Modeling the Effect of Solar Ion Irradiation of Troilite with SDTrimSP – Implications for (16) Psyche. G.M. Minesinger[1], J.M. Christoph[2], C.A. Dukes[1], C. Bu[3], and L.T. Elkins-Tanton[2], [1]Laboratory for Astrophysics and Surface Physics, University of Virginia, Charlottesville, VA 22904 (gmm9uf or cdukes@virginia.edu), [2]School of Earth & Space Exploration, Arizona State University, Tempe, AZ 85287, [3]Astrophysics Laboratory, Columbia University, New York, NY 10027.

Introduction: The NASA Psyche mission, launching in 2022, will visit for the first time the Solar System's largest M-type asteroid, (16) Psyche [1,2]. Psyche resembles the exposed metallic core of a protoplanet after differentiation and impact loss of the silicate crust, though its precise geochemistry is unknown. Current models suggest a volumetric composition of predominately Fe-Ni metal (30 - 60%) with silicate and opaque materials, including troilite, comprising the remainder, given an average porosity of ~20% [2]. To infer the planetary geology of the surface, the Psyche mission will carry a gamma-ray and neutron spectrometer (GRNS) and dual visible-near infrared multispectral imagers. Due to its thin exosphere, Psyche is directly exposed to space weathering processes, such as solar-ion sputtering, resulting in ongoing surface changes that complicate mineralogical interpretation.

Troilite (FeS) is a sulfide expected to be found on Psyche, in conjunction with kamacite and taenite metal phases. Thus, to understand weathering effects on surfaces like Psyche, we have experimentally examined the chemical, optical, and morphological effects of solar ions on two polished thick sections of meteoritic troilite (Toluca and Canyon Diablo) with 1 keV hydrogen (H^+) and 4 keV helium (He^+) [3]. We detected depletion of sulfur over the course of irradiation using in-situ X-ray photoelectron spectroscopy (XPS). To better understand the depletion mechanism, here we simulated ion-induced physical sputtering with SDTrimSP 6.0, a 1D Monte Carlo simulation that uses the binary-collision approximation to model atomic-collision processes for projectiles incident on amorphous targets, both gaseous and condensed [4].

Experiment: Similar to Ziegler's SRIM [5], SDTrimSP can output ion ranges, sputtering yields, reflection coefficients, damage cascades, target composition as functions of depth or fluence, and specific target atom/molecule information such as: trajectories, energies, exit angles, vacancies, and displacements for comparison with measured parameters [6-8]. Additionally, SDTrimSP actively updates the target composition and includes thermal, pressure-driven and ion-enhanced diffusion, as well as carbon-based chemical sputtering that allow a more rigorous simulation of the ion-solid interaction.

Our experimental XPS spectra [3] can be used to tune various SDTrimSP models, which allowed us to investigate how surface binding energy (U_s) and diffusion affect the physical sputtering process.

SDTrimSP simulations were run at the flux of 1.8×10^{13} ions cm^{-2} s^{-1} to a fluence of 3.6×10^{18} ions cm^{-2} (average laboratory values). After preliminary studies, the simulated surface oxide composition was identified and modeled by 4 nm (Toluca) and 15 nm (Canyon Diablo) oxide layers for each sample, both atop 300 nm of troilite–deeper than the ion range. A thin layer (0.2 nm) of adventitious carbon was added on the very surface of the modeled samples, simulating the contamination due to atmosphere-exposure seen in highly surface-sensitive XPS spectra [9].

Results: Initial runs with kinetic sputtering alone could not reproduce the magnitude of XPS-measured sulfur depletion. Therefore, we evaluated how the surface binding energy (U_s) affects the FeS composition with ion irradiation by modifying the atom-specific parameters in SDTrimSP. We found that the target composition with irradiation was not strongly dependent on the U_s after independently (*isbv = 1*) varying U_s from 0 to 5 eV for sulfur and also by using a weighted average of U_s based on surface atomic fraction (*isbv = 2*) (Fig. 1). Negligible differences were observed between these model variations.

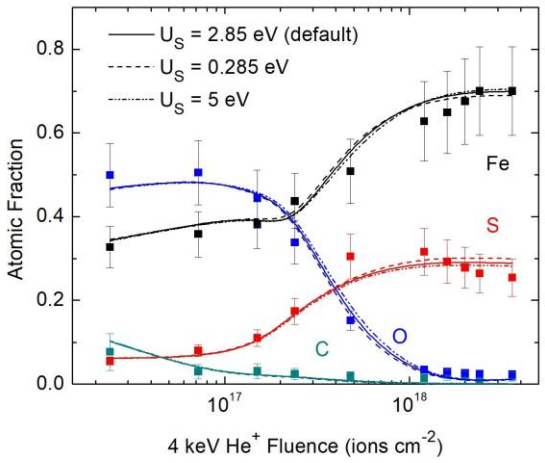

Fig. 1: The surface binding energy of sulfur (U_s) has minimal effect on the resulting compositional changes due to 4 keV He^+ irradiation of troilite in SDTrimSP. Points are XPS data [3], curve is model with isbv = 1.

The role of radiation-enhanced S-diffusion was investigated by enabling/disabling diffusion in SDTrimSP, then adjusting the diffusion coefficient for

sulfur. The inclusion of damage-driven diffusion in the model was critical to matching the experimental data, suggesting that ion-induced diffusion played a vital role in establishing S:Fe equilibrium values (Fig. 2).

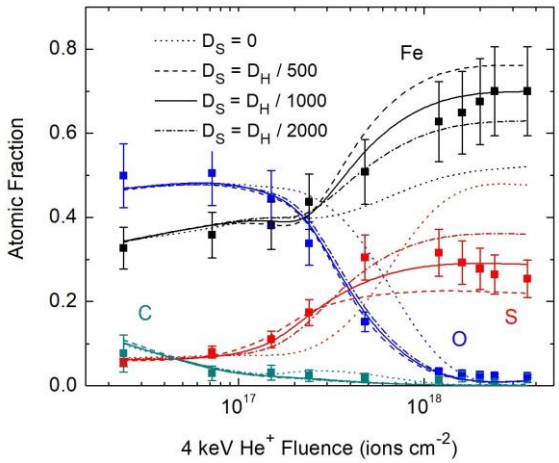

Fig. 2: Inclusion of ion-enhanced diffusion in SDTrimSP (curves) is critical to replicate the sulfur depletion in troilite after 4 keV He^+ irradiation measured by XPS [3].

No published values are available for sulfur diffusion through troilite. Thus, we extracted these values from SDTrimSP-XPS data best fits. Using order of magnitude estimations, we identified the optimal damage-driven sulfur diffusion coefficient as $\eta_T = 1.0 \times 10^3$ Å^4 per atom (Fig. 2), which implied a sulfur-diffusion coefficient through irradiated amorphous FeS to be approximately 7.6×10^{-22} cm^2 s^{-1} at 300K.

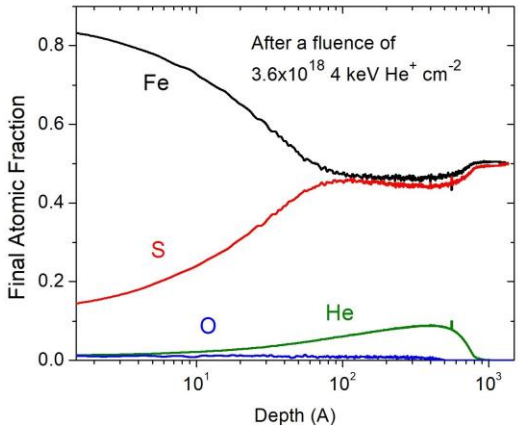

Fig. 3: SDTrimSP elemental distribution for troilite after 3.6 × 10^{18} He^+ cm^{-2} as a function of depth, with the implanted He.

The FeS altered layer–the region directly below the surface through the ion range–was inspected in the SDTrimSP simulation (Fig. 3). The resulting profile was well-matched to high-resolution transmission electron microscopy measurements of 4 keV He^+ irradiated synthetic FeS: significant Fe-enrichment at the irradiated troilite surface (2-3 nm) with S-depletion throughout the outermost ~10 nm [10]. Similar features were also identified in natural Itokawa FeS grains exposed to the solar-wind, with vesicles appearing throughout the damaged region to a depth of ~50 nm [11].

Using parameters deduced from the experiment-calibrated work, we modeled the solar-ion-induced sulfur depletion of troilite within Psyche's regolith. Simulations utilized a 4% He^+ and 96% H^+ solar ion flux of 2.38×10^7 ions cm^{-2} s^{-1}, similar to Psyche at 2.9 A.U. (Fig. 4). We estimate an exposure time of ~10^3 Earth-years is required for troilite on (16) Psyche to reach equilibrium sulfur depletion (S:Fe = 0.06).

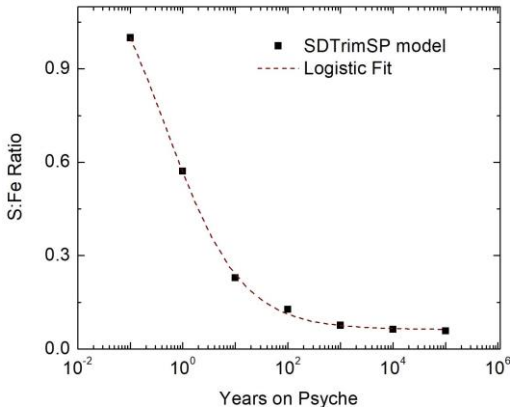

Fig. 4: SDTrimSP simulation shows sulfur-loss occurs rapidly on (16) Psyche with exposure to solar-wind ions, reaching equilibrium in ~10^3 (Earth-) years.

Conclusion: SDTrimSP is a useful modeling tool, as it quantitatively confirmed XPS-detected ion-induced sulfur depletion of troilite, and allowed predictions for Psyche's regolith. SDTrimSP can thus be used to predict the impact of solar-ion irradiation on regolith materials of other airless planetary bodies, and may be beneficial for further investigations of space weathering impacts.

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References: [1] D. Y. Oh et al. (2017), *Development of the Psyche Mission for NASA's Discovery Program*. [2] L.T. Elkins-Tanton et al. (2020), *JGR* 125, e2019JE006296. [3] J.M. Christoph et al. (2021), 52th LPSC. [4] A. Mutzke et al.(2019), *SDTrimSP Version 6.00 IPP 02/19 Garching.* [5] J.F. Ziegler et al. (2010), *NIM* B268, 1818. [6] P.S. Szabo (2020). *Astrophys. J* 891, 100. [7] R. Stadlmayr (2018). *NIM B430*, 42-46. [8] K. Wittmaack & A. Mutzke (2017). *J. Appl. Phys.* 121. [9] S. Sinha & M. Mukherjee (2018). *Vacuum v.* 148, 48-53. [10] L. P. Keller et al. (2013), LPSC44 #1719. [11] Matsumoto (2018). *The Meteoritical Society LXXXI* Abstract #6096.