Experiments and modeling of enhanced liquid-metal erosion

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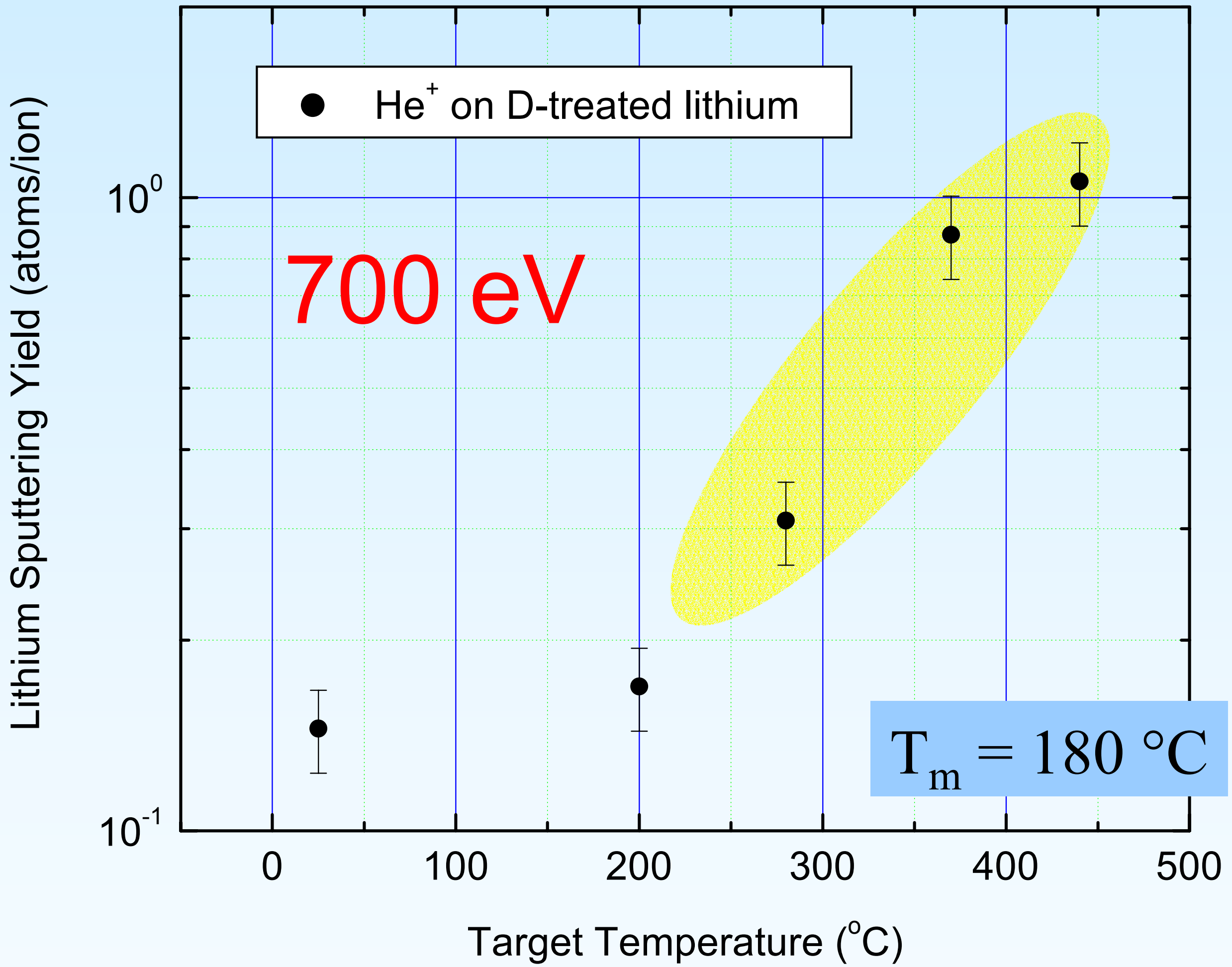
Outline of Talk

- Where do we stand with liquid-metal erosion experiments?
- Scope of liquid metal erosion work in IIAX
- Experimental setup of IIAX (Ion-surface Interaction Experiment)
- Measurements of liquid Sn sputtering
- Enhancement of liquid lithium erosion with target temperature: An atomistic model
- Conclusions and Future Work

IIAX data on lithium sputtering yield temperature dependence from oblique He^+ bombardment

- Enhanced erosion of lithium measured for temperatures higher than melting temp. for lithium, tin-lithium and tin
- Ad-hoc models for liquid lithium with smooth surface in VFTRIM-3D suggest several temperature-dependent mechanisms[1] are important



1. J.P. Allain, M.D. Coventry, D.N. Ruzic, J. Nucl. Mater. 313-316 (2003) 645

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What do we know from PMI experiments on the erosion from liquid metals?

- Liquid-metals do not erode much differently compared to solid state near the melting point
- So far: liquid Li, Sn-Li, Ga and Sn show signs of erosion enhancement (particularly lithium) *with* rise in temperature
- Liquid lithium maintains very high secondary ion sputtered fractions across all temperatures studied so far (200-450 °C)
- 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
- In IIAX experiments no signs of bubble formation except in liquid Sn-Li erosion experiments. Need more experiments to determine bubble formation effects for liquid lithium and other liquid-metals

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Conjectures on possible mechanisms responsible for erosion enhancement

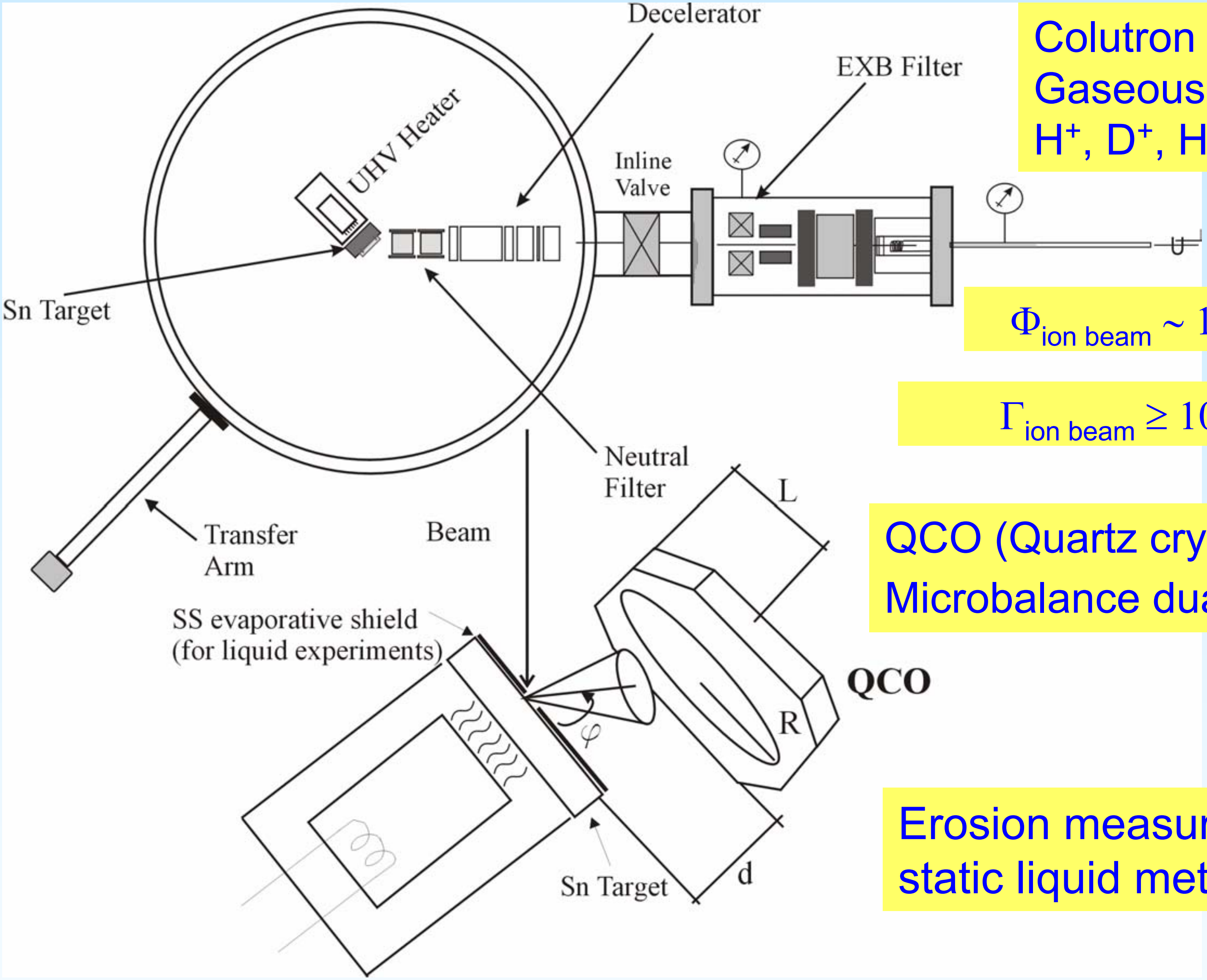
- Bubble formation of implanted He or D could precipitate into nano-size bubbles reaching the surface and emitting a non-linear amount of material
  - Need more experiments to determine the role of bubble formation on the *enhancement* of lithium erosion in a 200 °C window.
- Localized rise in temperature (in the form of thermal or elastic spikes) could lead to a larger Li yield due to its low vapor pressure (a rise of 200 ° C could do this)
- Other models for liquid metals?... fluid dynamics model of sputtering?
  - **M.M. Jakas, E.M. Bringa, R.E. Johnson, Phys. Rev. B 65 (2002) 165425-1**
- Surface stratification of liquid metal (S. Rice, et al.)

Mechanisms we (Allain-Ruzic) believe explain enhancement

- Near-surface energy deposition to “weakly-bonded”, mobile lithium atoms lead 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 *hot* 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 is important to explain the measured enhancement
- Surface stratification (characteristic of liquid-metals) could in fact play a role in the enhancement of erosion

Scope of Experimental Work in IIAX

Liquid Lithium	Eo (eV) 200-1000	T (°C) 25-425	D-treated	Non D-treated
H^+	✓	✓	✓	
D^+	✓	✓	✓	✓
He^+	✓	✓	✓	✓
Li^+	✓	✓	✓	
Liquid Tin-lithium	**Eo (eV) 200-1000**	**T (°C) 25-425**	**D-treated**	**Non D-treated**
D^+	✓	✓	✓	
He^+	✓	✓	✓	✓
Li^+	✓		✓	
Liquid Tin	**Eo (eV) 200-1000**	**T (°C) 25-425**	**D-treated**	**Non D-treated**
H^+	✓	.		✓
D^+	✓	✓		✓
He^+	✓	✓		✓



Colutron ion source for both Gaseous and metal species: H^+, D^+, He^+, and Li^+

$\Phi_{\text{ion beam}} \sim 10^{15} - 10^{18}$ ions/cm^2

$\Gamma_{\text{ion beam}} \geq 10^{14}$ ions/cm^2/sec

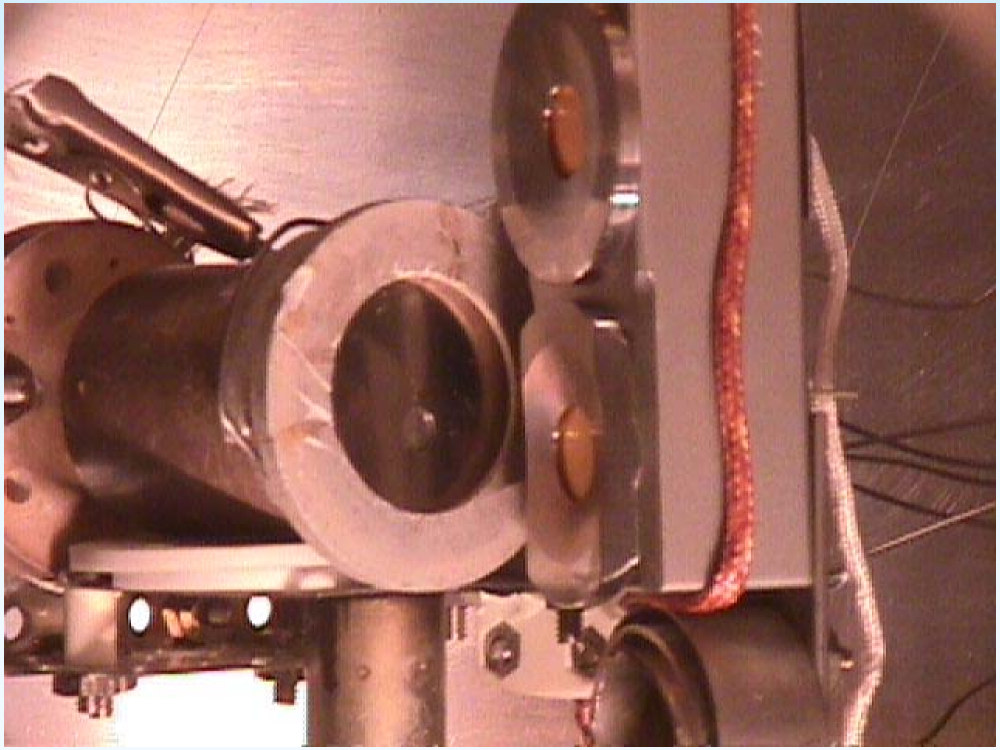
QCO (Quartz crystal oscillator Microbalance dual unit, $\pm$ 0.1 Å)

Erosion measurements on static liquid metals

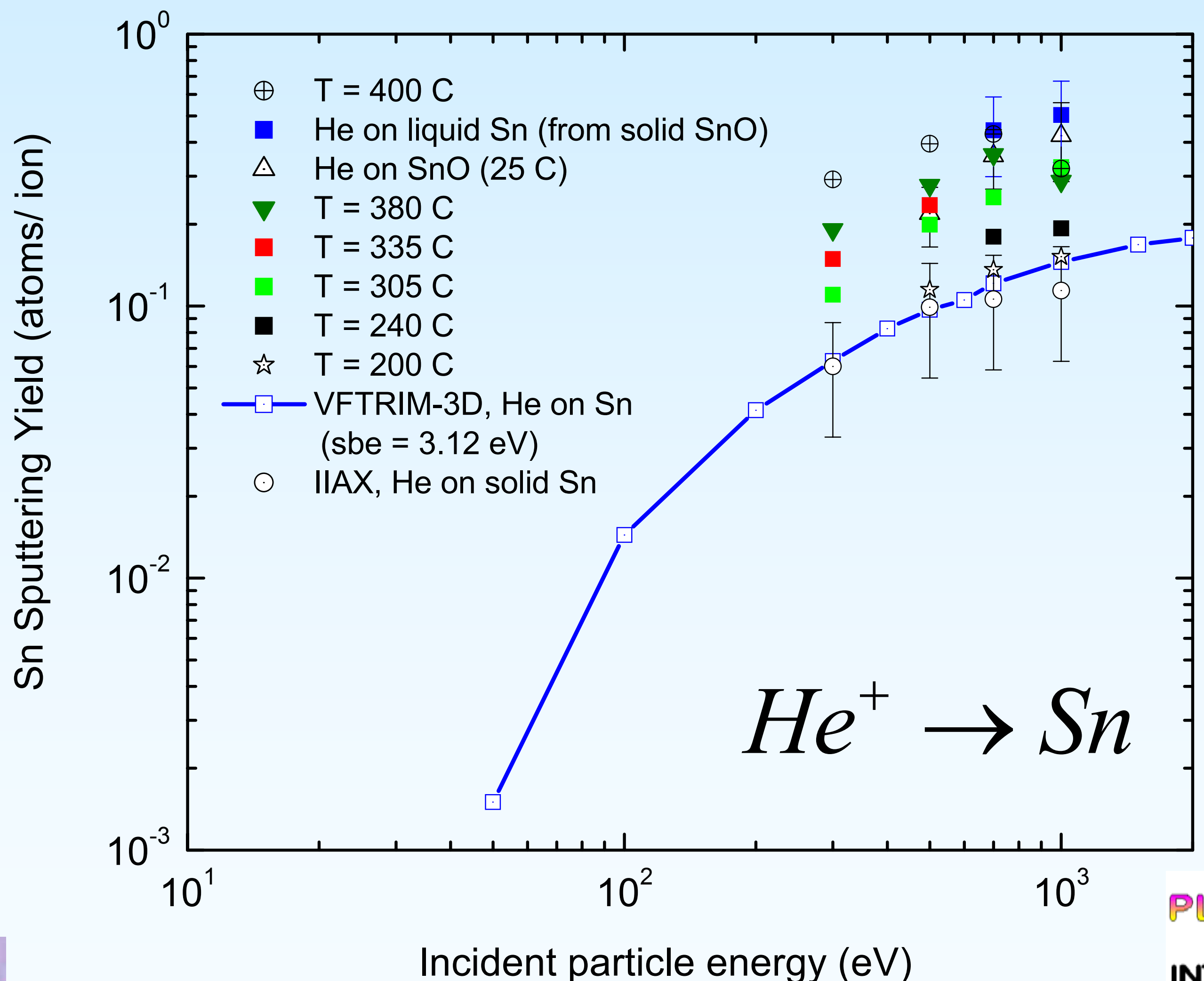
J.P. Allain, M.D. Coventry, D.N. Ruzic, J. Nucl. Mater 313-316 (2003) 641.
M.D. Coventry, J.P. Allain, D.N. Ruzic, J. Nucl. Mater 313-316 (2003) 636.

In-situ sputtering diagnostics and heater system

- A cleaving arm is designed to remove thin oxide layer formed on liquid-metal sample
- The DCU-QCM is used here to address temperature variation in background
- Both evaporation and sputtering are measured with quartz crystal microbalance



Sn sputtering vs incident particle energy by He^+ bombardment



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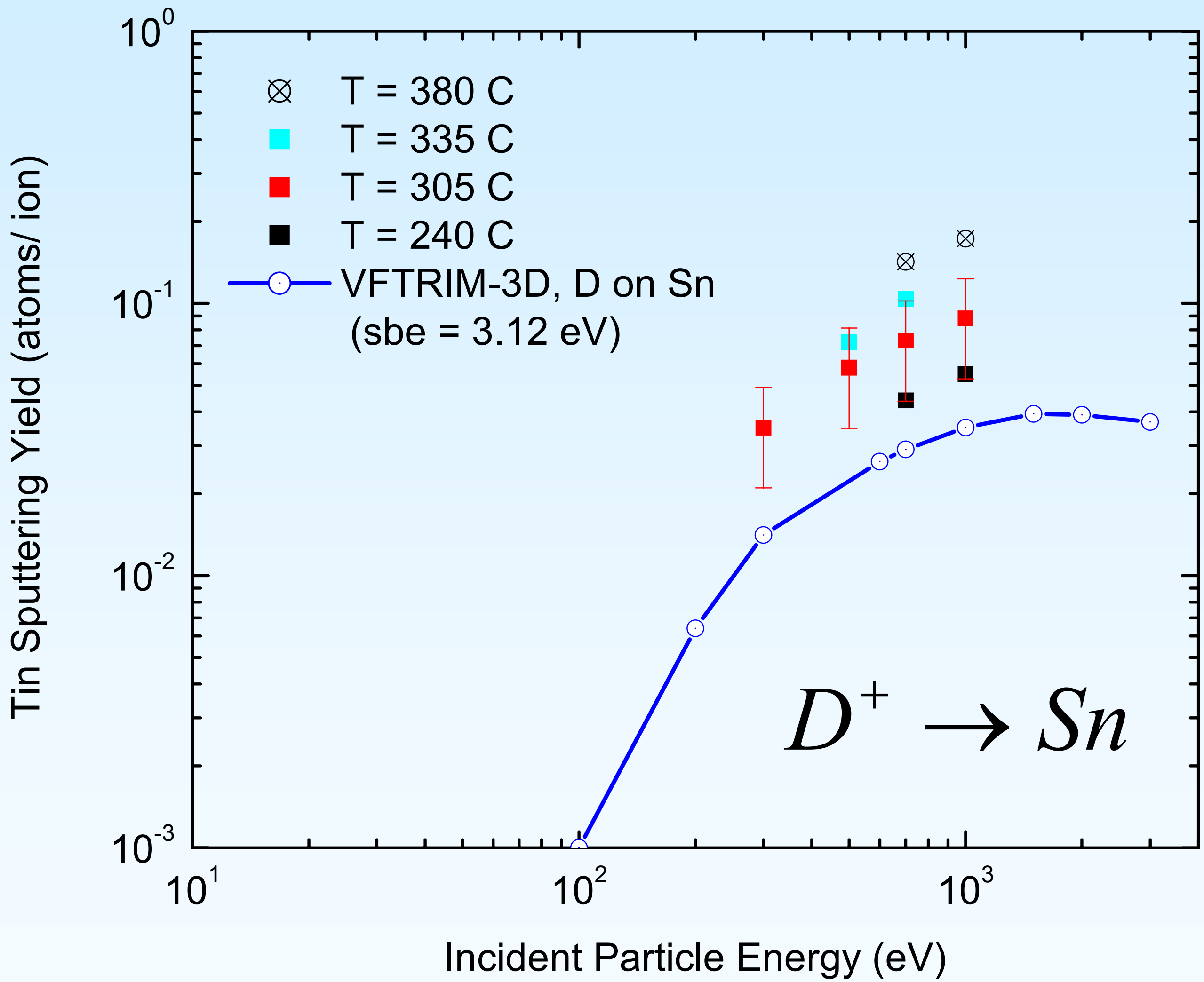

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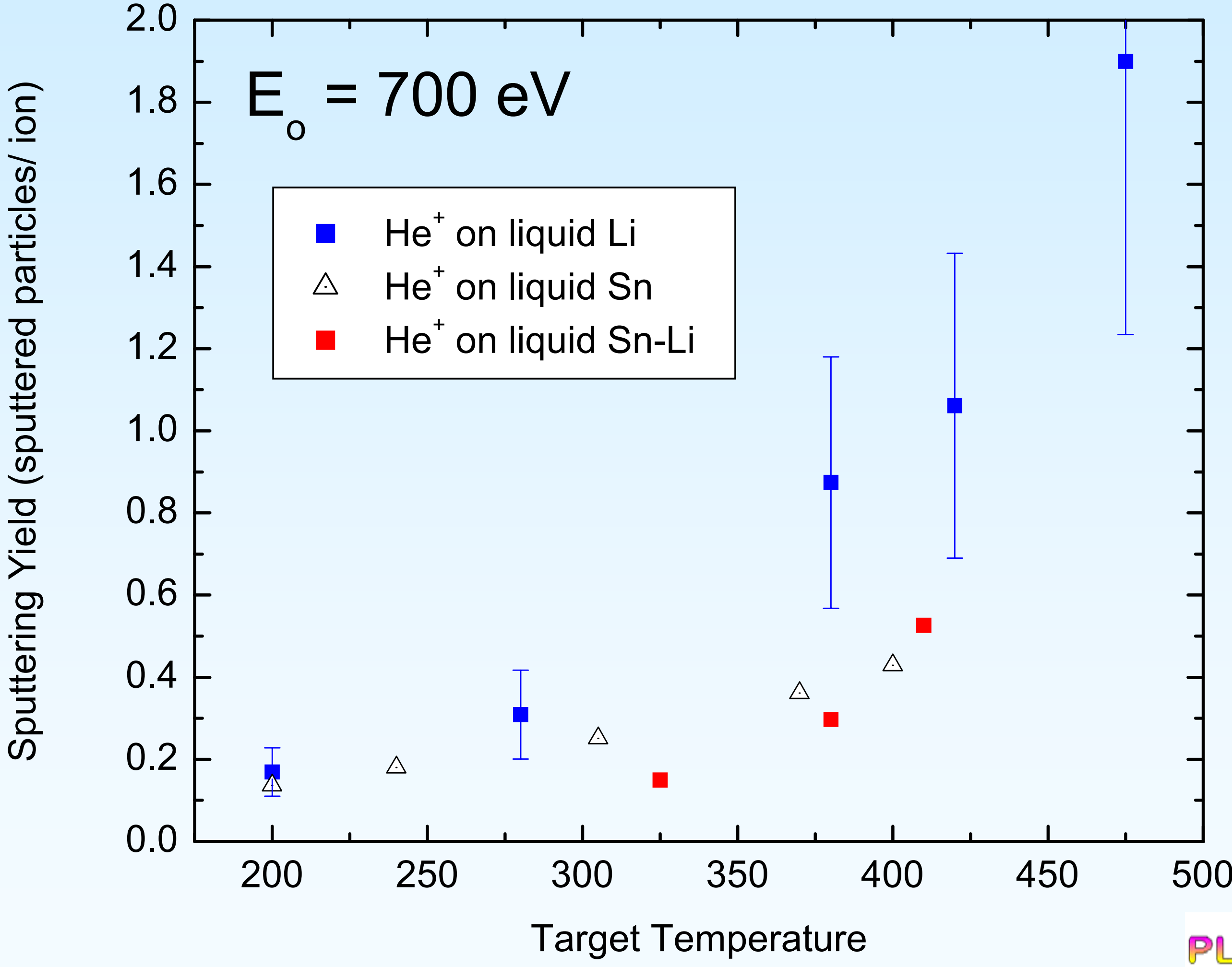
Comparison of Sn sputtering with SnLi and Lithium from He^+ bombardment



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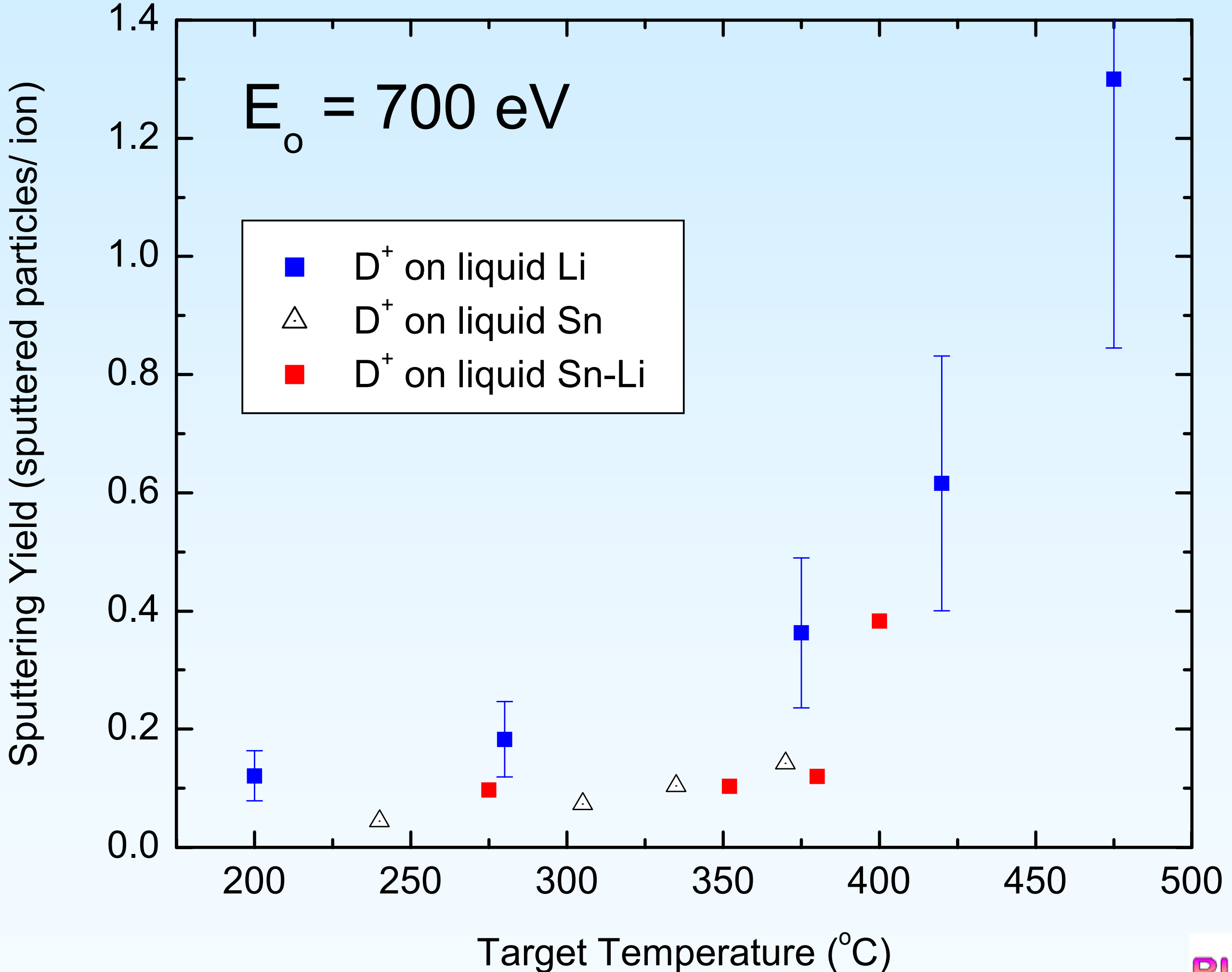
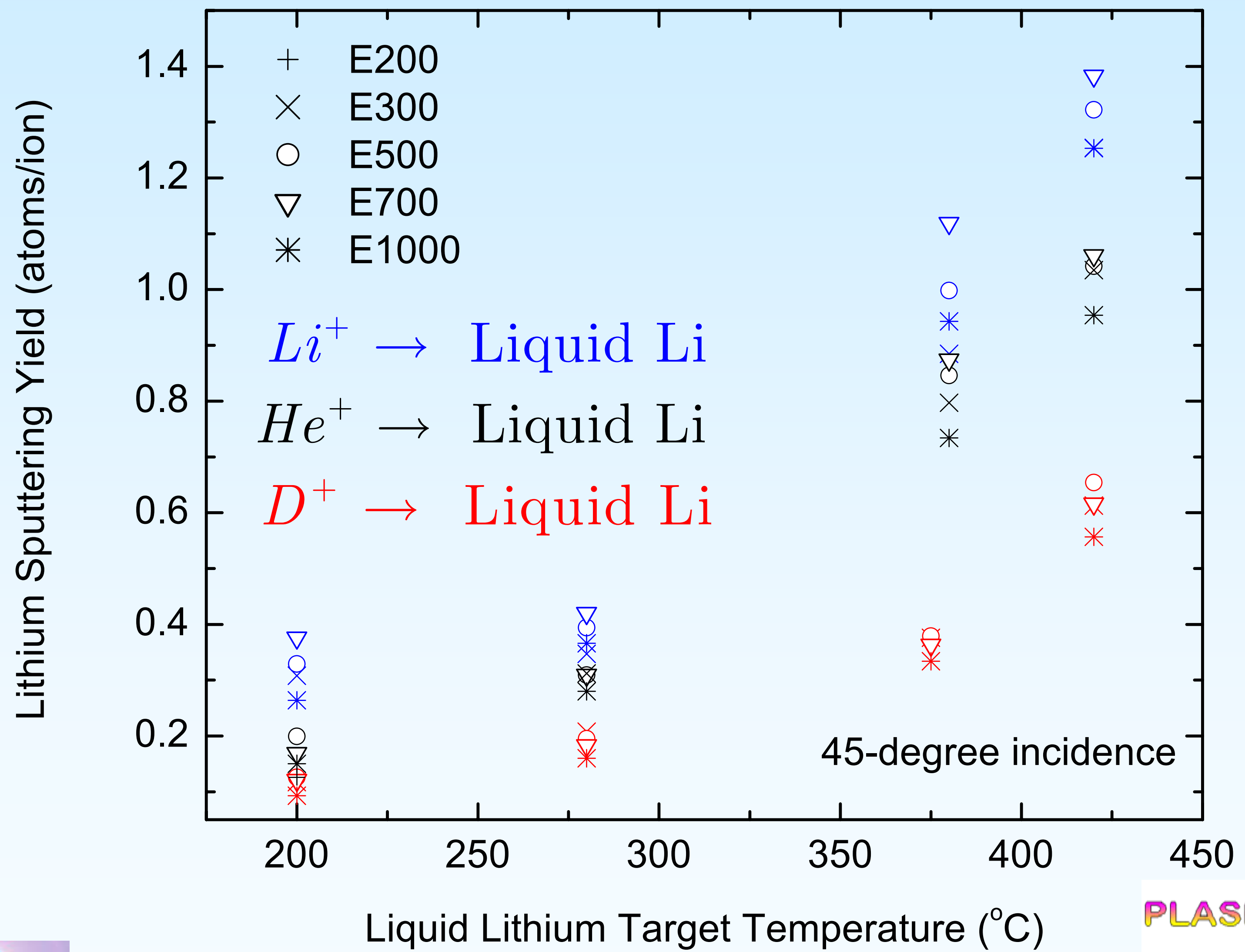


IIAX temperature-dependent yields for various incident particle energies



MD-TRIM liquid Li erosion enhancement modeling studies

- Lithium erosion enhancement is studied using molecular dynamics of Li bombardment from liquid Li†
- Near-surface energy cascades are found from MD results for a variety of system temperatures
- The recoil energy and angular distributions are implemented in a Monte Carlo code (modified VFTRIM-3D) to obtain absolute lithium sputtering yields for comparison with experimental Li erosion data
- In addition, the surface binding energy from MD is implemented in VFTRIM-3D for temperatures at 473 and 653 K

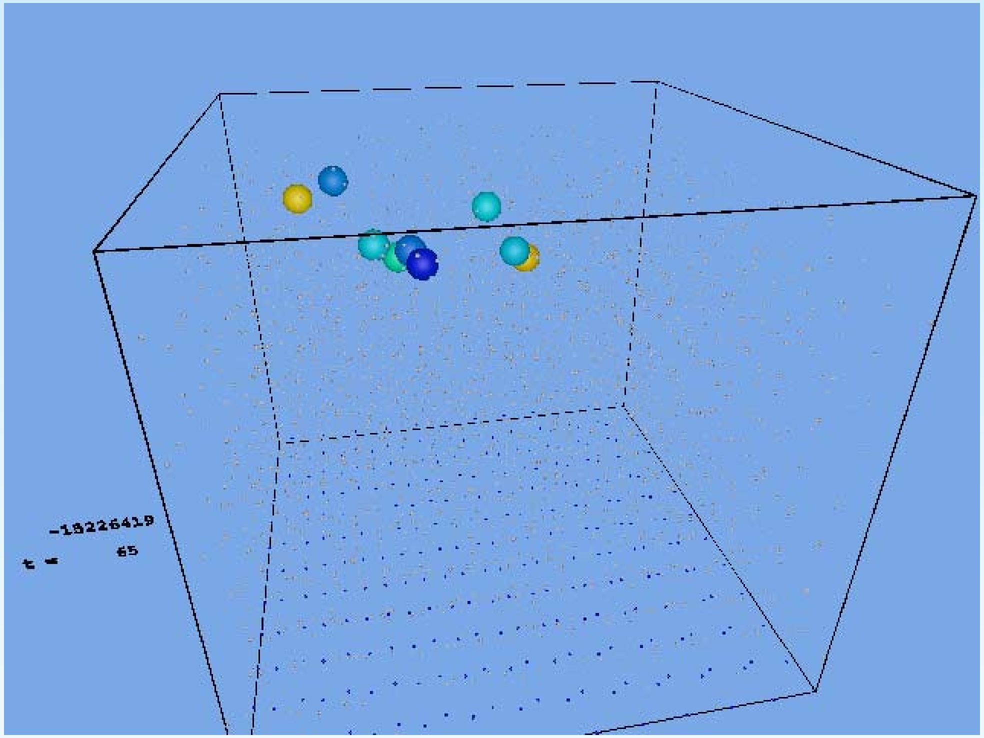
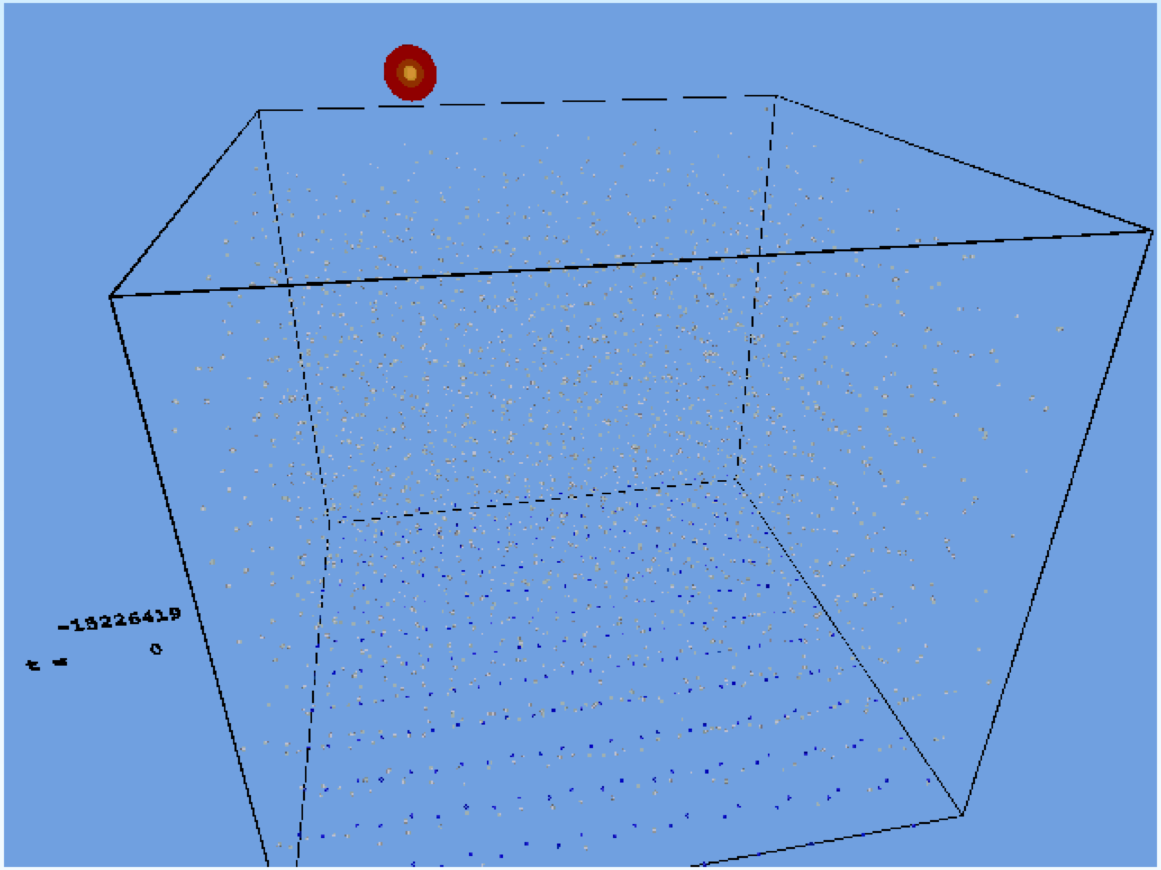


Figure shows near-surface energy cascade of recoils from a 100 eV, 45-deg. incident Li atom. Colors represent energy magnitudes (red – highest, blue – coldest). Only atoms with 10*kT eV or more are shown.

† L.E. Gonzalez, private communication, 2002
L.E. Gonzalez, J. Phys. Conds. Matter 5 (1993) 4283.

Near-surface energy cascade of a 100 eV 45-deg. Li particle



T = 473 K

Concluding Remarks

- Liquid-metals do not erode much differently than in their solid state just above the melting point
- Lithium erosion is enhanced 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
- Ion fraction of sputtered species for liquid lithium and liquid tin-lithium are 55%-65% compared to <10% for solid phase tin-lithium and tin
- Molecular dynamics simulations coupled to Monte Carlo codes such as TRIM (MD-TRIM) show promise in being able to elucidate key physical mechanisms responsible for measured enhanced erosion in low-energy charged particle bombardment of liquid-metals

PMI research of liquid-metal erosion: What lies ahead?

- Key experiments needed in liquid-metal PMI erosion research:
  - Bubble formation and its role on erosion enhancement
  - Understanding the influence of the surface chemical state on erosion, backscattering and surface charge dynamics
  - Study of erosion enhancement on other materials (i.e. Ca,Mg) as a function of temperature
  - ITER related: reduction of methane erosion by lithium treatment of hydrogen-saturated graphite
- Molecular dynamics modeling of liquid-metal erosion incorporating surface stratification at the liquid-vapor interface
- Exploit strengths of both MD and BCA codes in a hybrid model (e.g. MD-TRIM) to understand and predict non-linear erosion phenomena such as: temperature-dependent enhanced erosion

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