3D-SIMULATIONS OF SPUTTERING AND ION REFLECTION FROM REGOLITH SURFACES.

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Introduction: Ion fluxes from the solar wind and from planetary atmospheres represent a key component of the space weathering of airless bodies [1]. The energy deposition of ion impacts on a planetary surface contributes to exospheres of Mercury and the Moon [2], to the formation of nanophase Fe or to the amorphization of near-surface layers [3]. Furthermore, the implantation of volatiles by impinging ions [4], as well as ion scattering from the surface have recently also been of interest [5,6]. Due to impact-angle dependencies and possible shadowing, most of these phenomena are affected by the surface roughness. In this context, the grain-like regolith created by prolonged weathering of planetary bodies represents a stark contrast to an ideally flat surface. To improve our understanding of space weathering, more investigation of the ions' interaction with the regolith is required. While models of the sputtering of regolith have been formulated [7], recently developed 3D codes allow an extended simulation of the interaction between ions and planetary regolith [8]. We therefore employ a regolith model in SDTrimSP-3D and present first simulation results regarding sputtering and ion reflection for the interaction with solar wind ions.

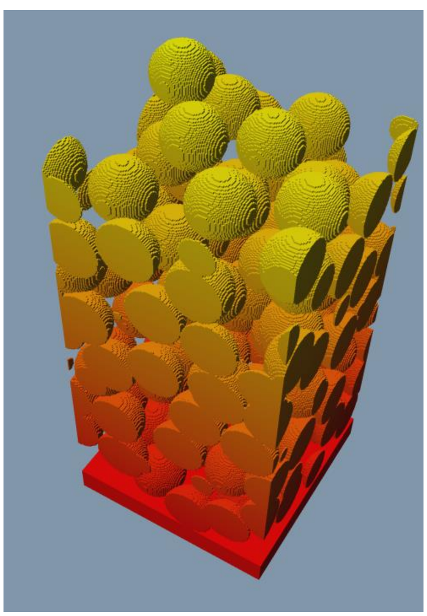

Figure 1: An example for the regolith input used in SDTrimSP simulations. Spheres appear cut off due to the periodic boundary conditions of the simulation cell.

Regolith Model in SDTrimSP-3D: SDTrimSP-3D is an expansion of SDTrimSP, a program that simulates the interaction of ions with a solid based on the Binary Collision Approximation (BCA). Within the BCA, this process is treated as a sequence of scattering events between two atoms. All projectile ions and recoil atoms are followed through the solid until they are either stopped or leave the solid again. With material properties from tabulated inputs, quantities such as ion ranges, reflection coefficients or sputtering yields can be computed. SDTrimSP furthermore allows dynamic simulations of target changes under ion irradiation. SDTrimSP-3D combines these capabilities with a cubic cell structure to simulate a three-dimensional surface morphology. For this first simulation, we implement a regolith structure in SDTrimSP-3D by approximating the grains as spheres of equal size. This model allows a full simulation of the sputtering process, including redeposition of sputtered atoms at other grains or multiple impacts by locally reflected ions. The spatial distribution of the grains is determined by an algorithm similar to the method used by Kulchitsky et al. [9]: Grains are dropped into a box under the influence of gravity and variable cohesive sticking leads to different porosities of the final structures. An example for a regolith target used in an SDTrimSP-3D simulation is presented in Figure 1.

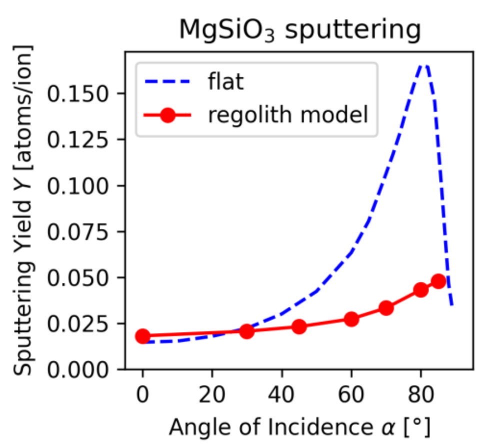

Figure 2: Total sputtering yields of enstatite ($MgSiO_3$) under 1 keV H irradiation. Simulation results for a flat surface from SDTrimSP-1D (blue) are compared to regolith model results from SDTrimSP-3D (red).

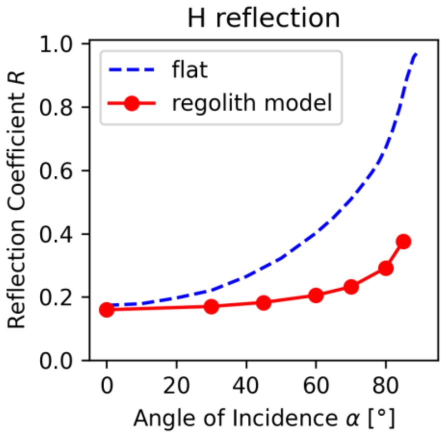

Figure 3: H reflection coefficients from 1 keV H irradiations of enstatite ($MgSiO_3$). Reflection from regolith (red) decreases for non-normal incidence angles compared to a flat surface (blue).

Simulation Results: Using the spherical regolith model, the irradiation of enstatite ($MgSiO_3$) by 1 keV H ions was simulated under different angles of incidence. Figure 2 compares the total sputtering yields from SDTrimSP-3D (averaged from about 20 different regolith target setups) to the angular dependence for a flat surface from SDTrimSP-1D. Regolith sputtering yields are slightly increased under quasi-normal incidence ($\alpha < 30°$), but significantly decreased under oblique incidence ($\alpha > 30°$). Such behaviors are commonly observed for rough surfaces due to varying local incidence angles and redeposition of sputtered material at other surface features [10, 11]. However, this result differs from the model of Cassidy and Johnson [7], where a decrease would also be predicted for normal incidence. For the H reflection coefficients of 1 keV H irradiation of $MgSiO_3$, which are depicted in Figure 3, the pronounced angular dependence of the flat sample is suppressed for the regolith structure. Instead, a decrease to the normal incidence reflection coefficient of a flat surface at about 20% is observed for the majority of impact angles. This is in very good agreement with observations of reflected neutral solar wind hydrogen from planetary regolith: For example, a solar wind H neutral reflection coefficient of 0.16 ± 0.05 was deduced from Chandrayaan-1 measurements [6].

Discussion: The regolith simulations with SDTrimSP-3D can reproduce spacecraft measurements of reflection coefficients, which supports the validity of the presented approach. Substantial decreases in sputtering yield and reflection coefficients, as they have been observed for other very rough or porous structures [12], are not found for regolith. Instead, a significant part of the ion-surface interaction occurs at the uppermost part of the regolith. As the exact form of regolith grains will influence the interaction with incoming ions, the presented observations will further be tested with simulations of different non-spherical grain shapes and varying grain sizes, as well as considering varying solar wind energies.

References: [1] Hapke B. (2001) *JGR: Planets, 106*, 10039-10073. [2] Wurz P. et. al. (2007) *Icarus, 191*, 486-496. [3] Poppe A.R., Farrell W.M., Halekas J.S. (2017) *JGR: Planets, 123,* 37-46. [4] Lucey P.G. et. al. (2021) *Geochemistry*, 125858. [5] Wieser M. et al. (2009) *Planet. Space Sci.*, *57*, 2132-2134. [6] Vorburger A. et. al. (2013), *JGR: Space Phys.*, *118,* 3937-3945. [7] Cassidy T.A., Johnson R.E. (2005) *Icarus*, *176,* 499-507. [8] Von Toussaint U., Mutzke A., Manhard A. (2017) *Phys. Scr.*, *2017,* 014056. [9] Kulchitsky A.V. et. al. (2018) *JGR: Planets, 123,* 972-981. [10] Küstner M. et. al. (1999) *J. Nucl. Mater. 265*, 22-27. [11] Cupak C. et. al. (2021) *Appl. Surf. Sci.*, *570*, 151204. [12] Li Y. et. al. (2016) *Nucl. Fusion*, *57,* 016038.