Understanding surface kinetics of InGaN epitaxy: Applications towards advanced photovoltaics

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ABSTRACT

Indium-gallium-nitride alloys (InGaN) is a unique semiconductor ternary alloy system with direct bandgaps covering the entire UV to IR solar electromagnetic radiation spectrum at earth surface. Thus is an alloy system ideal for advanced next-generation photovoltaic applications.

Realization of this goal requires polarization engineered heterostructure design [1], as well as, the ability to achieve high quality InGaN epilayers and heterostructures in the entire composition range [2]. The latter is a challenging task, complicated by the unconventional epitaxy surface mechanism of InGaN. While RF-plasma assisted molecular beam epitaxy is the method of choice to realize device-quality InGaN heterostructures, the nature of the fundamental kinetics mechanisms involved (indium desorption and InGaN decomposition) need to be fully understood to achieve control and optimization of the epitaxy.

Regarding the indium desorption from III-N (0001) surface mechanisms, we employed detailed reflection high-energy electron diffraction (RHEED) experiments with density functional theory (DFT) and hybrid Monte-Carlo/quasi-continuous modeling methods to reveal and quantify the underlying physical mechanisms of the indium surface bilayer [3]. We found that while the bilayer desorbs in a layer-by layer mode, the desorption mechanisms from the bottom and top layers are significantly different. In the case of bottom monolayer, desorption follows approximately a ¾ order monotonic Polyani-Wigner relation, which is attributed to the dependence of adatoms binding on their first neighbors and to contributions from two different monolayer phases. In the case of the top monolayer, desorption has a non-monotonic dependence on coverage, with maximum desorption occurring at ~0.55 coverage. This was associated with the liquidus status of the top monolayer and its consequent continuous restructuring during the desorption process.

Furthermore, the surface-driven decomposition of InGaN epilayers was studied and the relevant mechanisms will be discussed.

REFERENCES

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