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Modeling Limits of BCA for Sputtering Regolith

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Angular distributions of sputtered ejecta are critical inputs for simulating regolith sputtering on airless bodies, where surface topography and porosity determine if particles escape or redeposit. We present new analysis and simulations demonstrating that, although current binary collision approximation (BCA) frameworks can reliably predict either total sputter yields or angular distributions for minerals, they cannot reproduce both simultaneously. This is a limitation with direct implications for exosphere and surface-evolution models that require realistic, three-dimensional ejecta plumes. Using SDTrimSP[1] for flat targets, SPRAY[2] for AFM-resolved rough surfaces, and SDTrimSP-3D[3] for porous regolith analogs, we quantify how morphology and binding energies control plume tilt and shape via a dedicated three-dimensional lobe-fitting approach designed for full-plume implementation in modeling tools. This framework addresses the need to move beyond simplified cosine laws and to incorporate azimuthal structure when propagating sputtered particles in regolith and exosphere simulations.

Across surface morphologies, rough and porous targets deflect ejecta toward the surface normal, reducing the strongly forward-facing plumes typical of flat surfaces and introducing geometry-mediated effects such as shadowing and redeposition that reshape both yield and energy distributions. In this regime, we find a robust tradeoff between reproducing sputter yield and plume tilt: the "compound/hybrid" binding-energy model[4] capable of matching experimental mineral yields[5] fails to reproduce the experimentally observed forward tilt at oblique incidence on flat and, more significantly, on rough surfaces (Fig. 1). Conversely, adopting increased surface-binding energies (SBEs) informed by recent molecular dynamics work[6] strengthens the forward tilt and better matches rough-surface angular data but underestimates absolute mass yields by factors of 3–4.

Figure 1: Model–data comparison of sputter yields and angular distributions for $MgSiO_3$ under 4 keV He irradiation. ***Left****: SDTrimSP model yields that result from the Jäggi et al. (2023) hybrid binding energy model (HB-C, blue dashed) with the increased surface-binding case (SB-C) based on Morrissey et al. (2024) surface binding energies, compared to the Biber et al. (2022) laboratory measurements (black, with 2 SD errors).* ***Center****: Normalized mass yield polar distributions from a flat surface at an incidence angle α_{in} = 60° for said simulations.* ***Right:*** *Analogous to the center figure, but for a rough pellet surface.*

Methodologically, we map flat-surface SDTrimSP ejecta to measured roughness via ray tracing in SPRAY and construct porous regolith stacks in SDTrimSP-3D, then fit the resulting plumes with a single- or tri-lobe model that captures central and side "winglet" components associated with single-collision recoils (Fig. 2). This procedure allows for consistent comparison to laboratory angular data

and direct use of fitted plumes in forward models. For rough surfaces, the simulations confirm a forward tilt relative to the sample surface normal but with magnitudes that depend sensitively on the binding-energy scheme. Only the higher-SBE case reproduces the observed forward-tilted distributions. For porous targets, preliminary comparisons and prior 3D simulations indicate stronger backscattering, further emphasizing the need for morphology-aware angular inputs in regolith sputtering models.

*Figure 2: Comparison of O sputter ejecta distributions sputtered from a rough surface (SPRAY) by 4 keV He at an incidence angle of α_{in} = 75° from the surface normal (black arrow) resulting from (**left**) the Jäggi et al. (2023) hybrid binding energy (HB) model and from (**right**) a surface binding energy (SB) model with increased binding energies from Morrissey et al. (2024), fitted by a central plume (blue) and two forward-facing "winglet" plumes (red).*

These findings have two key implications. First, exosphere and regolith models should incorporate full 3D angular distributions rather than rely on simple cosine laws, especially for rough and porous substrates where plume tilt and azimuthal structure are non-negligible. Second, the inability to match yield and angle concurrently suggests missing physics in BCA implementations—most notably, yield-enhancing processes such as molecule and cluster sputtering that are not represented in single-atom BCA ejecta—and cautions against parameter tuning. In practice, our results recommend using binding-energy models that best reproduce angular distributions when plume directionality controls transport and redeposition, while acknowledging that total yields must then be corrected for non-BCA processes if absolute source strengths are required.

In summary, angular distribution data are indispensable for realistic regolith sputtering simulations, yet existing BCA parameterizations cannot simultaneously reproduce experimental mass yields and angular distributions across flat, rough, and porous mineral surfaces. This demonstrates a fundamental limitation of current BCA-based models for planetary surfaces and motivates hybrid or extended frameworks that incorporate missing yield mechanisms while retaining accurate, morphology-dependent plume geometry.

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