SIMULATION-DERIVED THERMAL DIFFUSION PARAMETERS IN TEMPERATURE-DEPENDENT DEPLETION OF POTASSIUM ADSORBED ON MAGNETITE. G. Killian[1] C.A. Dukes[1], and C. Bu[2],
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Introduction: Ground observations and observations of the MErcury Surface, Space ENvironment, GEochemistry, and Ranging (MESSENGER) Spacecraft of Mercury's exosphere have revealed a substantial variation in column densities of Na and K, ranging in values of 10^6-10^{12} atoms cm^{-2} and 10^4-10^9 atoms cm^{-2}, respectively [1,2]. Furthermore, a temporal and spatial-dependent variation in Na/K abundance ratios has been measured to fall within a significantly broad range of 22 to 400 [3,4]. For comparison, the lunar Na/K abundance ratio has been measured at ~6 [5]. The temperature fluctuations of the Hermean surface (ranging from 100-700K) may be an underlying motivator for mechanisms responsible for this exospheric variation in combination with ion irradiation [6].

Mercury's regolith surface experiences continuous radiation (photons, electrons, and ions) from the sun, where solar-wind ions (and electrons) are generally focused toward the high latitudes by the planetary magnetic field. Solar-ion irradiation has a multitude of effects, including compositional and optical changes in the regolith, with concurrent ejection of secondary ions and neutrals, along with backscattering of primary solar-wind ions.

In this work, we explore the thermal dependence of sputtering and mineral compositional change for vapor-deposited amorphous potassium on magnetite, relevant to Mercury's exospheric kinetics. We explore the effects of thermal diffusion and radiation-enhanced diffusion parameters of X-ray photoelectron spectroscopy (XPS) data for of potassium in magnetite, adsorbed on magnetite at multiple temperatures are modeled with the chemical physics simulation software Static /and Dynamic Trim for Sequential and Parallel computing (SDTrimSP) [7].

SDTrimSP is a static or dynamic target-updating Monte Carlo simulation software developed by W. Eckstein and collaborators the Max-Planck Institute for Plasma Physics to model ion irradiation effects on amorphous targets based on binary collision approximation [8]. By matching the starting composition of the XPS target with the simulated target and imposing the same sputtering parameters (incident ion energy, target temperature, etc), the diffusion input parameters of SDTrimSP can be varied until the output of the simulation matches the XPS data with reasonable fidelity. The set of diffusion parameters with the highest fidelity to the XPS data may yield insight on the dependence of regolith temperature on potassium sputtering from the Hermean surface.

Experimental Methods: XPS data was obtained of 4keV He^+ ions incident on a target consisting of a potassium monolayer adsorbed on a rough-cut magnetite (Fe_3O_4) sample at 110 K, 200 K, 300 K, and 400 K as seen in Figure 1 [9]. Note the small oxygen increase with fluence below 1E16 He^+ cm^{-2} , followed by the gradual increase of atomic composition, as well as the rapid decline in potassium at <$5x10^{15}$ ions/cm^2.

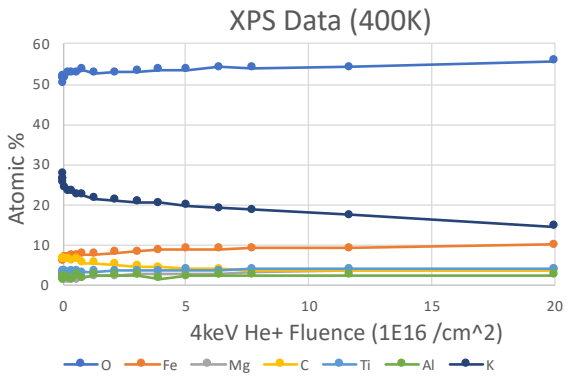

Figure 1: *Atomic percent composition as a function of fluence of XPS data*

To initially model the XPS data, the same target at 400K was replicated in SDTrimSP with 4 keV He^+ ions incident on the magnetite at similar flux/fluence parameters with no diffusion. After each simulation was conducted, the atomic composition of the surface-most 10nm was weighted using each photoelectron inelastic mean-free path (IMFP) to simulate the weighting observed in XPS data, which loses sensitivity with increasing photoelectron origin depth. Simulations are subsequently compared to the data in general trend of atomic composition. Discrepancies will be adjusted by variation in atomic surface binding energy and diffusion, where parameters will be gradually modified in sequential models, noting the shift in fidelity with the XPS data after each attempt. This process will be repeated until all diffusion parameters have been characterized, such that the simulation output resembles the XPS data for each temperature.

Results: Initial SDTrimSP simulations of the target irradiation at 400K yield promising likeness of trends to the XPS data.

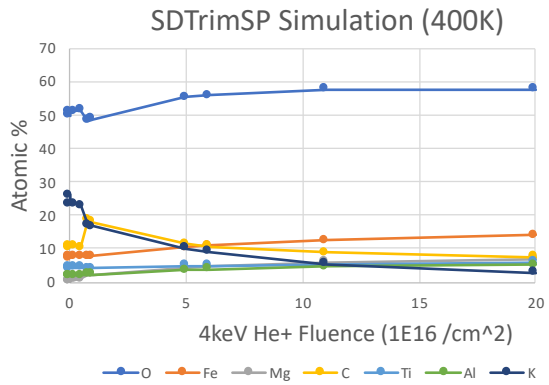

Figure 2: *Atomic percent composition as a function of fluence in SDTrimSP simulation*

As observed in the XPS data, the oxygen atomic composition displays a small feature in the < $1x10^{15}$ ions/cm^2 fluence range, followed by a gradual increase. More importantly, the potassium shows a highly sloped-decrease, followed by a more gradual reduction, although the minimum of potassium atomic composition occurs at much lower levels than seen in the XPS data, perhaps due to surface roughness effects. The effect of roughness will be investigated using SDTrimSP 2D. Iron, aluminum, and magnesium follow the XPS data with great fidelity, with deviation limited to <0.5% atomic composition at any fluence.

Discussion: While the potassium atomic composition trend exhibits general likeness between XPS data and the simulation, fidelity is limited by the extent through which the trend continues—potassium atomic composition in XPS observations is seen to reach equilibrium at fluences of ~$15x10^{15}$ ions/cm^2, whereas the SDTrimSP simulations continue decreasing beyond ~$5x10^{15}$ ions/cm^2. Since the simulations were conducted without diffusion parameters, effects such as thermal diffusion and radiation enhanced diffusion, or surface roughness, may therefore be the responsible mechanisms for differences between simulation and XPS measurements. Future simulations will independently vary both diffusion thermal and radiation enhanced diffusion in SDTrimSP simulations to identify to what extent either parameter is responsible for the limit of decline in XPS measurements, but not observed in simulation. Should these efforts prove successful, irradiation of adsorbed Ca and Na will then be analyzed in the same manner.

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