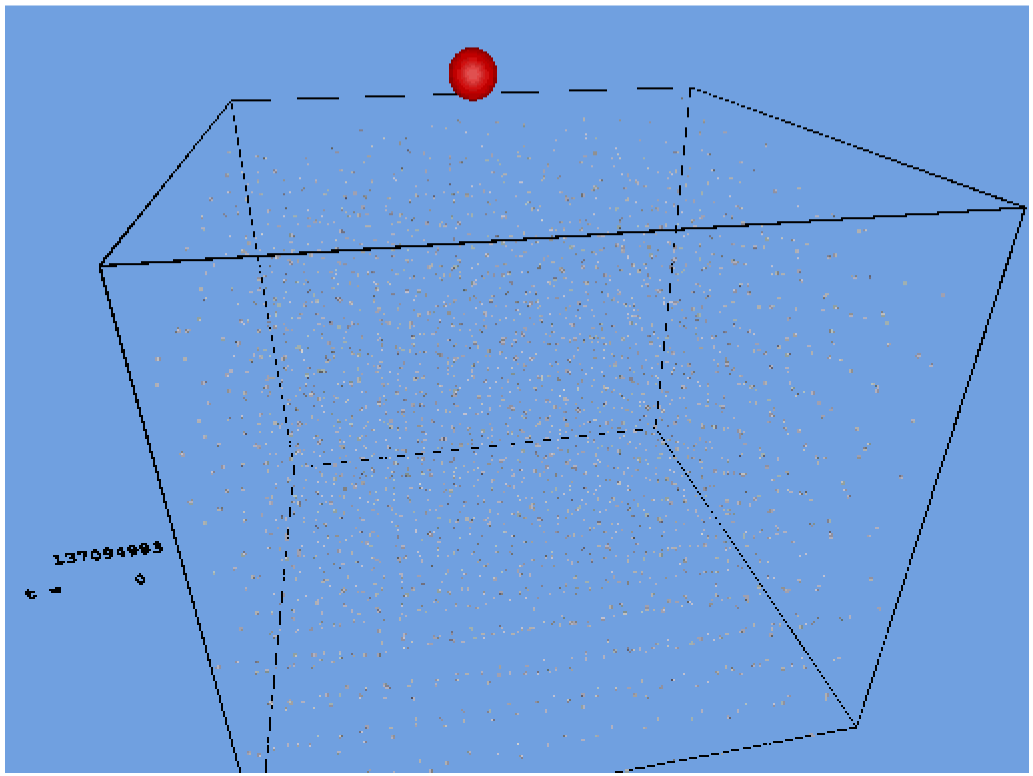
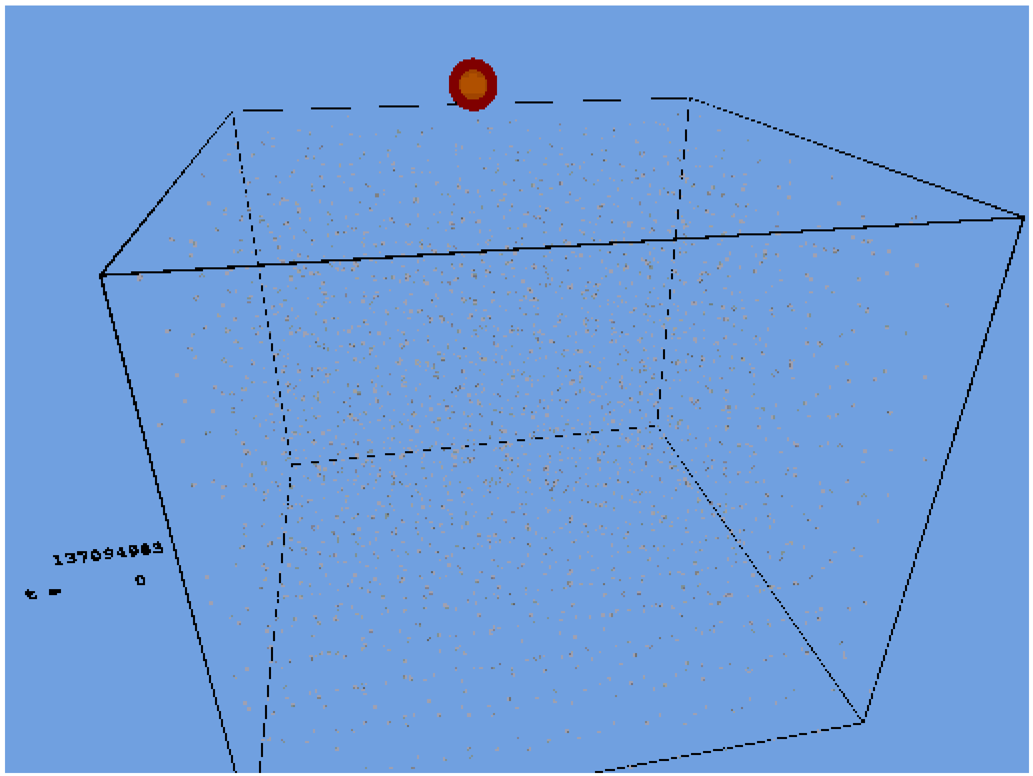
Details of collision cascade for 100 eV 45-deg at 473 K



Details of collision cascade for 100 eV 45-deg at 473 K (faster)



Same flight but at higher T (100 eV 45-deg. at **653** K)



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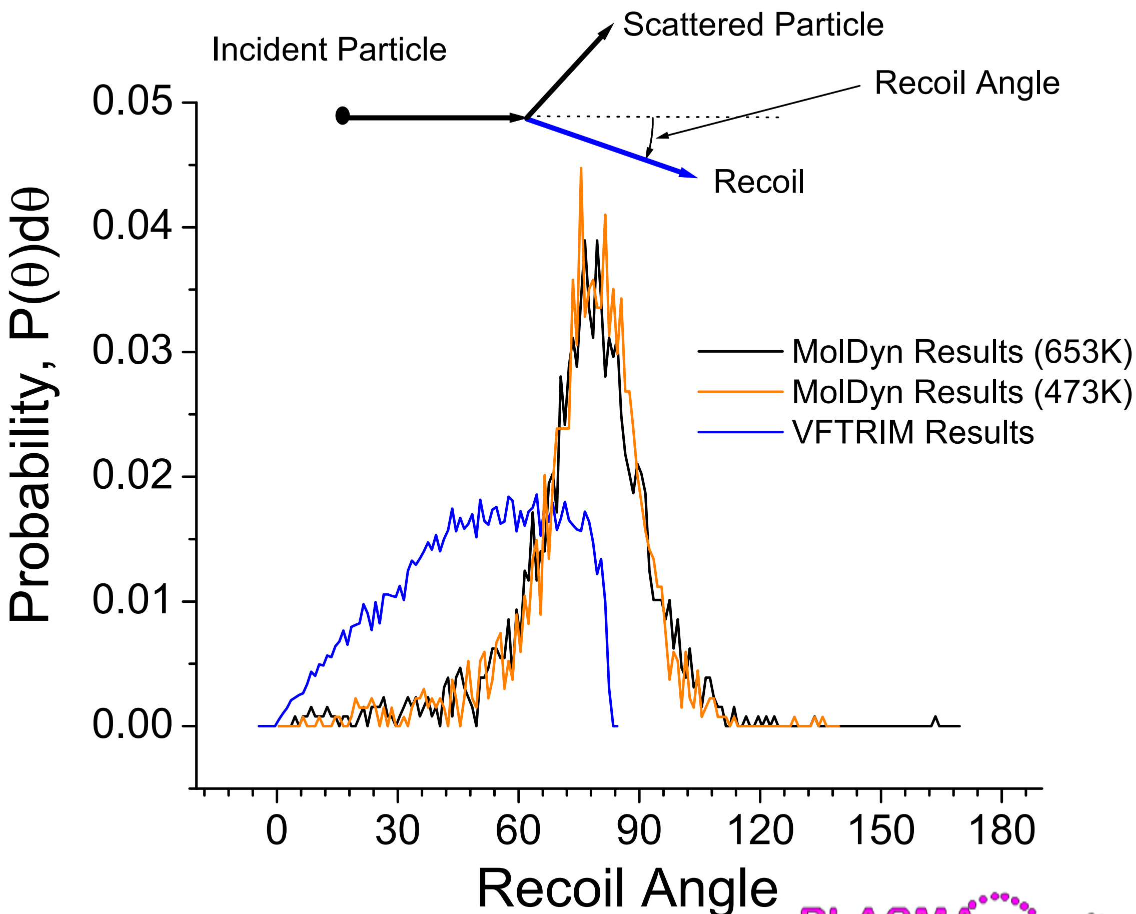
Our new code: MD-TRIM

- Principle Objective: Develop model(s) 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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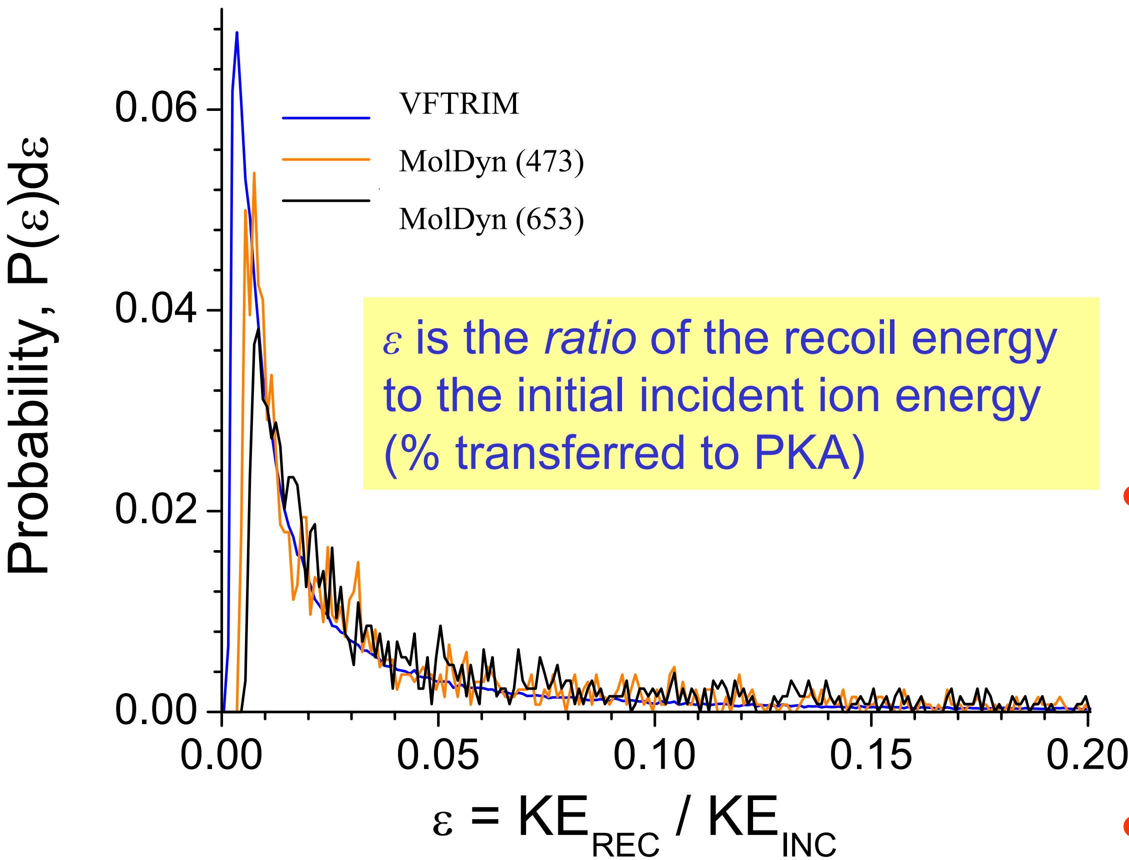
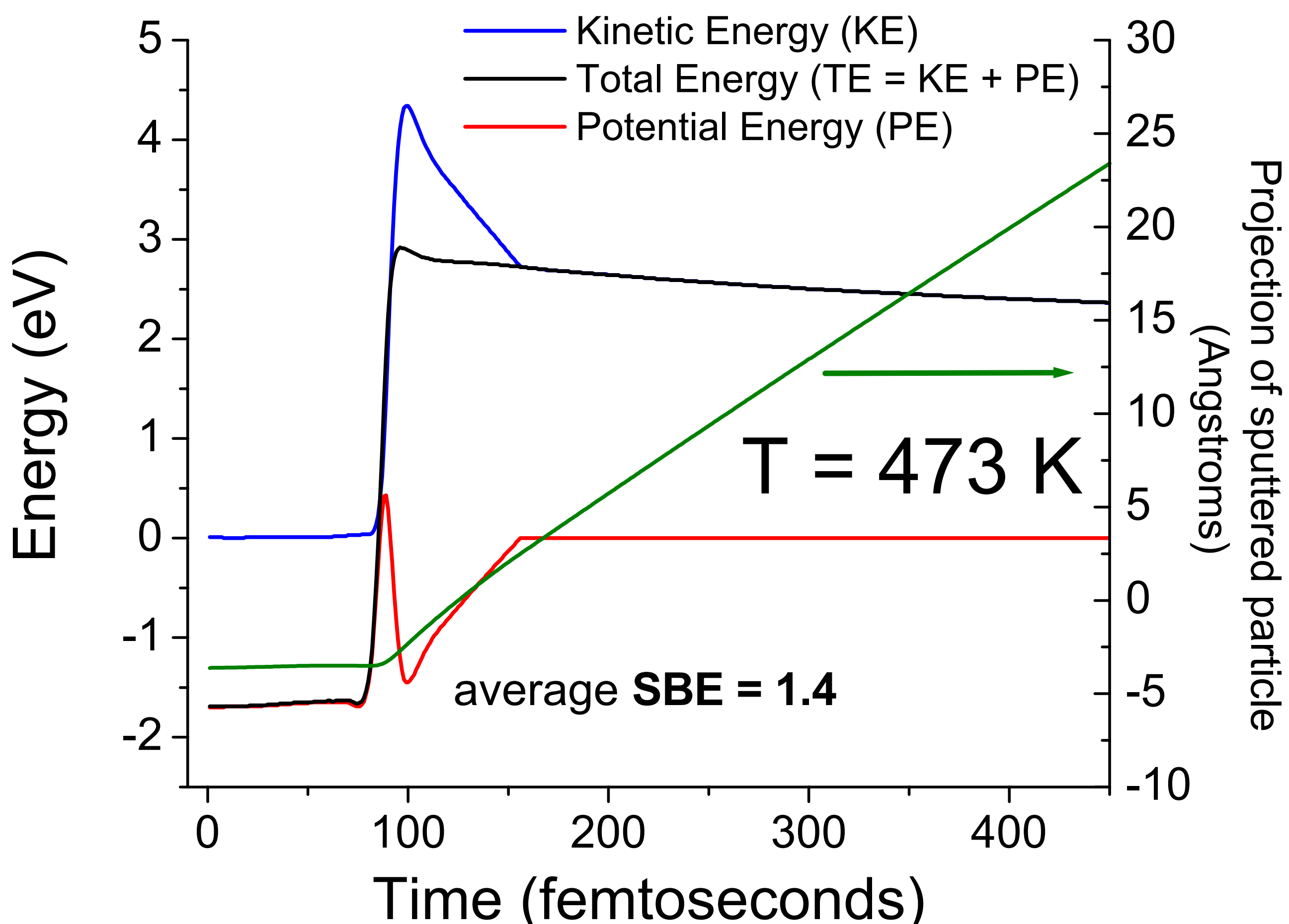
Recoil energy distribution from MD simulations



- 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

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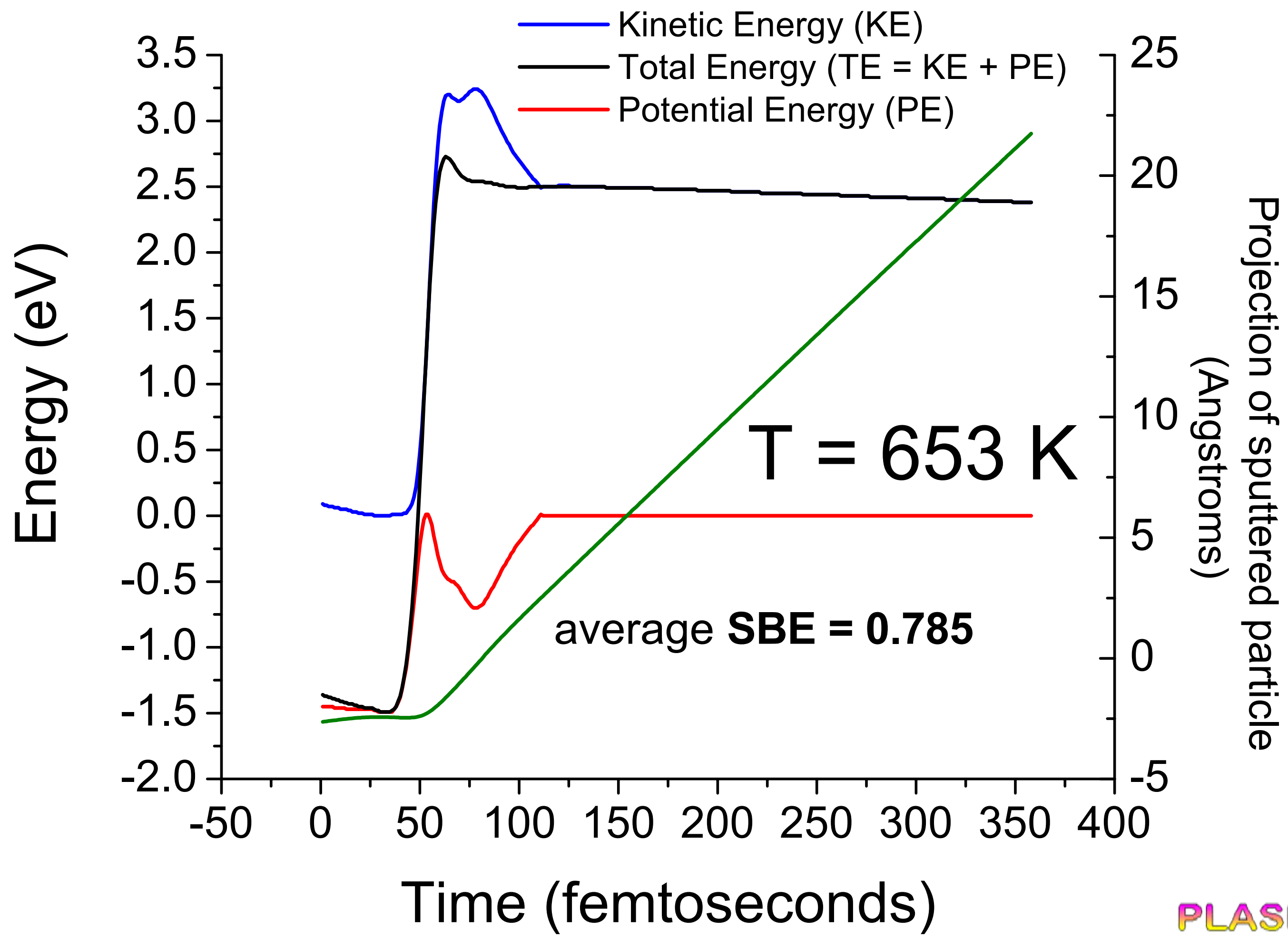
Surface binding energy from MD simulations at 653 K is lower !



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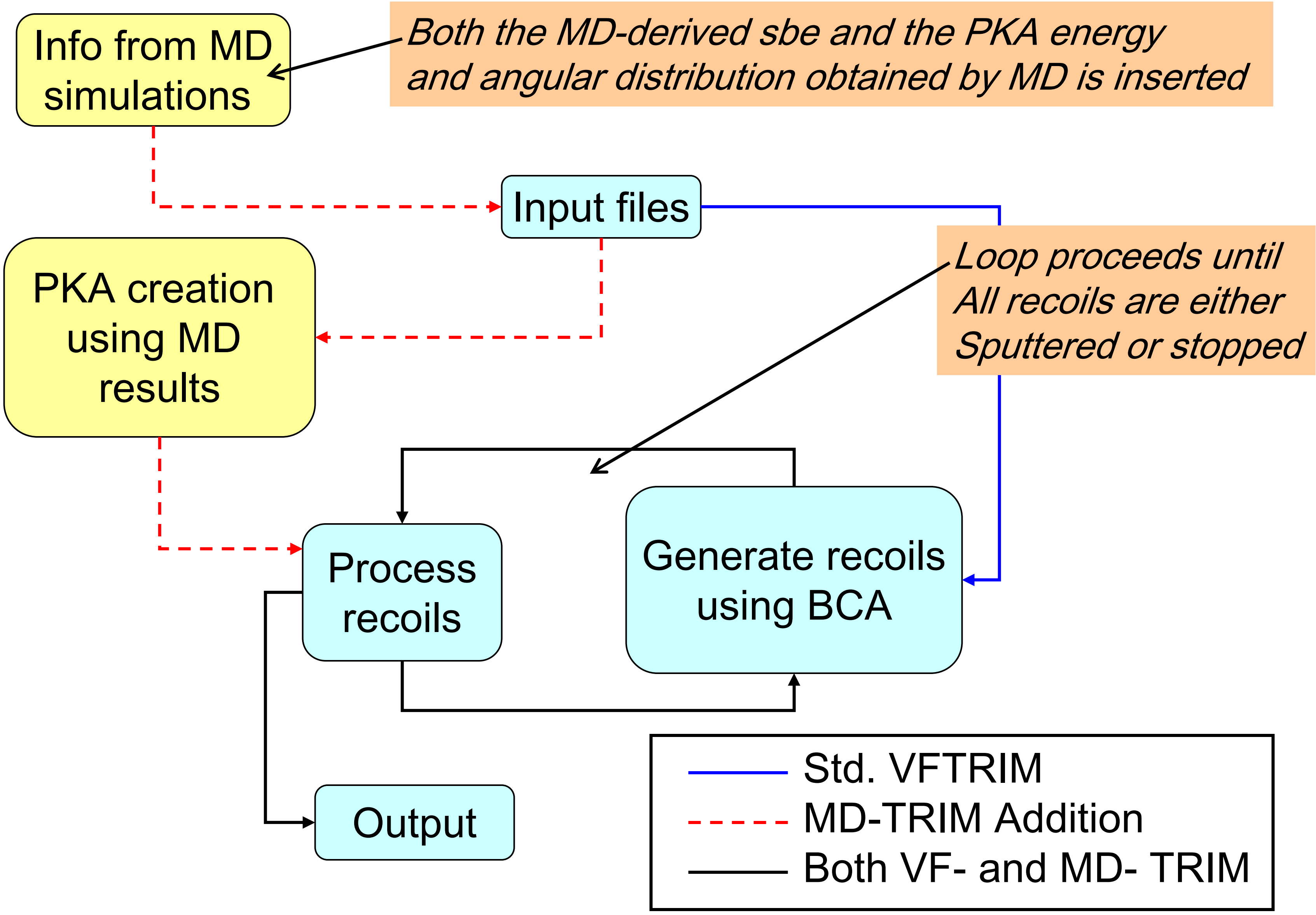
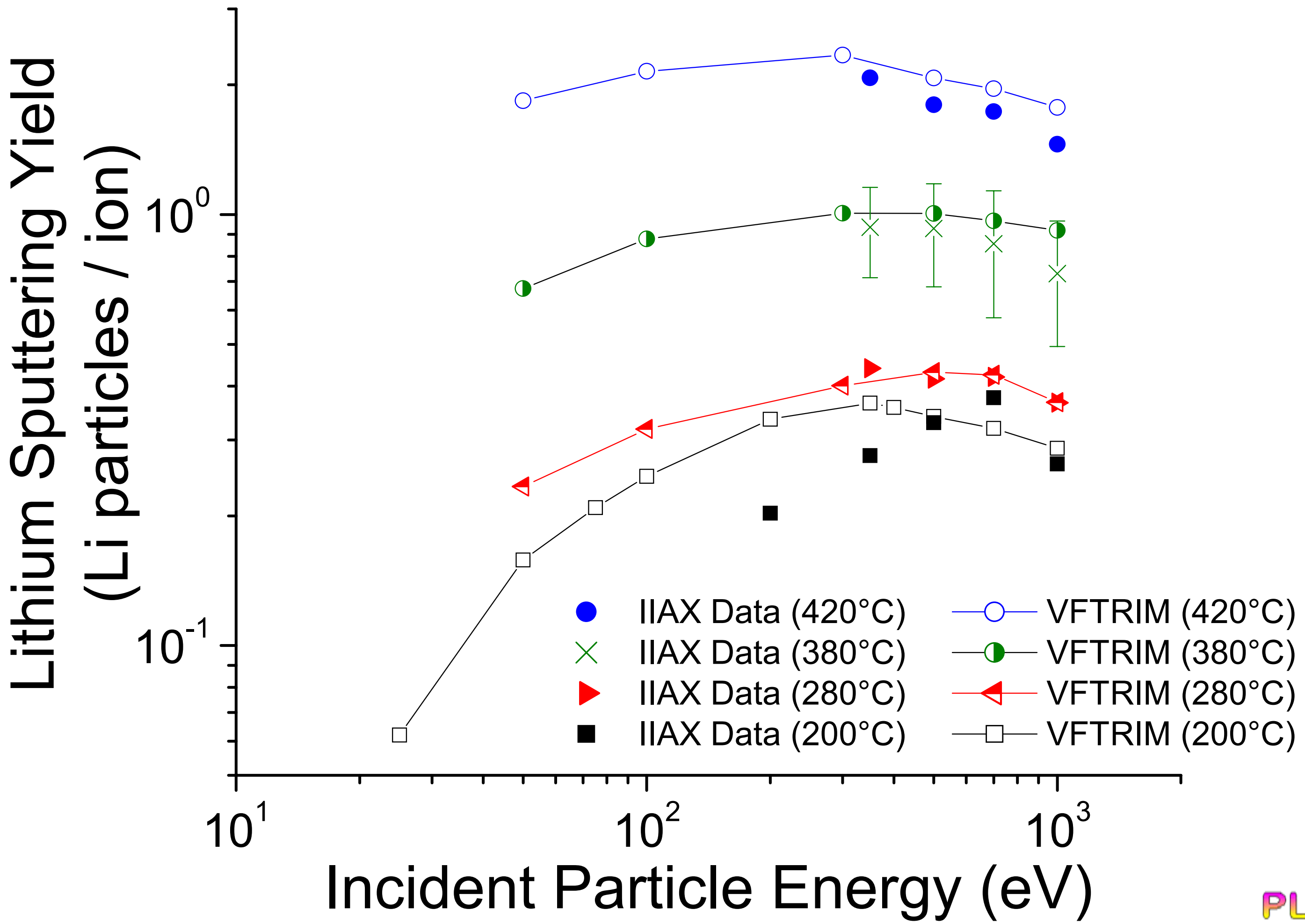


Info from MD simulations
Both the MD-derived sbe and the PKA energy and angular distribution obtained by MD is inserted
Input files
PKA creation using MD results
Loop proceeds until All recoils are either Sputtered or stopped
Process recoils
Generate recoils using BCA
Output
Std. VFTRIM
MD-TRIM Addition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

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



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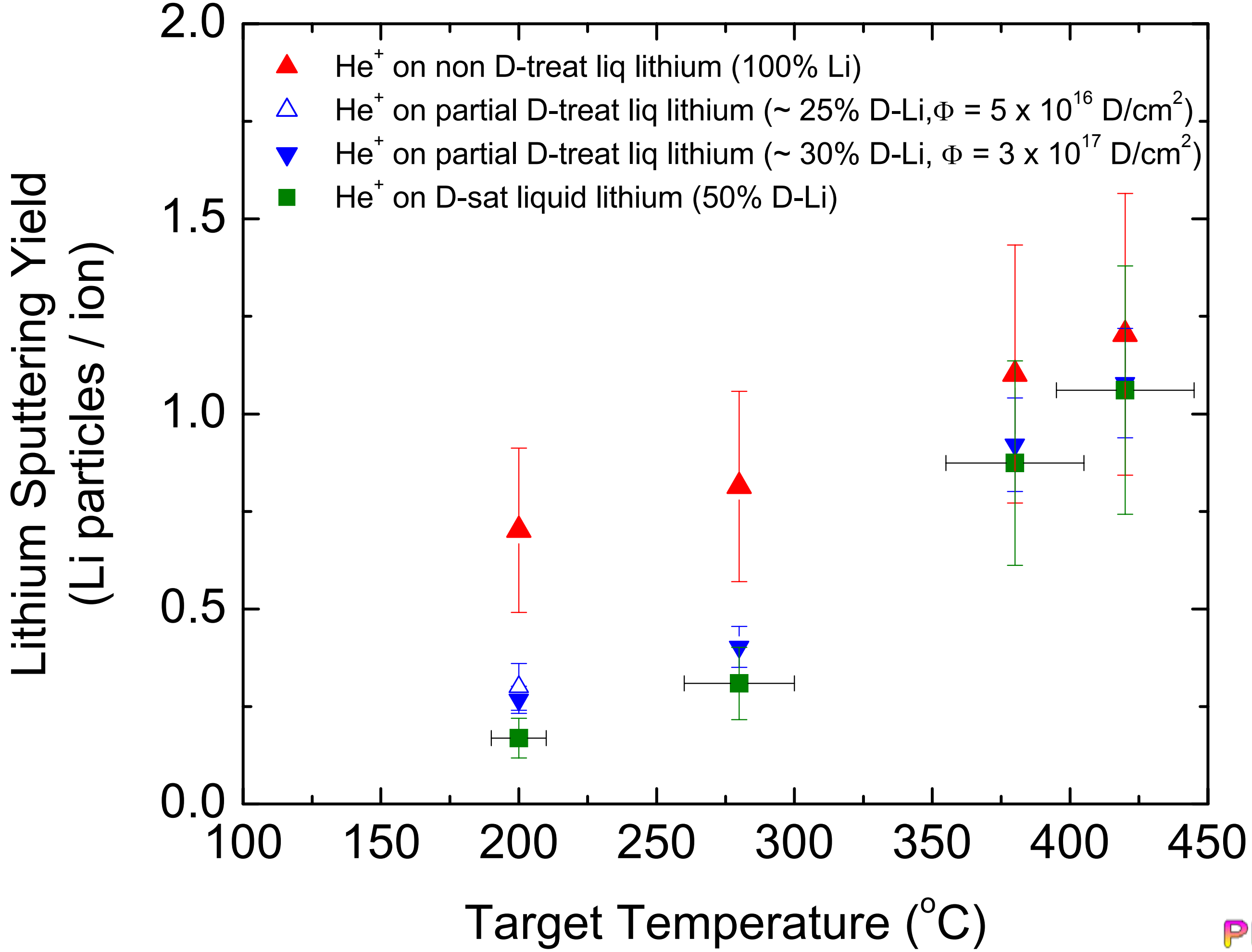
D-treatment of liquid Li surfaces versus target temperature (He^+)



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MD-TRIM Results

Estimated Experimental Results : 0.8 1.2

sbe \ PKA Dist. Type	VFTRIM (Std. Ver.)	VFTRIM (BCA Dist.)	MD-TRIM Results 473°K (MD Dist.)	MD-TRIM Results 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

The Allain-Ruzic model appears to fit and explain liquid-metal erosion enhancement with temperature

- The characteristics of the near-surface energy cascade are important in explaining the enhanced nature of physical sputtering of material measured in experiments. The cascade can not be treated in a binary fashion and is temperature dependent
- How a particle that is sputtered is bound to its neighboring atoms is crucial in being able to model a reasonable “surface binding energy”. It is a sensitive function of temperature.

Future work

- Long temporal mechanisms: thermal sputtering, ion-induced evaporation
- Effects of hydrogen isotope implantation on near-surface cascade dynamics and Li erosion
- liquid-vapor interface: liquid-metal stratification
- Other interactions: inert gases and liquid Li (e.g. He, Ne, Ar)

Acknowledgements

- G. H. Miley, NPL Associates, Inc (STTR funding Phase II) DE-FG02-01ER86134
- ALPS/DOE funding
- Undergraduate students: Jason Tillery, Matt Hendricks, Ian Treviranus

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