Comment on "Molecule Formation During Sputtering by Two-Body Associative Ionization with Diabatic Curve Crossing"

A model for the formation of excited molecular ions has recently been proposed by Snowdon, Heiland, and Taglauer.[1] Experimental evidence for the model is presented with the identification of N_2^+ molecular emission in the wavelength range 400–430 nm, observed during the bombardment of Si by 0.5 to 6 keV N_2^+. The purpose of this Comment is to demonstrate that these spectral features are those from the SiN $B^2\Sigma$-$X^2\Sigma$ system.

We have bombarded intrinsic, p-type and n-type single crystals of Si with 7 keV N_2^+ under UHV conditions and have observed the photon emission. The spectrum observed was similar to that shown by Snowdon, Heiland, and Taglauer.[1] Spectral features observed in the region 400–430 nm, during the bombardment of intrinsic Si are shown in Fig. 1. Prominent peaks are at 411.7 ± 0.2, 414.2 ± 0.2, and 417.2 ± 0.3 nm. Identical spectra were also observed from the other Si targets.

These peaks are compared in Fig. 1 with known band heads for the red degraded SiN $B^2\Sigma - X^2\Sigma$ system[2] (incorrectly designated the $A^2\Sigma - X^2\Sigma$ system in Ref. 2) and show an excellent correspondence for the (0,0), (1,1), and (2,2) vibrational transitions. SiN is one of the ejected species expected because of the high count rate measured for the SiN^+ secondary ions. The intensity distribution and band degradation show excellent agreement with that found previously[3] for SiN bands excited in a *high-frequency discharge* despite the fact that the rotational features were not resolved in our experiment with an instrument resolution of 0.4 nm. When we bombarded Ge with N_2^+ under identical conditions, no emission bands in the range 370–430 nm were observed. This negative result further supports our identification of the spectral features shown in Fig. 1 as belonging to the SiN $B^2\Sigma - X^2\Sigma$ system.

Snowdon, Heiland, and Taglauer[1] have preferred to identify their tabulated features with selected high rotational states of the N_2^+ vibrational spectrum which is also shown in Fig. 1. Their model of N_2^+ formation results from an electron-loss mechanism which takes place no more than 0.5 nm from the surface. However,

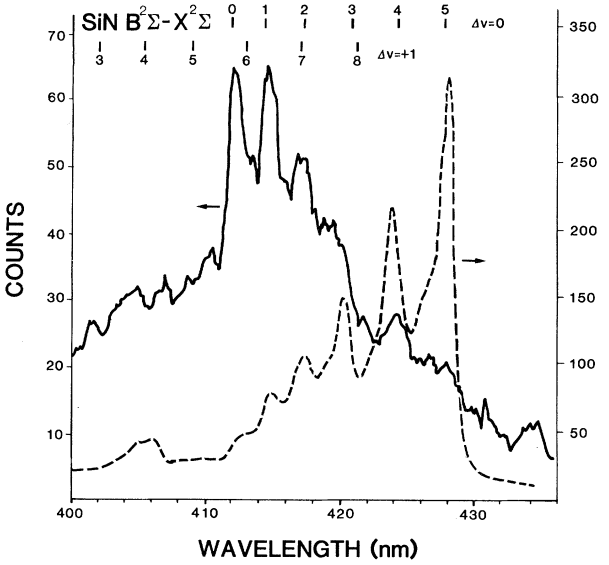

FIG. 1. SiN vibrational spectrum (solid line) due to N_2^+ bombardment of intrinsic Si, and N_2^+ vibrational spectrum (dashed line) due to electron bombardment of N_2 gas. The band heads of SiN are shown at the top.

such a highly rotationally excited molecule would have a very high probability for losing its rotational energy to the surface[4] and would be unlikely to survive in the excited state to decay radiatively.

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