SDTrimSP Simulations of Solar Wind Sputtering on Mercury: A Sensitivity Study to Establish a Best-Practice

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Background: Solar Wind on the Surface of Mercury

- Sun emits stream of charged particles
- Solar wind (SW) comprised of ~95% H+
- SW sputtering is a potentially important source of Mercury's exosphere
- Most common models use binary collision approximation (SDTrimSP)
- SDTrimSP has many user-specific inputs that are not consistent across previous SW studies[1,2,3]
- Reliable sputtering methods are needed for accurate models for Mercury's surface

Methodology:

Purpose: We have conducted a detailed sensitivity study into SDTrimSP parameters to produce a best-practice for simulating SW impacts onto Mercury's surface.

- Within SDTrimSP we will focus on several important user-specified parameters:
  - Oxygen surface binding energy
  - ISBV (method of dealing with compound SBE)
  - Static vs. Dynamic Simulations
  - 1 keV/amu protons vs. capturing impact energy distribution
  - 90-degree (normal) impacts vs. cosine angular distribution of impacts
- Simulated H+ impacts onto anorthite
- Focused on constraining oxygen SBE due to high overall abundance
- Quantify the effect of each parameter on overall yield, elemental yield, and surface composition

Results:

1. Effect of SBE on Sputtering Yield

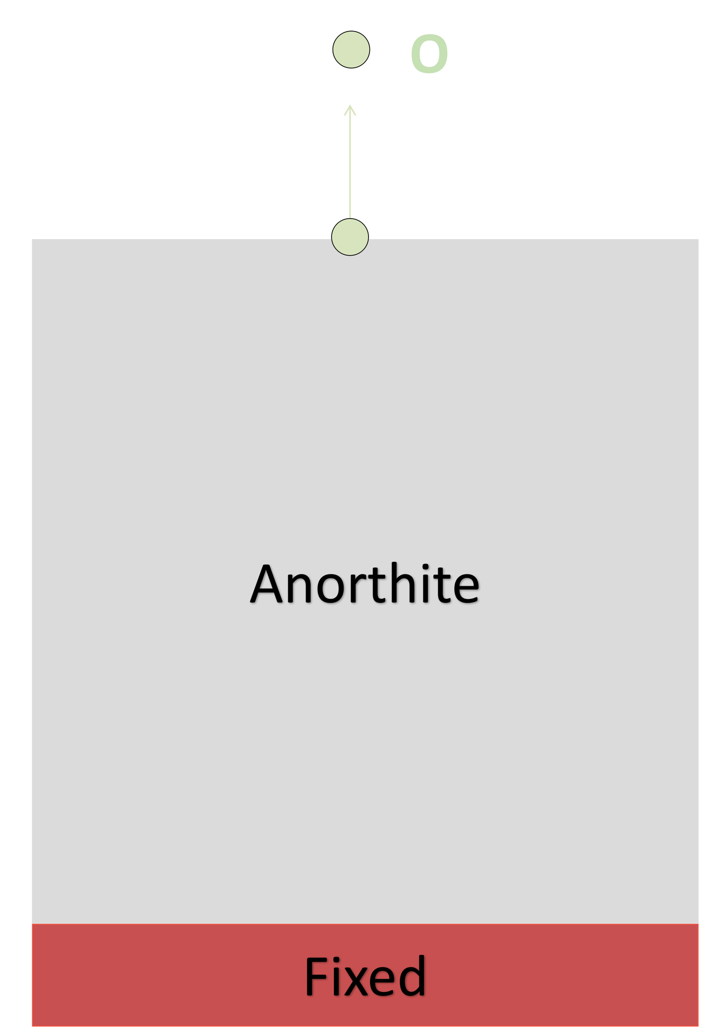
Elemental Yield (10-3 atoms/ion) (ISBV = 1)				
	Static			
	Oxygen SBE			
Anorthite Comp.	1	2.6	6.5	8.3
Al	1.2	1.3	1.2	1.2
Ca	3.3	3.3	3.1	3.2
Si	1.6	1.5	1.6	1.5
O	52.0	17.1	5.0	3.7
Overall	58.1	23.2	10.9	9.6
O yield proportion	89.6%	73.9%	46.0%	38.5%

- Previous studies recommend O SBE between 1-6.5 eV based on experimental fits to other silicates
- Overall and O yields strongly dependent on SBE
- Properly constraining SBE key to realistic results

Results:

2. Quantifying Anorthite SBE via Molecular Dynamics (MD)

- SBE typically derived from fitting SDTrimSP yield to experiment
- MD simulations used to find SBE of O from anorthite surface
- Iterative approach with a reactive potential used to find minimum energy needed to remove a surface O atom
- O SBE of 8.3 eV from anorthite – higher than fit for wollastonite (6.5eV)[2]
- MD quantified value significantly higher than SDTrimSP recommended value (1 eV)[1]



Results:

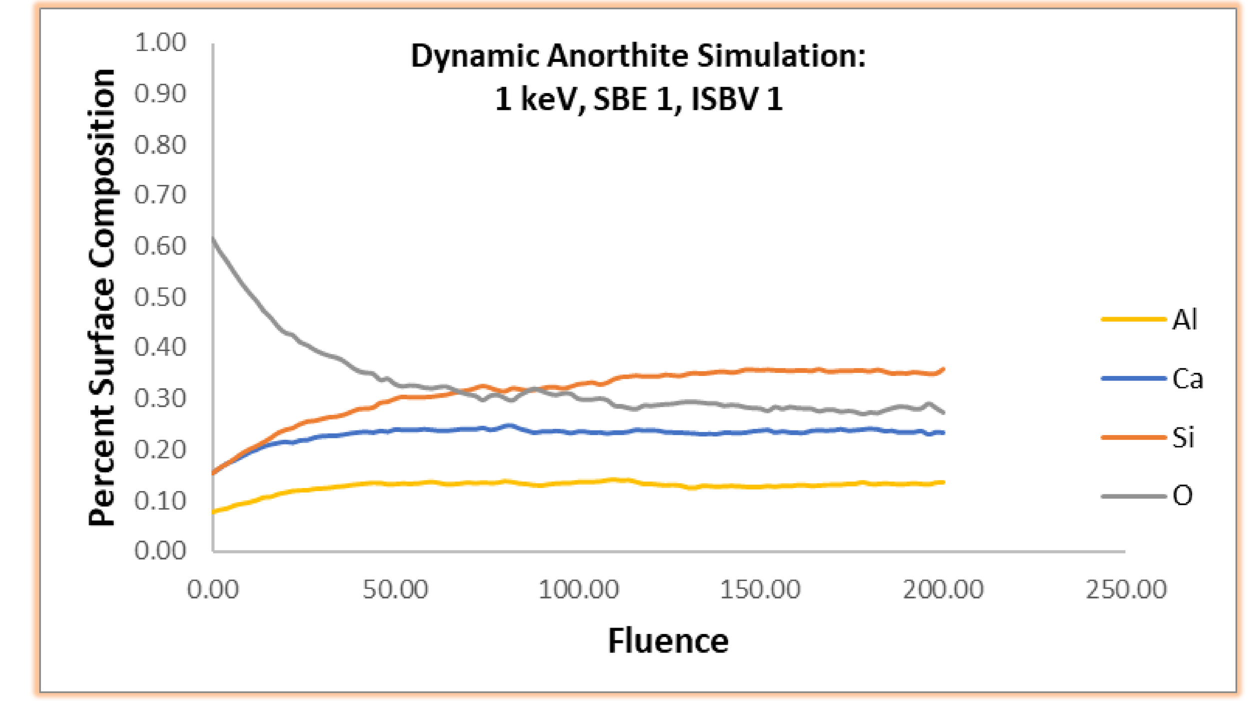
3. Mineral Specific O Surface Binding Energies-Dynamic

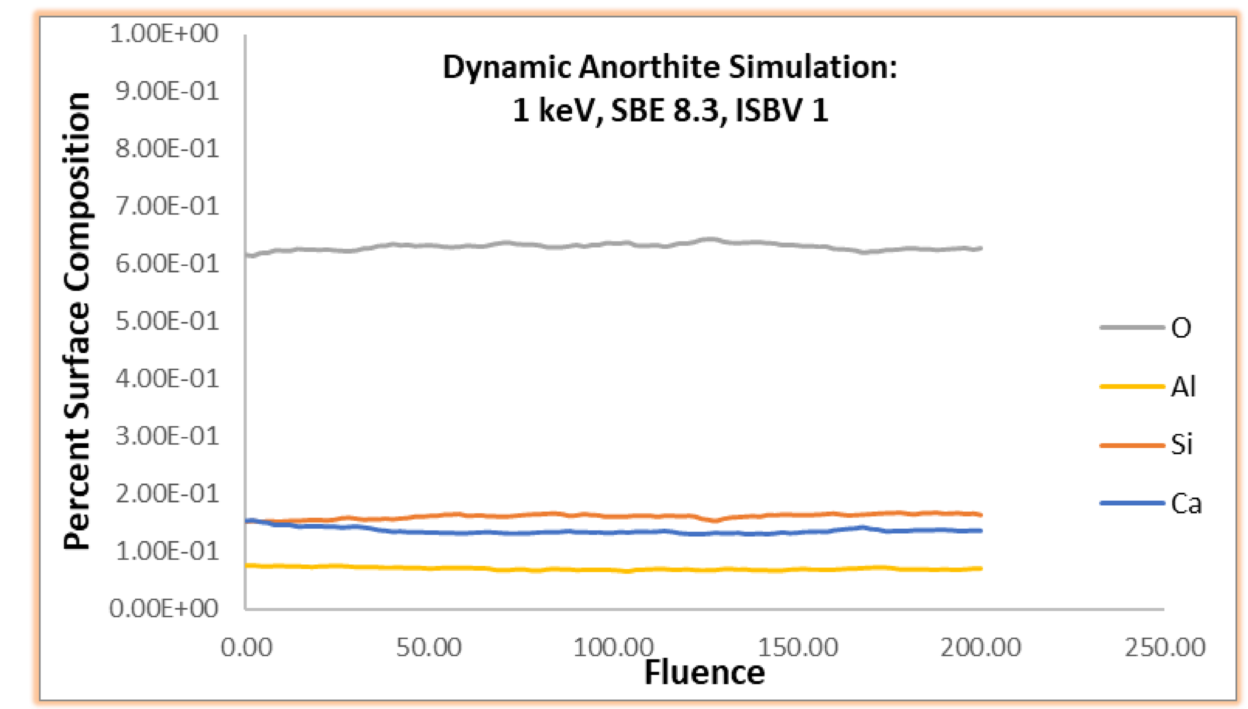
Elemental Yield (10-3 atoms/ion) (ISBV = 1)				
	Dynamic			
	Oxygen SBE			
Anorthite Comp.	1	2.6	6.5	8.3
Al	2.0	1.6	1.2	1.1
Ca	4.8	3.9	2.9	2.8
Si	3.1	2.6	1.8	1.7
O	17.1	11.8	5.1	3.9
Overall	26.9	19.8	10.9	9.5
O yield proportion	63.5%	59.6%	46.5%	41.1%

- Dynamic simulations allow composition to change with fluence
- Previous results suggest static vs dynamic not important[2]
- At low O SBE large difference between static and dynamic results
- For dynamic simulations, all element yields depend on O SBE

Results:

4. Effect of SBE on Surface Composition





- Dynamic simulation results visualize the direct correlation between surface composition and SBE
- At low SBE there are large surface composition changes with fluence
- At higher SBEs limited change in percent surface composition
- SBE parameter did not influence damage production

Conclusions and Best Practice Recommendations:

- SDTrimSP simulations of SW sputtering are highly dependent on input parameters
- Important to consider the overall yield, elemental yield, and surface composition
- We demonstrate the large importance of SBE and static vs. dynamic simulations
- We have used MD to quantify the O SBE from anorthite – mineral specific
- Based on these findings we recommend the following:
  - O SBE of 8.3eV
  - ISBV 1
  - Dynamic simulations
- Future work will consider other parameters, the formation of damage