## Materials Science & Engineering Doctoral Defense

Interaction of Charge Carriers with Defects at Interfaces and Grain Boundaries in Compound Semiconductors

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## **Abstract**

Realization of efficient photovoltaic cell with high bandgap in an economically viable manner is one of the technological advances that could accelerate the development of human civilization. A material needs to be engineered that has high bandgap, has relatively inactive defects, is thermodynamically stable in ambient conditions and is economically viable for mass manufacturing. This work focuses on a material system made of gallium, indium, and phosphorus – hereafter referred to as GalnP. GalnP based photovoltaic cells, in single crystalline form, have demonstrated excellent power conversion efficiencies. Growth of single-crystal GalnP in prohibitively expensive. While growth of polycrystalline GalnP is expected to lower its cost of production, polycrystalline GalnP is expected to have a lot of defects, about which not a lot is known at this time. This work presents the first study of synthesis, and structural and optoelectronic characterization of polycrystalline GalnP thin films.In addition, this work models the best performance of solar cells achievable with a particular grain size and the recombination velocities needed to achieve it. Effect of defect characteristics at the surface and layer properties like doping and thickness that affect the recombination velocities are also modelled. Recombination velocities at the free surface of single crystalline GalnP and after deposition of various high-k dielectric layers on GalnP is experimentally quantified using time resolved photoluminescence decay measurements. In addition, bulk lifetime, and surface recombination velocity of effectively passivated single crystal AllnP-GalnP based double heterostructures is also measured. All these studies enabled the development of a novel passivation method for polycrystalline thin films. A novel passivation method, named – aluminum assisted post deposition treatment, is introduced that has demonstrated improvement in the minority carrier lifetime of polycrystalline GalnP to nearly 40 ns at 80K. During the development of the passivation process, aluminum diffusivity in GalnP is also quantified using TEM-EDS line scans. Introduction, development, and demonstration of this novel passivation mechanism in polycrystalline GalnP could initiate the development of a new family of passivation treatments to improve the optoelectrohic response of many other polycrystalline compound semiconductors.