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Plasma Liquid-Metal Interaction Experiments and Modelling

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1. Introduction

The ability of flowing metal plasma facing components (PFCs) to withstand the extreme conditions of future tokomaks has been recognized. The flowing liquid retention experiment (FLIRE) facility at the University of Illinois measures the retention properties, both for helium (ash pumping) and hydrogen (recycling regime, tritium inventory), of candidate liquid PFCs, such as lithium. Results of deuterium absorption measurements in flowing lithium are presented[1].

Sputtering yields and reflection coefficients from pure and hydrogenated lithium surfaces under low-energy, light-particle bombardment have been modeled with molecular dynamics (MD) simulations. The effects of surface temperature, incident energy and angle, and the hydride concentration on the sputtering yields and reflection coefficients are shown and compared with experimental results from the ion-surface interaction experiment (IIAX) and from standard binary collision codes such as TRIM[2].

Flowing liquid tin is also being considered for divertor PFCs. Modeling of a liquid tin divertor requires knowledge of self-sputtering and D^+ and He^+ sputtering yields. In IIAX, Quartz-crystal microbalances measured the sputtering yields from tin ions and a range noble gas ions with energies ranging from 300 to 1000 eV incident at 45°[3] to elucidate a physical understanding of the temperature dependent mechanisms involved. Experimental results are compared to VFTRIM simulations.

2. Results

<u>FLIRE-TDS:</u> In the FLIRE[4] experiments discussed here, approximately 400 g of Lithium was flowed through an upper chamber on a set of ramps, where it was exposed to deuterium gas at a specified pressure, and into a lower chamber where prompt release was measured. Two runs are discussed: (1) at 7.5×10^{-5} Torr at an average speed of 44 cm/sec for a duration of 30 sec. and (2) at 1 Torr and an average speed of 22 cm/sec for a duration of 60 seconds. The upper chamber flow path and the lower chamber were maintained at a temperature of 230°C.

After measuring the prompt release in the lower chamber for 5 minutes, the lithium is transferred to the thermal desorption spectroscopy (TDS) chamber which is maintained initially at 250°C. The temperature program used for the TDS studies in FLIRE is a ramp of 2 °C/min, starting at 250 °C and finishing at 600 °C. At the moment of transferring Li (5 min into the scan) from the lower chamber to the TDS chamber, there is a weak release of deuterium. This indicates that a deuterium concentration between 0.1 and 0.2% was trapped during the exposure and released when the temperature was raised in a step-wise manner. The bounds on concentration correspond to equilibrium concentrations of 0.1% at 230°C (initial temperature) and 0.2% at 250°C (TDS temperature).

A wetted wall tower model[5], which assumes a saturated hydrogen concentration at the liquid surface (50% atomic fraction of hydrogen) and diffusion into the bulk, indicates that an average deuterium concentration of ~3% is expected for typical FLIRE conditions. Clearly, the model overestimates the amount trapped, which is not surprising since it assumes all H is in the form of atomic H and not molecular H_2.

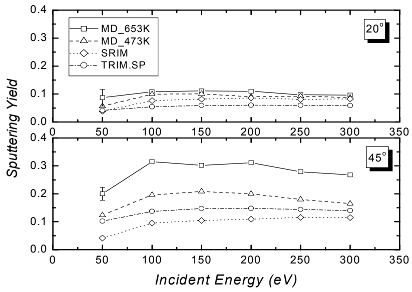
To verify this conclusion, the TDS chamber was cleaned, and the lithium charge was transferred to the TDS chamber after exposure to 1 Torr of D_2. Despite the orders of magnitude higher pressure, the deuterium pressure trace still exhibited a peak between 230 and 250°C, hence the absorbed deuterium concentration was still between 0.1 and 0.2%.

<u>MD Calculations:</u> Recent experiments, IIAX at UIUC[6] and PICSES at UCSD[7,8,9], show enhancement of sputter erosion with increasing surface temperature. Codes based on the binary collision approximation (BCA) (e.g. TRIM) can't model these temperature effects; therefore, MD modeling is widely used to study the issues related to PFC materials since MD includes temperature effects, as well as cascade effects.

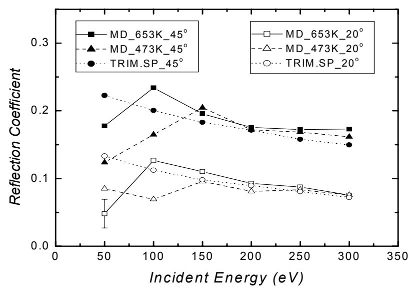
A MD code, MolDyn[10], was improved to handle the lithium/deuterium system. First, the liquid Li-Li potential was obtained with the neutral pseudoatom method[11] by considering both structural and dynamical properties. This potential was developed for liquid lithium MD calculations and is effective for high temperatures ranging from 470K to 843K. We used the singlet ab initio potential[12] splined with the universal potential at small distances for the D-Li interatomic potential. This potential enables accurate predictions to be made of the scattering of the alkali metal atoms by deuterium atoms[13,14].

In order to simulate a surface consisting of liquid PFC material, the original surface (BCC) was gradually heated to 473K or 653K over a long time until equilibrium was reached.

The sputtering yield and reflection coefficient of D incident on Li as a function of energy for two different temperatures are shown in Figure 1, along with results from TRIM. Surface temperature has little effect on the average energy of sputtered atoms, but affects the energy distribution of the sputtered atoms (see Figure 1). There are two peaks for the energy distribution, a low-energy stimulated-evaporation component and the more typical Thompson energy distribution contribution. Higher surface temperature increases the stimulated-evaporation low-energy peak. This has also been seen experimentally[6-9].



(a)



(b)

Figure 1. (a) The sputtering yield as the function of incident energy, and (b) The reflection coefficient as the function of incident energy. The error bars shown are representative of the statistical error for every point.

<u>IIAX:</u> IIAX[15,16] uses a Colutron[17] ion gun system to deliver a mono-energetic, velocity-filtered, low-energy ion beam, currently at a 45°, to a target. Material sputtered from the target can be collected using a quartz-crystal microbalance dual crystal unit (QCM-DCU), which monitors the amount of material deposited. From the measured mass deposited on the crystal and with the use of VFTRIM[18] to estimate other parameters, an absolute sputtering yield was calculated. Figure 2 displays sputtering data over a wide range of temperatures and for two different ion species (Ne^+ and Ar^+). The data show evidence of the suppression of temperature-enhanced sputtering[6,8,19,20,21,22]. Extending the masses heavier (see Figure 2) shows an even more strongly suppressed enhancement curve for the neon bombardment and no evidence for temperature enhancement outside of the error bars for Ar^+ bombardment for this particular range of temperatures.

This apparent lack of temperature enhancement of heavy-ion sputtering of liquid tin initially seemed to contradict previous results for light-ions seen for tin and other liquid metals. However, if one considers the energy density in the collision cascade, light-ion bombardment will keep more energetic atoms near the surface than heavy-ion bombardment.

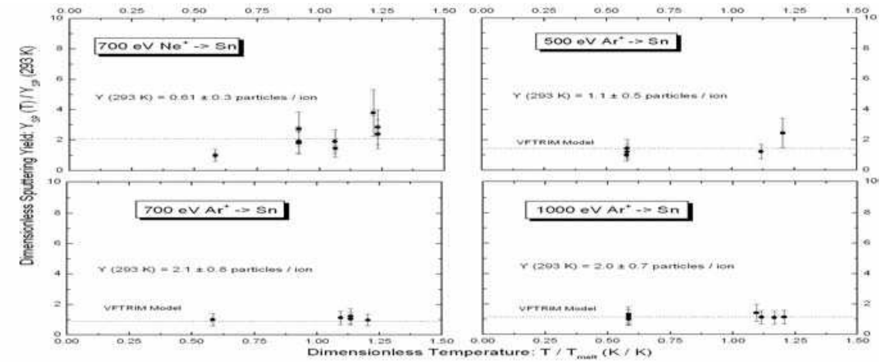


Figure 2: Experimental results for heavy-ion bombardment of tin at 45° incidence. Also shown is the dimensionless sputtering yield found using VFTRIM[18].

If tin self-sputtering is temperature-independent at least up to temperatures of interest (1300°C), then tin still has the same finite self-sputtering as found for the room temperature case[23]. This would place the sole restriction on the operating temperature of a liquid tin divertor surface from an erosion perspective on light ion sputtering which has been explored more in depth[6,22].

3. References

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