Liquid metal sputtering data/models & DIII-D DiMES analysis

J.P. Allain, J.N. Brooks, D.G. Whyte

Plasma Facing Components (PFC) Meeting Oak Brook, Illinois November 18, 2003



Argonne National Laboratory



A U.S. Department of Energy Office of Science Laboratory Operated by The University of Chicago



Liquid metal sputtering data/models & DIII-D DiMES analysis

- Lithium erosion mechanisms: Models and Data
- NSTX Low and High-power cases: sputtering
- Quiescent plasma Li-DiMES experiments: erosion
- Measurements on ionization and sputtered Li velocity distributions
- Modeling of physical sputtering
- Erosion/redeposition analysis with WBC/REDEP
- Conclusions







What we know about liquid-metal surface mechanisms

- No significant difference in sputtering from the solid to liquid state when temperature is near melting point
- Non-linear increase in sputtering from liquid-metal when temperature is about 50% higher than melting point (accounting for evaporation)
- Two-thirds of lithium sputtered particles are in the charged state
- Implanted hydrogen leads to a ~ 40% decrease in *lithium* sputtering
- High retention of hydrogen in liquid lithium (PISCES-B results)







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 temperaturedependent mechanisms¹are important









Lithium erosion enhancement measured in various experiments





IIAX temperature-dependent yields for various incident particle energies







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





Liquid-metal erosion mechanisms

- 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
- 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







Other possible mechanisms responsible for erosion enhancement

- Formation of surface adatoms with lower binding to surface (Doerner, et al.)
- Bubble formation of implanted He or D could precipitate into nanosize 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 $\Lambda T \sim 200$ °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







Temperature-dependent Liquid Lithium Models

- **Radiation Activated Adatom Sublimation (RAAS)** model (Doerner, et al.)
 - Assumes adatom formation on a liquid surface and obtains activation energy from MD modeling
 - Scales erosion to incident flux

Allain-Ruzic model

- Utilizes near-surface spatial distribution of energy cascade from MD models
- Can predict temperature dependence of erosion

Other models

Sigmund, Vaulin, others with: Y(T) = A*T^{-1/2} exp(-B/T)



Office of Scienc





Empirical Y(T) model (Allain) for NSTX erosion/redeposition studies

- Empirical fits made to calibrated VFTRIM-3D runs
- Fits are completed for sputtering yields of lithium as a function of:
 - Incident particle energy
 - Surface temperature
 - Incident angle
- The fit is made to a temperature-dependent function (from P. Sigmund model)
- Empirical fits used in WBC/REDEP transport code







Energy-dependent sputtering yields for liquid lithium (low-energy levels)









Sputtering yields for liquid lithium at higher incident energies



of Energy





Li-DiMES experiments under quiescent plasma conditions



- DiMES with a 2.5 cm lithium spot as PFC in quiescent plasma discharges
- Plasma diagnostics and atomic lithium visible spectroscopy
- Diagnostics near outer strike point (OSP) with swept plasmas







Quiescent plasmas in Li-DiMES experiments



- Electron temperatures ~ 5-25 eV
- Electron densities ~ 0.03 1.80 × 10¹⁹ m⁻³







Li-DiMES sputtering of D⁺ on lithium







Li-DiMES able to measure erosion mechanisms in both PF and SP regions









Neutral Li line intensity vs distance from Li-DiMES center

- Private flux
 bombardment in Hmode plasma
- Electron temperatures are low, ~ 1eV
- Electron densities ~ 10²⁰ m⁻³
- Ionization occurs a centimeter away and is confirmed with WBC/REDEP modeling data







Calculated Li I (671 nm) brightness with OSP on DiMES center









Li-DiMES code/data photon emission comparison, solid lithium

D.G. Whyte, J.N. Brooks and J.P. Allain



Good agreement code/data







Summary and Conclusions

- Atomistic simulations helping elucidate erosion enhancement effects in liquid-metals and hot solids (e.g. Be)
- Further experiments/modeling needed:
 - Testing effect of bubble formation on erosion enhancement in liquid metals
 - Charge dynamics of candidate LM PFCs
 - Low-energy reflection (need atomistic modeling with proper surface potentials)
- NSTX cases modeled with calibrated surface models
- Li-DiMES erosion results from quiescent plasmas
 - Measured yield ~ 10% for T_e ~ 20 eV
 - Sputtered Li readily ionized near surface







Acknowledgements

PMI Group at the UIUC, D.N. Ruzic

 See: J.P. Allain, et al. JNM 313-316 (2003) 641 and M.D. Coventry, et al. JNM 313-316 (2003) 636

PISCES-B group

• See: R.P. Doerner, et al. JNM 313-316 (2003) 383

C. Wong and the DiMES team

 See: SOFE 2003 paper titled: "DiMES Contributions to PMI Understanding" C.P.C. Wong, et al. for more details





