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Dopant Adsorption and Incorporation at Irradiated GaN Surfaces[1] QIANG SUN, Princeton University, ANNABELLA SELLONI, Princeton University, THOMAS MYERS, West Virginia University, W. ALAN DOOLITTLE, Georgia Institute of Engineering — Mg and O are two of the common dopants in GaN, but, in spite of extensive investigation, the atomic scale understanding of their adsorption and incorporation is still incomplete. In particular, high-energy electron irradiation, such as occurring during RHEED, has been reported to have an important effect on the incorporation of these impurities, but no study has addressed the detailed mechanisms of this effect yet. Here we use DFT calculations to study the adsorption and incorporation of Mg and O at the Ga- and N-polar GaN surfaces under various Ga, Mg and O coverage conditions as well as in presence of light or electron beam-induced electronic excitation. We find that the adsorption and incorporation of the two impurities have opposite surface polarity dependence: substitutional Mg prefers to incorporate at the GaN(0001) surface, while O prefers to adsorb and incorporate at the N-polar surface. In addition, our results indicate that in presence of light irradiation the tendency of Mg to surface-segregate is reduced. The O adsorption energy on the N-polar surface is also significantly reduced, consistent with the experimental observation of a much smaller concentration of oxygen in the irradiated samples.

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