Nitrogen chemical environments after N_2^+ bombardment on $GaInP_2$: theoretical X-ray emission study

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$GaInP_2$ is a promising photocathode material for solar hydrogen production if its corrosion problem can be resolved [1]. Recently our collaborators succeeded in improving the corrosion resistance of $GaInP_2$ photocathodes by N_2^+ bombardment. In order to better understand the origin of the protection mechanism, we developed a theoretical method to calculate X-ray emission spectra of Nitrogen K-edge. From the comparison with the experimental spectra of well-defined nitride materials, we were able to identify appropriate broadening scheme. Also relative shift of core level depending on chemical environment is taken into account. It turns out that the electronic state of incorporated nitrogen couples with both localized and delocalized states, and that it varies depending on its chemical environment. In particular, when nitrogen forms bonds with anions such as P and N, new peaks rise up at the low-energy side. These are attributed to localized states and would not be visible in spectral feature derived from N-metal bonds. These peaks explain observed features in the experimental spectra in the low-energy regime once appropriate energy dependent lifetime broadening is applied.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

[1] O. Khaselev and J. A. Turner, *Science* **280**, 425 (1998).