Simulating Solar-Wind-Ion Sputtering of Sodium from Silicate Minerals: The Importance of the Surface Binding Energy L.S. Morrissey[1], O.J. Tucker[2], R.M. Killen[2], S. Nakhla[1], D.W. Savin[3], ([1]Memorial University of Newfoundland *A1C 5S7, St. John's, Newfoundland Labrador, Canada,* [2] NASA Goddard Space Flight Center Greenbelt, Maryland, 20771, United States, [3] Columbia Astrophysics Laboratory, Columbia University, New York, New York, 10027, United States)

Introduction: Na and He are the most abundant confirmed neutral species in Mercury's exosphere. Whereas the source of He is from the solar wind (SW) itself, the source of the Na is potentially due to sputtering from silicates on the Hermean surface (1, 2). As SW ions impact the surface, they deposit energy, leading to sputtered atoms both from the surface and within the substrate (3, 4). The sputter yield and angular and energy distributions of the sputtered atoms depends on the energy of the incoming SW and the composition of the surface being impacted. Understanding the role SW ions play on surface sputtering of Mercury is critical to any exosphere model.

The most common sputtering models use the binary collision approximation (BCA) and thus consider sputtering to be a result of binary collision cascades (5). These models can be used to predict the energy distribution and yield of sputtered atoms as a function of incoming ion type, energy, and angle, with only modest computational requirements. A fundamental physical parameter for BCA models is the surface binding energy (SBE) of atoms in the substrate (6, 7). The SBE is a user defined value in SDTrimSP (8), a BCA sputtering simulation tool, and in the commonly referenced Thompson energy distribution of the sputtered atoms (9). Despite the clear importance of the SBE in simulating sputtering, its actual value is not well understood for many substrates. For single component substrates the SBE is often approximated as the heat of sublimation for the atoms in the substrate (10). However, previous research has suggested that this approach can underestimate the SBE by 20-40% (7). More importantly for planetary science, there is no universal approach to estimating the SBE for multicomponent substrates. This uncertainty is particularly enhanced for sputtering of Na. On the low end, Leblanc and Johnson (11) suggested a value of 0.27 eV based on sulfate data. SDTrimSP recommends using the pure heat of sublimation of each atomic species to predict the SBE for sputtering from a compound, 1.1 eV (8). However, this approach assumes that the SBE is independent of the bonds formed with the other atoms within the substrate In contrast, Lammer et al. (12) predict a value between 2-2.65 eV but note that this is not well determined due to a lack of experimental data. Given that BCA methods rely on a user defined SBE, this can be a significant source of error for sputtering predictions from complex substrates.

To address this issue, we have performed molecular dynamics (MD) simulations to better constrain the SBE of Na from silicates. We then consider the effect these modified inputs have on predicted yield and energy distributions of sputtered Na due to SW impacts.

Methods: MD simulations were conducted to better constrain the SBE of Na on the surface of a crystalline Na_2SiO_3 silicate substrate. In each case a Na atom in the substrate was given a specific amount of energy and its subsequent position and remaining energy was tracked as a function of time. An iterative method was used to determine the minimum energy needed to remove one Na atom completely from the substrate. Simulations were conducted using a many-body reactive potential (ReaxFF) that was previously shown to be suitable for a variety of sodium silicate crystals and glasses (13).

BCA models were then used to determine how this modified SBE value affected the predicted yield and energy distribution of sputtered Na. First, the commonly referenced Thompson distribution was used to determine the energy distribution as a function of SBE as per equation 1:

$$J(E) = C\frac{E}{(E+E_b)^3}\left\{1-\left[\frac{(E+E_b)}{E_{max}}\right]^{1/2}\right\}. \quad (1)$$

Here C is a normalization constant, E is incoming ion energy, E_{max} is the maximum energy that can be transferred in a binary collision and E_b is the SBE of the substrate. The peak in this distribution corresponds to half the SBE. We also used SDTrimSP to calculate the sputtering yield and energy distribution for a series of ion and Na-bearing target combinations. To capture the most common components of the SW, 1 keV H^+ and He^{2+} impacts were simulated on a Na_2SiO_3 substrate.

Results: Results from MD simulations determined an SBE of 4.1 eV for Na from the silicate surface. This was confirmed for 5 different Na atoms located on the substrate surface. In contrast, the individual cohesive energy of pure Na is only 1.1 eV. Therefore, SBEs from a compound can be drastically different than their atomistic cohesive energies. The SBE of a specific atom is instead a function of the compound in which the atom is bound.

The newly predicted Na SBE value was then used to determine the sputtering yield and energy distribution of the sputtered atoms using SDTrimSP and the Thompson energy distribution. We find that increasing the SBE from 0.27 to 4.1 eV had a significant effect on predicted energy distribution (Fig. 1). For example, increasing the SBE from 0.27 to 4.1 eV broadened the sputtered atom energy distribution and lead to an increase in the peak energy by a factor of over 15. Therefore, the characteristics of sputtered atoms are highly dependent on the SBE used for the simulations. Yield results from SDTrimSP will also be presented. Overall, this study highlights the large range of suggested SBE values and demonstrates the potential of MD to better understand and constrain these values, though laboratory measurements are still needed to benchmark these calculations. In summary, an accurate SBE is critical to obtaining realistic models of SW sputtering into the Hermean exosphere.

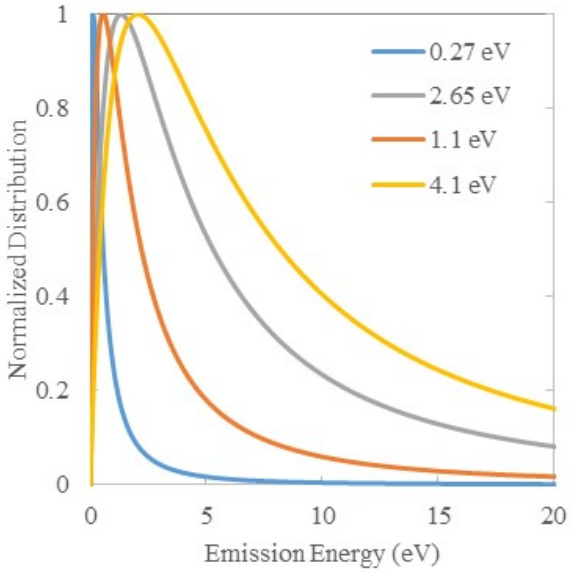

Fig 1. Energy distribution of sputtered Na atoms as a function of SBE, normalized at the peak for each distribution.

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