Surface Sputtering by Ion Irradiation: Benchmarking Binary Collision Approximation and Molecular Dynamics Models to Laboratory Measurements

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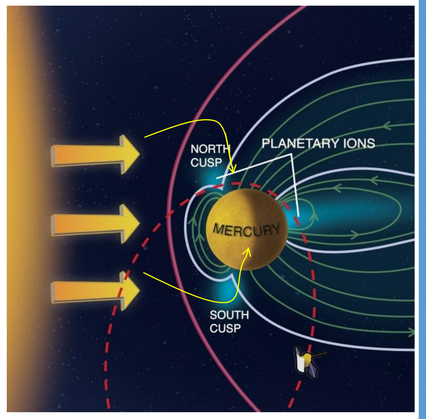
Background: Planetary Science Motivation

- Sun emits stream of charged particles known as Solar wind
- Solar wind comprised of ~95% H^+, ~5% He^{++}
- Energy between ~0.1 – 10keV – can potentially lead to surface sputtering
- Ion sputtering contributes to Hermean exosphere
- Reliable sputtering data is needed



Knowledge Gap

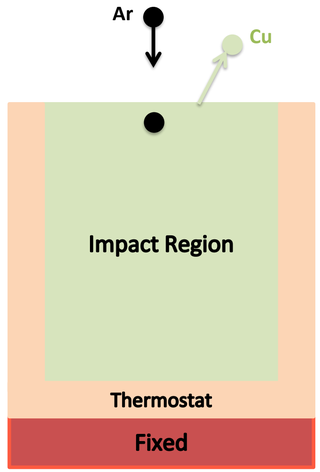
- Lab work is complex and expensive – theoretical models needed
- Binary Collision approximation (BCA) often used
  - User defined surface binding energy (not well understood)
  - Ignores many-body effects
- In contrast Molecular Dynamics (MD) models all interactions during cascade
  - Includes chemical and thermal effects
  - Surface binding energy computed directly
  - Accounts for damage and crystallinity
  - Limited research comparing to experimental

Purpose: Before models can be used to simulate planetary surface impacts, they should be verified by comparison to pre-existing experimental values.

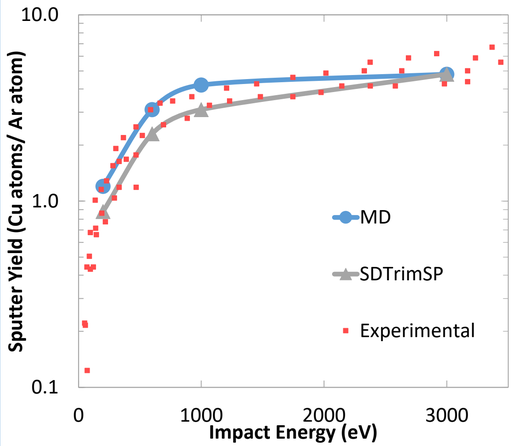
We compare predicted sputtering yield and energy distributions from BCA and MD to experimental results for Ar on Cu impacts

Methodology

- Cu impacted by Ar at normal incidence using MD and BCA methods
- Impact energy between 200-1000eV
- MD simulations use hybrid interatomic potential

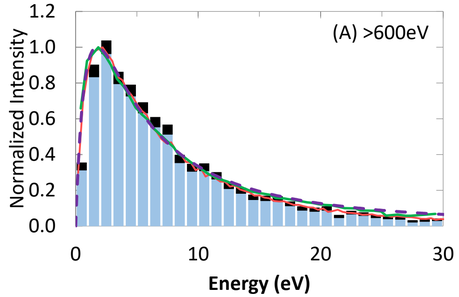


Results: Sputtered particle energy distribution

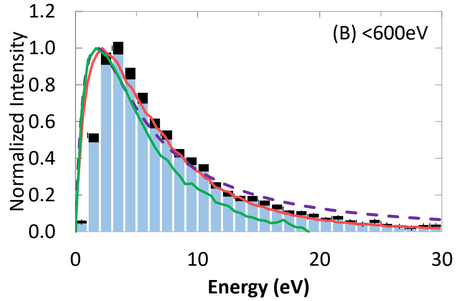


- SDTrimSP and MD agree with experimental range
- SDTrimSP consistently lower than MD

Results: Sputtered particle energy distribution



- Good agreement with experiment and BCA/MD models



- Experiment narrows
- Good agreement between SDTrimSP and MD

MD results normalized to 1 (**+/- error**), Experimental results, SDTrimSP Thompson Distribution

Implications and Conclusions:

- Low energy collisions do not become isotropic – error in Thompson
- MD/SDTrimSP in better agreement but still discrepant
- Experimental results sample only normal emission – system issue?
- Previous studies have shown dependence on angle of emission
- For oblique emission angles peak shifts and distribution broadens
- MESSENGER FIPS data has shown H^+ impacts on Mercury across low and high energies
- MD and SDTrimSP can be used to simulate SW impacts with complex Hermean surface