



## Simulating Solar-Wind-Ion Sputtering of Sodium from Mercury's Surface: The Importance of the Surface Binding Energy

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**Introduction:** Na, Ar and He are some of the most abundant confirmed neutral species in Mercury's exosphere. Whereas the source of He is from the solar wind (SW), 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 from the substrate (3, 4). The yield and energy distributions of the sputtered atoms depends on the energy of the impacting ions and the composition of the impacted surface. Understanding the role SW ions play on surface sputtering of Mercury is critical to any exosphere model (3).

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 impacting angle. 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, 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 substrate atoms (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 where the Na is likely bonded to other atomic species. SDTrimSP recommends using the pure heat of sublimation of each atomic species as the SBE for sputtering from a compound, which is 1.1 eV for Na (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.

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 the predicted yield and energy distributions of sputtered Na due to SW impacts.

**Methods:** MD simulations were conducted to determine the SBE of Na for various crystalline silicates: sodium metasilicate ( $\text{Na}_2\text{SiO}_3$ ), sodium orthosilicate ( $\text{Na}_4\text{SiO}_4$ ), and albite ( $\text{NaAlSi}_3\text{O}_8$ ). An iterative method was used to determine the minimum energy needed to remove one Na atom completely from the substrate surface. Simulations were conducted using a many-body reactive potential that was previously shown to be suitable for a variety of sodium silicate crystals (13).

BCA models were then used to determine how the resulting SBE values affected the predicted yield and energy distribution of sputtered Na. The commonly referenced Thompson distribution was used to determine the energy distribution vs. SBE. SDTrimSP was used to calculate the sputtering yield of Na vs. SBE. To capture the most common components of the SW, 1 keV  $\text{H}^+$  and  $\text{He}^{2+}$  impacts were simulated on sodium silicate surfaces.

**Results:** The MD simulations yielded a range of SBEs from sodium silicates: 2.6 eV for sodium orthosilicate, 4.4 eV for sodium metasilicate, and 7.9 eV for albite. 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. These results show that the SBE of a specific atom is a function of the compound in which the atom is bound.

The newly predicted Na SBE values were 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 1.1 to 7.9 eV had a significant effect on predicted energy distribution (Fig. 1). Therefore, the characteristics of sputtered atoms are highly dependent on the SBE used for the simulations. Similarly, the Na yield from albite was highly dependent on the Na SBE (Fig. 2). For example, the Na yield from albite for a 1keV H impact decreased by a factor of almost 15 when the SBE was increased from 1.1 eV to the SBE for Na from albite (7.9 eV). Overall, this study demonstrates that the SBE within in a compound can be significantly different than the monatomic cohesive energy. The results demonstrate 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 contribution to the Hermean exosphere.

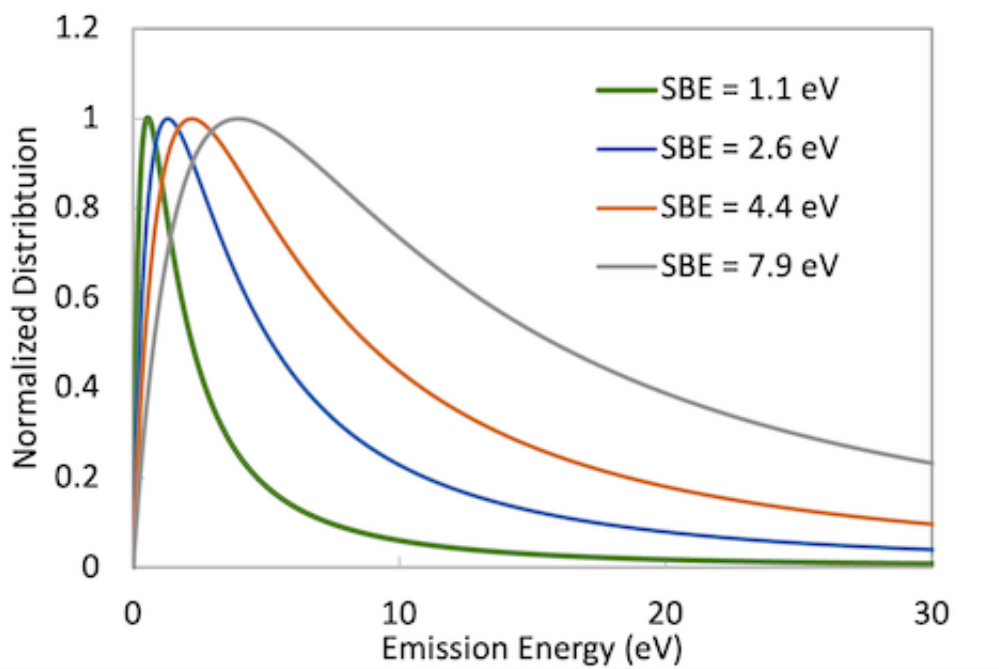


Fig 1. Normalized Energy distribution of sputtered Na atoms as a function of SBE

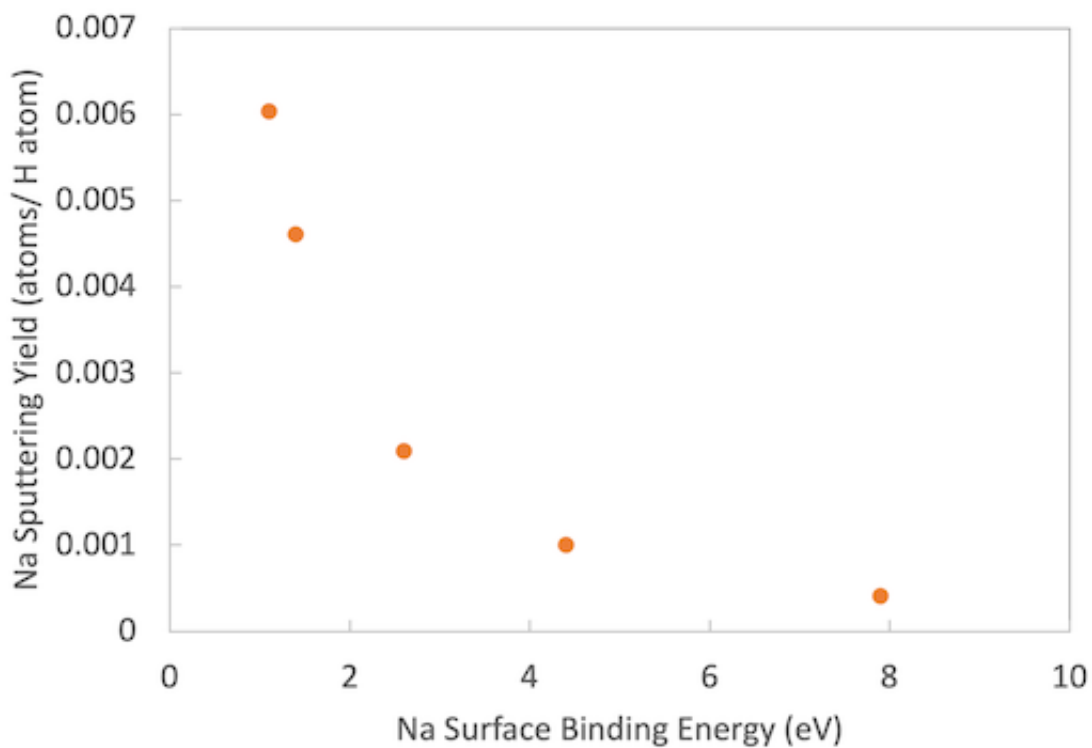


Fig 2. Sodium sputtering yield as a function of surface binding energy

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